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ABSTRACT

Eigenvalues of a finite graph are defined as the eigenvalues of its adjacency matrix. A growing body of evidence links structural and spectral properties of graphs. This thesis makes contributions to two areas in this field. Both areas are concerned with eigenvalue extrema for certain classes of graphs and the structure of the extremal graphs.

Let G be a finite graph and let $\lambda_1 \geq \lambda_2$ be its two largest eigenvalues.

Our first subject is the structure of connected trivalent graphs which minimize the eigenvalue gap $\lambda_1 - \lambda_2$. This investigation is motivated by experimental observations made two decades ago by Bussemaker et al. on connected trivalent graphs with 14 or fewer vertices. Generalizing their empirical conclusions, we describe the exact structure of the extremal graphs. Our result supports the intuitive idea that the eigenvalue gap is related to the sturdiness of interconnections within the graph; the interconnections will be the most fragile for our long, "path-like" extremal graphs.

Our second subject is the spectral generalization of certain classical results in extremal graph theory. The classical results concern the quantity $ex(n, \mathcal{H})$, defined to be the maximum number of edges in graphs G on n vertices which do not contain as a subgraph any graph H from the set $\mathcal{H}$. Analogously, we define $spex(n, \mathcal{H})$ to be the maximum spectral radius $\lambda_1(G)$ over the same class of graphs G.

In the spectral analogue of Turán's theorem, we show that among graphs having clique number at most t, i.e., not containing K_{t+1} as a subgraph, Turán's graph $T(n,t)$ has maximal spectral radius and that it is the unique extremal graph.

It is easy to see that

$$2 \cdot ex(n, \mathcal{H})/n \leq spex(n, \mathcal{H}), \qquad (*)$$

and that there are graphs H for which the set $\{spex(n, \{H\}) \cdot n/\, ex(n, \{H\}) : n > 0\}$ is not bounded. We show, however, that if $\mathcal{H}$ does not contain bipartite graphs, then

the two sides of $(*)$ are asymptotically equal; we do this by proving that

$$\lim_{n\to\infty} spex(n,\mathcal{H})/n = 1 - 1/t$$

where t is one less than the minimum chromatic number of graphs in $\mathcal{H}$. The fact that the right-hand side is equal to the limit of the extremal density $\lim_{n\to\infty} ex(n,\mathcal{H})/\binom{n}{2}$ is the Erdős-Stone-Simonovits theorem.

The case of bipartite excluded subgraphs is not nearly as well understood; even for complete bipartite graphs $K_{s,t}$, in most cases the correct order of magnitude of the function $ex(n,\{K_{s,t}\})$ is not known. Nevertheless, we show that the order of magnitude of $spex(n,\{K_{s,t}\})$ is not greater than the conjectured order of magnitude of $2 \cdot ex(n,\{K_{s,t}\})/n$ for complete bipartite graphs.

Returning to the case of $\mathcal{H} = \{K_{t+1}\}$, we prove a stability result for our Spectral Turán theorem for the cases $t = 2, 3$, which shows that if the spectral radius of a graph not containing K_{t+1} is close to the bound, then the graph is close to Turán's graph.

Our last result states that "graphs with hereditarily bounded average degree have small spectral radius." The trivial bound for the spectral radius in terms of the number of edges m is $\lambda_1 \leq \sqrt{2m}$, which may be improved upon only slightly in general. We show, however, that if the graph has hereditarily bounded average degree, then this may be improved to $\sqrt{m}$ asymptotically, which we show to be tight. More specifically, we show that if $r, t \in \mathbb{N}$ and G is a graph satisfying $|E(H)| \leq t|V(H)| + r$ for every subgraph $H \leq G$, then

$$\lambda_1(G) \leq (t-1)/2 + o(1) + \sqrt{tn}.$$

This result implies that

$$\lambda_1(G) < 1 + o(1) + \sqrt{3n},$$

for graphs embeddable on a fixed surface, improving upon previous bounds by a constant factor.

A number of problems arise from these results. They are discussed in the final chapter of this thesis.

CHAPTER 1

INTRODUCTION

1.1 Brief exposition of the subject

Let G be a graph on n vertices and let $A_G = (a_{ij})$ be its adjacency matrix, an $n \times n$ symmetric matrix given by $a_{ij} = 1$ whenever $\{i, j\}$ is an edge of G, and 0 otherwise. The eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ of A_G are called the eigenvalues of G, their multiset is called the *spectrum* of G. λ_1 satisfies $\lambda_1 \geq |\lambda_i|$ for all i and is called the *spectral radius* of G.

In this thesis, we investigate some extremal problems related to the spectrum of a graph G, given that G satisfies some combinatorial conditions. Specifically, we consider two types of problems: the minimum *eigenvalue gap* $(\lambda_1 - \lambda_2)$ for connected trivalent graphs and bounds on the spectral radius of graphs with restricted subgraphs.

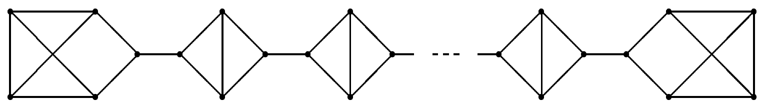
Trivalent graphs with minimum eigenvalue gap. Trivalent graphs are regular graphs of degree 3. For these, it follows easily that $\lambda_1 = 3$. We define the *eigenvalue gap* of regular graphs to be the difference $\lambda_1 - \lambda_2$; the gap is positive if and only if G is connected. This quantity was first investigated by Fiedler in 1973, who called it the *algebraic connectivity* of G. It is in some sense a measure of the strength of the interconnections of G (cf. Section 1.2.1 and references there).

In Chapter 3, we consider the eigenvalue gap of trivalent, connected graphs. In 1976, Bussemaker, Čobeljić, Cvetković, and Seidel [19] enumerated all 621 connected trivalent graphs with at most 14 vertices. They ordered the graphs lexicographically by their spectra and remarked that:

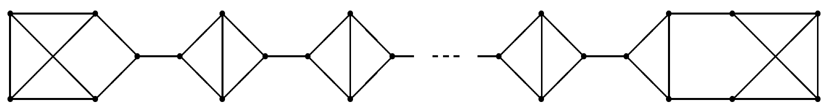
> "Our table shows that there is a strong relation between the second eigenvalue and the connectivity of a graph. This is not surprising in view

of [Fiedler [46]]. But the inequalities in [46] are not sharp in the case of cubic graphs and the whole question needs further consideration."

This observation is the motivation for our work involving trivalent graphs. Let Γ_n be connected trivalent graph on $n \geq 10$ vertices given by:



whenever $n \equiv 2 \pmod 4$, and



whenever $n \equiv 0 \pmod 4$.

In the enumeration of Bussemaker et al., the first graph appearing for each $n \geq 10$ is Γ_n. In Chapter 3 we prove the conjecture implicit in their paper:

Theorem 3.1 *For $n \geq 10$, the graph Γ_n is the connected trivalent graph with minimum eigenvalue gap, and it is the unique such graph.*

We also make the observation that Γ_n has maximum diameter among connected trivalent graphs on $n \geq 10$ vertices, and that for $n \equiv 2 \pmod 4$ it is unique with this property.

Bounds on the spectral radius. The spectral radius satisfies the following inequality:

$$\frac{2m}{n} \leq \lambda_1,$$

where n is the number of vertices and m is the number of edges in G. In Chapter 4 we investigate upper bounds on the spectral radius of graphs given that they do not contain certain subgraphs. The inequality above then shows that our results strengthen classical results in extremal graph theory.

Let $\mathcal{H}$ be a set of graphs. Let $ex(n, \mathcal{H})$ be the maximum number of edges in graphs G with n vertices not containing any graph in $\mathcal{H}$ as a subgraph. Analogously, we define $spex(n, \mathcal{H})$ to be the maximum spectral radius of graphs on n vertices over the same class of graphs G. (If $\mathcal{H} = \{H\}$, we write $ex(n, H)$ and $spex(n, H)$ for $ex(n, \{H\})$ and $spex(n, \{H\})$.) The quantities are linked by the inequality

$$2 \cdot ex(n, \mathcal{H})/n \leq spex(n, \mathcal{H}). \qquad (*)$$

We start our investigation with the case $H = K_{t+1}$, i.e., graphs having clique number at most t (for basic graph theoretic definitions, see Section 2.1). Turán's graph $T(n, t)$ is defined as the unique complete t-partite graph where all t color classes are of size either $\lfloor n/t \rfloor$ or $\lceil n/t \rceil$. Turán's theorem states that $ex(n, K_{t+1}) = |E(T(n, t))|$, and that $T(n, t)$ is the unique extremal graph. We prove the following spectral analogue in Section 4.3:

Theorem 4.2 (Spectral Turán theorem) *Let G be a graph with n vertices not containing K_{t+1} as a subgraph. Then*

$$\lambda_1(G) \leq \lambda_1(T(n, t)).$$

Equality holds if and only if G is the Turán graph $K(n, t)$.

This strengthens a result of Wilf [89], who showed that $\lambda_1(G) \leq (1 - 1/t)n$. This bound agrees with our tight bound if and only if $t|n$.

There are easy examples of graphs for which the set $\{spex(n, \{H\}) \cdot n / ex(n, \{H\}) : n > 0\}$ is not bounded; we show, however, that if $\mathcal{H}$ does not contain bipartite graphs, then the two sides of $(*)$ are asymptotically equal. In Section 4.4 we prove:

Theorem 4.22 (Spectral Erdős-Stone-Simonovits theorem) *Let $\mathcal{H}$ be a set of (nonempty) graphs, and let $t = \min_{H \in \mathcal{H}} \chi(H) - 1$. Then*

$$\lim_{n \to \infty} spex(n, \mathcal{H})/n = 1 - 1/t.$$

The fact that the right-hand side of the equation above is equal to the limit of the extremal density $\lim_{n \to \infty} ex(n, H)/\binom{n}{2}$ is the Erdős-Stone-Simonovits theorem.

The case of bipartite excluded subgraphs is much less understood; even for complete bipartite graphs H, in most cases the correct order of magnitude of the function $ex(n, H)$ is not known. Nevertheless, we show that the order of magnitude of $spex(n, H)$ is not greater than the conjectured order of magnitude of $ex(n, H)$ for complete bipartite graphs. Kővári, Sós, and Turán [64] showed that

$$2 \cdot ex(n, K_{s,t})/n \leq ((t-1)^{1/s} + o(1))n^{1-1/s}.$$

In Section 4.2, we prove the following spectral strengthening of their bound:

Theorem 4.7 (Spectral Kővári-Sós-Turán theorem)

$$spex(n, K_{s,t}) \leq ((t-1)^{1/s} + o(1))n^{1-1/s}.$$

Erdős [38, 39] and Simonovits [79] independently showed that Turán's theorem is stable in the following sense: if G is a graph with clique number at most t having almost as many edges as the Turán graph $T(n,t)$, then by removing only a few edges from G, it can be made a subgraph of $T(n,t)$. We prove the following spectral version of this for $t = 2, 3$ in Section 4.5:

Theorem 4.8 (Spectral stability theorem) *For all $\varepsilon > 0$ and for $t = 2$ or 3, there exist constants $c = c(t)$ and $N = N(\varepsilon, t)$, such that for all graphs G on $n \geq N$ vertices with clique number at most t and spectral radius satisfying*

$$\lambda_1(G) \geq (1 - 1/t)n(1 - \varepsilon),$$

G can be made t-partite by removing at most $c\varepsilon n^2$ edges, and it can be made a subgraph of $T(n,t)$ by removing at most $c\sqrt{\varepsilon}n^2$ edges.

We now consider graphs with low density. For fixed positive integers t and r, let $\mathcal{H}_{t,r}$ be the set of all graphs on at least t vertices with the property that $|E(H)| > t \cdot |V(H)| + r$. We investigate $spex(n, \mathcal{H}_{t,r})$, showing that the trivial bound of $\sqrt{2m}$ can be improved to $c(t,r) + \sqrt{m}$ for these graphs, where $m = tn$ is the number of edges and $c(t,r)$ is a constant depending on t and r. In Section 4.6 we prove the following theorem:

Theorem 4.9 *Let $t \in \mathbb{N}$ and $r \geq -\binom{t+1}{2}$. If G is a graph on n vertices with the property that $|E(H)| \leq t \cdot |V(H)| + r$ for all subgraphs H on at least t vertices, then*

$$\lambda_1(G) \leq (t-1)/2 + \sqrt{(t+1)t + 2r} + \sqrt{tn},$$

and asymptotically,

$$\lambda_1(G) \leq (t-1)/2 + \sqrt{tn} + o(1),$$

where the $o(1)$ refers to $n \to \infty$ while r and t are fixed. Furthermore, the asymptotic bound is tight.

We also show that the unique extremal graph for $r = -\binom{t+1}{2}$ is the graph with t vertices of degree $n-1$, all other vertices of degree t.

As a consequence of this result, we obtain the following bounds:

Corollary 4.10 *Let G be a graph embeddable on a surface of Euler characteristic χ. Then*

$$\lambda_1(G) < 1 + \sqrt{6(2-\chi)} + \sqrt{3n},$$

and asymptotically,

$$\lambda_1(G) < 1 + \sqrt{3n} + o(1),$$

where the $o(1)$ refers to $n \to \infty$ while χ is fixed.

This improves upon previous bounds given by Hong [60] by a constant factor for all surfaces other than the plane; for the plane, we improve his result by an additive constant.

A number of problems arise from our results. These are discussed in Chapter 5.

1.2 History

1.2.1 Combinatorial versus spectral properties of graphs

The study of relations between spectral properties and combinatorial properties of graphs has been the subject of hundreds of papers (we refer the reader to the monographs [23, 28, 30], the survey article by Schwenk and Wilson [78], and the bibliographies there). Graph spectra have direct applications to Markov chains, random generation, Hückel theory in molecular quantum mechanics, and to monomer-dimer systems in thermodynamics [33, 50, 54, 56, 62, 73, 81].

The spectrum of a graph G encodes many properties of the graph, yet any precise encoding still remains elusive. Numerous results have given explicit relationships between a graph's spectrum and combinatorial properties, such as number of edges, maximum degree, chromatic number [27, 35, 57, 88], clique number [89], Hamiltonicity [86, 75], toughness [3, 15], etc. More recent developments even connect spectral properties of matrices related to the adjacency matrix to topological properties, such as planarity [25] and linkless embedability in $\mathbb{R}^3$ [69].

These relationships established to date shed light on the strong correlation between graphs and their spectra; many offer insight into the larger scheme of this correlation, yet there is still much to learn. Most inequalities, while tight in many instances, are very weak in others.

As an example of such results, an important theorem of A. J. Hoffman [57] provides the following lower bound on the chromatic number $\chi(G)$ of a graph

$$\chi(G) \geq 1 - \lambda_1/\lambda_n.$$

This result is related to the remarkable polynomial-time algorithm given by Grötschel, Lovász, and Schrijver [51] to compute the chromatic number of perfect graphs. No purely combinatorial algorithm is known.

Spectral radius. The spectral radius of graphs can be thought of as some sort of averaging of the degrees of the vertices. It satisfies the inequalities

$$\frac{1}{n}\left(\sum d_i^2\right)^{1/2} \leq \lambda_1 \leq d_{\max}\,.$$

Equality on the right implies that G is regular. Equality on the left holds if and only if the graph is either regular or if it is bipartite and the degree of a vertex is determined by its color class (the inequality on the left was observed by Hoffmeister [58]).

The spectral radius arises in topological dynamics, where it is related to the entropy of a topological system given by Markov shifts (cf. [87]). In topological dynamics, one studies the asymptotic properties of continuous maps. A standard simplifying trick is that of symbolic dynamics: reducing to a relatively simple topological space and a continuous map. A particularly interesting class of models is the Markov shifts. Let $Y = \{0, 1, \ldots, k-1\}$, with the discrete topology, and define

$$X = \prod_{-\infty}^{+\infty} Y,$$

with the product topology. The shift $T : X \to X$ given by $T(\{x_n\}_n) = \{x_{n+1}\}_n$ defines a topological dynamical system. Let A be a $k \times k$ matrix with entries in $\{0, 1\}$. Define

$$X_A = \{x \in X : a_{x_n, x_{n+1}} = 1, \quad \forall n \in \mathbb{Z}\}.$$

X_A is a compact subspace, invariant under the shift T. The restriction of T to X_A is called a topological Markov chain. We see that adjacency matrices of (directed) graphs with k vertices yield topological Markov chains, as these matrices have entries only in $\{0, 1\}$.

The entropy of dynamical systems has many formulations (cf. Bowen [13]), and as their definitions are quite involved, we refrain from any general definition, but mention an important result. Let A be an (irreducible) $\{0, 1\}$-matrix A, and let $T : X_A \to X_A$ be a Markov shift. Then the topological entropy $h(T)$ of the dynamical system is given by

$$h(T) = \log \lambda_1(A),$$

where λ_1 is the spectral radius of A. Topological Markov chains are important as a source of models for relevant diffeomorphisms, and as a model for which the topological entropy can be computed. They give added motivation to study the extremal values of λ_1.

Much research has been done trying to obtain upper and lower bounds for the spectral radius under various combinatorial constraints. Extremal graphs under various constraints have been characterized.

Spectra of trees were studied by Collatz and Sinogowitz [26], Heilmann and Lieb [56], Lovász and Pelikán [68], and others. They showed that the star alone has maximum spectral radius and the path alone has minimum spectral radius. This study was then taken a step further, to graphs with 1 and 2 cycles, and also to connected graphs with $n+t$ edges, for t fixed. For this last class of graphs, Cvetković and Rowlinson [31] confirmed a conjecture of Brualdi and Solheid [18] that for n large enough, the graph having maximal spectral radius has one vertex of degree $n-1$ and one vertex of degree $t+2$ (the remaining vertices have degree 1 or 2, as required).

For a given number m of edges (and no condition on the number of vertices), Brualdi and Hoffman [17] conjectured that the graph on t vertices, where $\binom{t}{2} \geq m > \binom{t-1}{2}$, consisting of K_{t-1} and one additional vertex of degree $m - \binom{t-1}{2}$ is the unique graph with maximal spectral radius; this was confirmed by Rowlinson [77].

Hong [59] bounded the spectral radius in terms of the number n of (non-isolated) vertices and the number m of edges of G as follows:

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

This bound was used by Cao and Vince [21] in their bounds on the spectral radius of planar and outer planar graphs.

The spectral radius of graphs with restrictions on the chromatic number $\chi(G)$ have been studied as well. Wilf [88] showed that $\chi(G) \leq \lambda_1(G)+1$. Cvetković [27] proved that $\lambda_1(G) \leq (1-1/\chi(G))n$, which was later improved by Wilf, who replaced $\chi(G)$ by $\omega(G)$, the clique number of G. In this thesis, we improve upon Wilf's result, obtaining the tight bound and determining all extremal graphs. Cvetković's result was improved in another direction by Elphick [35] who showed that $\lambda_1 \leq \sqrt{2m(1 - 1/\chi(G))}$, where m is again the number of edges. Hong used this result and the Heawood Coloring Theorem to give bounds on the spectral radius of graphs embeddable on surfaces (compact 2-dimensional manifolds). In Section 4.6 we improve upon these bounds.

For further information on the spectral radius, the reader is referred to the survey by Cvetković and Rowlinson [32] and the 3rd edition of the monograph by Cvetković et al. [30].

Eigenvalue gap. A particularly interesting application of graph spectra has been a linking of the eigenvalue gap with the interconnectedness of G, an intuitive, yet imprecise, concept. We think of graphs as being "highly interconnected" if large subsets of the graph cannot be cut off from the rest by a small number of edges; graphs with this property have small diameter. On the other hand, the interconnections are "weak" and "fragile" if the graph is easy to split, and can be disconnected at many places. Such graphs have large diameter.

Some interesting results exhibit a relationship between these concepts and the eigenvalue gap. The first relationship was noticed in 1973 by Fiedler [46], who bounded the connectivity of G above and below by functions of the eigenvalue gap of G (in fact, he called the gap the *algebraic connectivity* of G). Alon and Milman [4] and Tanner [84] bounded the gap above and Dodziuk and Kendall [34], and Alon [2] bounded the gap below, by functions of the isoperimetric ratio of G, a more global measure of connectivity. Similar relationships for the analogous, though somewhat different parameter of *electrical conductance* of graphs was shown by Sinclair and Jerrum [82]. These results may all be considered as discrete versions of Cheeger's inequality in differential geometry.

As a profound application of this relationship, Lubotsky, Phillips, and Sarnak [70], and Margulis [72] constructed explicit families of graphs having large girth and large chromatic number, thus "derandomizing" a celebrated probabilistic proof of existence of such graphs by Erdős [37]. To establish that the graphs have large chromatic number, they used Hoffman's result mentioned above.

These results also prove the existence of efficient algorithms for random generation. We want to prove that a random walk of polynomial length on certain graphs of exponential size will converge to an almost uniform distribution. Sinclair and Jerrum showed that the eigenvalue gap for the graphs they used implies the required bound on the electrical conductance. As a consequence, they showed that the permanent of a dense $\{0,1\}$-matrix may be estimated efficiently. (We refer to the monograph of Sinclair [81] and the article by Lovász [67].)

Chung [22], Mohar [74], Alon and Milman [4], and Haemers [55] have bounded the diameter of G above by functions of the gap, and Landau and Odlyzko [66] and McKay (see [74]) have bounded the diameter of G below by functions of the gap.

Unfortunately, all these results mentioned above yield little information if the gap is very small.

Bussemaker et al.'s table mentioned on page 1 suggests that this relationship is much stronger than the existing results indicate. Indeed, the graph with smallest gap has the largest diameter in each of their lists, and all graphs with maximum diameter have gap less than that of graphs with smaller diameter. Our results, determining the connected trivalent graph with minimum gap for all n, and showing that it has maximum diameter, support this stronger link.

1.2.2 Extremal graph theory

Extremal graph theory is the study of the asymptotic behavior of graph invariants. We do not attempt to do justice here to extremal graph theory, as that is beyond the scope of this thesis. We refer the interested reader to Bollobás's monograph [8] and his survey [9], as well as to the survey of Simonovits [80]. We mention here only those results which relate directly to this thesis.

Extremal graph theory started with Turán in 1941, although one could argue that Euler's result for planar graphs: $|E(G)| \leq 3 \cdot |V(G)| - 6$, was the first extremal graph theoretic theorem. Turán investigated the number of edges a graph G can have, given that it does not contain K_{t+1} as a subgraph, a special case of which ($t = 2$) had already been solved in 1907 by Mantel [71]. Turán showed that no such graph on n vertices can contain more edges than the *Turán graph* $T(n, t)$, and that this is the unique extremal graph. This graph has t sets of vertices of almost equal size (either $\lfloor n/t \rfloor$ or $\lceil n/t \rceil$), and edges connect all pairs of vertices in different sets. Aigner [1] has a nice survey of several interesting proofs of this theorem.

In 1946, Erdős and Stone [45] were able to extend Turán's theorem to the graphs $K_{t+1}(r)$, the complete $(t+1)$-partite graph with r vertices in each color class (this is $T(r(t+1), t+1)$ in our notation above). They showed that the number of edges in graphs not containing $K_{t+1}(r)$, depends asymptotically only on t and n, i.e.,

$$|E(G)| \leq (1 - 1/t)\binom{n}{2} + o(n^2).$$

Erdős and Simonovits [42] noticed that this same bound holds for any graph with chromatic number $t + 1$, and hence for arbitrary families of graphs $\mathcal{H}$ for which $t + 1 = \min_{H \in \mathcal{H}} \chi(H)$.

The extremal graphs for a given family of excluded $(t+1)$-chromatic graphs are not known in general and it is natural to ask whether the structure must be close to Turán's graph $T(n, t)$. Erdős [38, 39] and Simonovits [79] independently answered this question in the affirmative. In fact they even showed that the extremal graphs are stable in the sense that if G is a graph not containing a $(t + 1)$-chromatic graph H as a subgraph, and G has almost as many edges as an extremal graph, then by adding and subtracting only a small number of edges transforms G into a subgraph of the Turán graph $T(n, t)$.

A bipartite analogue to the problem considered by Turán was posed by Zarankiewicz [90] in 1951. The problem is to determine the maximum number of edges a graph may contain given that it does not contain the complete bipartite graph $K_{s,t}$ as a subgraph. The problem has become known as the *Zarankiewicz problem.* In 1954, Kővári, Sós, and Turán [64] gave an upper bound. They showed that for any such G, the following bound holds:

$$|E(G)| \leq (s-1)^{1/t} n^{2-1/t}/2.$$

There does not appear to be a simple extremal graph as in the case of Turán's theorem, and for $s = t > 3$, the question of whether or not this is the correct order of magnitude is still open. It is conjectured that this bound is asymptotically correct for all s and t.

What is known is that the order of magnitude of this bound is correct for $s = 2$ and all t (Klein, as reported by Erdős [36]), $s = 3$ and all t (Brown [16]), and all s and t satisfying $t \geq s! + 1$ (Kollár, Ronyai, and Szabó [63]). Furthermore, the bound is asymptotically tight for $s = t = 2$ (Erdős, Rényi, Sós [41] and Brown [16]) and for $s = 2$ and all t (Füredi [47]). In contrast, the best known lower bounds, due to Erdős and Spencer [43], using a probabilistic argument, gives only $\Omega(n^{1-2/(s+t)})$.

1.3 Publication status of the results in the dissertation

All major results are in the process of publication in specialized journals. The dissertation includes results obtained in collaboration.

Section 3.3 represents individual work without coauthors and has been accepted for publication in the *Journal of Algebraic Combinatorics* [53]. The remainder of Chapter 3 represents joint work with Clemens Brand and Wilfried Imrich [14].

Section 4.3 represents individual work without coauthors [52], as does Section 4.6. The remaining results in Chapter 4 were obtained in collaboration with the author's advisor László Babai [6, 7].

CHAPTER 2

PRELIMINARIES

2.1 Basic graph theory

In this thesis, we consider finite undirected graphs without loops or multiple edges. The definitions below reflect this convention.

A graph $G = (V, E)$ consists of a vertex set V and an edge set E, where every edge (element of E) is an unordered pair of distinct vertices (elements of V). Graphs denoted by the letter G will always have n vertices, $m \le \binom{n}{2}$ edges, and their vertex set will for simplicity be assumed to be the set $\{1, 2, \ldots, n\}$.

We say that vertices i and j are *adjacent* if $\{i, j\} \in E$. In this case we also say that i and j are *neighbors*. We denote this by $i \sim j$. We denote by $\overline{G}$ the *complement* of G defined as the graph on the same vertex set, where two vertices are adjacent in $\overline{G}$ if and only if they are not adjacent in G.

An *isomorphism* of two graphs is a bijection between their vertex sets which preserves adjacency as well as non-adjacency. Two graphs G and H are *isomorphic* if there is an isomorphism between them; in this case we write $G \cong H$. Self-isomorphisms of a graph are called *automorphisms*.

The *degree* of a vertex i is the number of neighbors of i and is denoted by $d(i)$ or d_i. The maximum degree of a vertex of G is denoted $d_{\max}(G)$. The *average degree* of G is

$$d_{\text{ave}}(G) = \frac{\sum_{i \in V} d(i)}{n} = \frac{2m}{n}. \tag{2.1}$$

The *density* of G is the ratio $m/\binom{n}{2} = d_{\text{ave}}(G)/(n-1)$.

A graph is *regular* if all vertices have the same degree. A *trivalent* graph is a regular graph of degree 3. By equation (2.1), a regular graph of odd degree must have an even number of vertices.

A *walk* of length k between vertices i and j is a sequence $i = u_0, u_1, \ldots, u_k = j$ of vertices such that u_{i-1} and u_i are neighbors for $i = 1, \ldots, k$. A *path* is a walk without repeated vertices. We view the paths $(u_0, u_1, \ldots, u_k)$ and $(u_k, \ldots, u_1, u_0)$ as identical.

The *distance* between i and j is the length of a shortest path between i and j; the distance is infinite if there is no such path. The *diameter* of the graph is the maximum distance between pairs of its vertices. The graph is *connected* if every pair of vertices has finite distance. Since the graphs we consider are finite, this statement is equivalent to the diameter being finite.

A set $F \subseteq E$ is said to cut the graph G if $(V, E \setminus F)$ is disconnected. In this case F is a *cut-set.* A *cut-edge* is an edge e of a connected graph such that $\{e\}$ is a cut-set. The *edge-connectivity* of a connected graph is the minimum size of its cut-sets; this number is zero if and only if the graph is disconnected.

A *closed walk* of length k is a walk $(u_0, u_1, \ldots, u_k)$ such that $u_0 = u_k$. A *cycle* of length k is a closed walk of length $k \geq 3$ without repeated vertices other than $u_0 = u_k$. The cycles $(u_0, u_1, \ldots, u_k)$, $(u_k, \ldots, u_1, u_0)$, and $(u_1, u_2, \ldots, u_k, u_0)$ are considered identical. The *girth* of a graph is the length of its shortest cycle.

The *complete graph* K_n has n vertices and all the $\binom{n}{2}$ pairs of vertices are adjacent. Complete graphs have density 1.

A graph is *bipartite* if its vertex set can be divided into two "color classes" ("red" vertices and "blue" vertices, say), such that vertices of the same color are never adjacent. A graph is bipartite if and only if all cycles have even lengths.

The *complete bipartite graph* $K_{s,t}$ is defined as follows: it has $s + t$ vertices and st edges; the st edges join each of the first s vertices with each of the last t vertices.

A *subgraph* $H = (T, F)$ of $G = (V, E)$ is a graph such that $T \subseteq V$ and $F \subseteq E$.

The edge $\{i, j\} \in E$ is *induced* by the subset $T \subseteq V$ if $i, j \in T$. The subgraph *induced* by the subset $T \subseteq V$ is the graph (T, F), where $F \subseteq E$ consists of all edges induced by T.

A subset $T \subseteq V$ is *independent* if no edge is induced by T. We say that $T \subseteq V$ is a *clique* if T induces a complete graph. The *clique number* $\omega(G)$ of G is the size of the largest clique $T \subseteq V$.

A *legal coloring* of a graph is an assignment of "colors" to each vertex such that vertices of the same color are never adjacent (each color class is an independent set). Colorings of the vertex set will tacitly be assumed to be legal and the adjective "legal" will be omitted. The *chromatic number* $\chi(G)$ of the graph G is the minimum number of colors for which there is a legal coloring. The graph G is bipartite if and only if $\chi(G) \leq 2$.

The complete t-partite graph $K_{n_1,\ldots,n_t}$ is a t-colored graph with $n = \sum_{i=1}^{t} n_i$ vertices such that the color classes have sizes $n_1, \ldots, n_t$, respectively, and each pair of color classes induces a complete bipartite graph (so the number of edges is $m = \sum_{1 \leq i < j \leq t} n_i n_j$).

2.2 Graph spectra

As general references for matrix theory, we refer the reader to the monographs by Gantmacher [48] and by Horn and Johnson [61]. In this thesis, vectors will appear in upright bold face, whereas italics will be used for scalars. Matrices will always be represented by capital letters. The all ones vector will be written $\mathbf{j} = (1, 1, \ldots, 1)^t$.

Before relating graphs to matrices, we recall our most frequently used tool from linear algebra, the Courant-Fisher theorem on symmetric real matrices.

Theorem 2.1 (Courant-Fisher theorem) *Let A be an $n \times n$ symmetric matrix over $\mathbb{R}$, and let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be its eigenvalues. Let $\mathbf{x}_i$ be an eigenvector for the i-th eigenvalue. Then*

$$\lambda_j = \max_{\mathbf{x} \perp \mathbf{x}_1, \ldots, \mathbf{x}_{j-1}} \frac{\mathbf{x}^t A \mathbf{x}}{\|\mathbf{x}\|^2} \qquad (1 \leq j \leq n),$$

and the maximum is attained precisely for eigenvectors corresponding to λ_j. *In particular,*

$$\lambda_1 = \max_{\mathbf{x}} \frac{\mathbf{x}^t A\mathbf{x}}{\|\mathbf{x}\|^2}.$$

Eigenvalues enter graph theory via the *adjacency matrix*.

The *adjacency matrix* of the graph G, denoted by $A = A_G$, is the $n\times n$ symmetric matrix $A = (a_{ij})$ where $a_{ij} = 1$ if vertices i and j are adjacent and $a_{ij} = 0$ otherwise. In particular, $a_{ii} = 0$ for all $i \in V$. The *eigenvalues of* G are the eigenvalues of A and their multiset is called the *spectrum of* G. The spectrum of G is independent of how the vertices of G are labeled (isomorphism invariant).

We note that since A is symmetric, the eigenvalues of A are real and will be denoted by

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n.$$

The trace of A is zero, therefore $\sum_{i=1}^n \lambda_i = 0$.

A vector $\mathbf{x} = (x_1, \ldots, x_n)^t \in \mathbb{R}^n$ can be viewed as an assignment of "weights" to the vertices: x_i is the weight of vertex i. Let $\mathbf{y} = A\mathbf{x}$, where $\mathbf{y} = (y_1, \ldots, y_n)^t$. Then

$$y_j = \sum_{i\sim j} x_i \qquad \text{for} \quad j = 1, \ldots, n. \tag{2.2}$$

(The summation extends over the neighbors of j.) In particular if $\mathbf{x}$ is an eigenvector corresponding to eigenvalue λ then we have

$$\lambda x_j = \sum_{i\sim j} x_i \qquad \text{for} \quad j = 1, \ldots, n. \tag{2.3}$$

The quadratic form $\mathbf{x}^t A\mathbf{x}$ also has a nice interpretation:

$$\mathbf{x}^t A\mathbf{x} = \sum_{i\sim j} x_i x_j. \tag{2.4}$$

The following well known facts follow easily from the Courant-Fisher theorem and equation (2.3). (See for example [29] and [49].)

Lemma 2.2 *(i)* $\lambda_1 \geq |\lambda_j|$ *for all* j.

(ii) λ_1 *has a nonnegative eigenvector.*

(iii) *If* G *is connected then* λ_1 *is simple (has multiplicity 1), and the corresponding eigenvector* $\mathbf{x}$ *is all-positive.*

(iv) *Let* $\mathbf{x}$ *be an all-positive eigenvector for the connected graph* G*. Then the corresponding eigenvalue is* λ_1 *and* $\mathbf{x}$ *is invariant under the automorphisms of* G*.*

(v) *If* G *is bipartite then its spectrum is symmetrical:* $\lambda_i = -\lambda_{n-i+1}$ $(i = 1, \dots, n)$*.*

(vi) *Conversely, if* G *is connected and* $\lambda_1 = -\lambda_n$ *then* G *is bipartite.*

(vii) $d_{\text{ave}} \leq \lambda_1 \leq d_{\max}$*. In the first inequality, equality holds exactly if* G *is regular; the same is true for the second inequality if in addition we assume that* G *is connected.*

(viii) *If* G *is regular of degree* d *then* $\lambda_1 = d$*. This eigenvalue is simple if and only if* G *is connected.*

As an illustration, let us prove item (vii).

For the first inequality, from the Courant-Fisher theorem we obtain that

$$\lambda_1 \geq \mathbf{j}^t A \mathbf{j} / \|\mathbf{j}\|^2 = 2m/n = d_{\text{ave}} .$$

If equality holds, then $\mathbf{j}$ must be an eigenvector and therefore G is regular.

For the second inequality, let $\mathbf{x} = (x_1, \dots, x_n)^t$ be a nonnegative eigenvector for λ_1 and let $x_j = \max_i x_i$. Then, by equation (2.3), $\lambda_1 x_j = \sum_{i \sim j} x_i \leq d_j x_j \leq d_{\max} x_j$. The case of equality is easily analyzed. □

We deduce one more important corollary.

Lemma 2.3 *Let* $H = (V, F)$ *be a proper subgraph of* $G = (V, E)$ *on the same vertex set* $(F \subset E)$*. Then*

(i) $\lambda_1(G) \geq \lambda_1(H)$*.*

(ii) If G is connected then $\lambda_1(G) > \lambda_1(H)$.

(iii) $\lambda_1(G) - \lambda_1(H) < \sqrt{2|E \setminus F|}$.

Proof: Items (*i*) and (*ii*) are immediate from the Courant-Fisher theorem. (For item (ii), use Lemma 2.2, item (iii).) For item (iii), let $K = (V, E \setminus F)$, and let B be the adjacency matrix of K. Then by the Courant-Fisher theorem, $\lambda_1(G) \leq \lambda_1(H) + \lambda_1(K)$. Moreover, $\big(\lambda_1(K)\big)^2 < \text{trace}(B^2) = 2|E(K)|$. □

The *Laplacian matrix* L of G is defined as $L = D - A$, where D is the diagonal matrix whose (i, i) entry is the degree of vertex i. L is singular, since $L\mathbf{j} = \mathbf{0}$. Moreover, L is positive semidefinite: $\mathbf{x}^t L \mathbf{x} = \sum_{i \sim j} (x_i - x_j)^2$. It follows that L has rank $n - 1$ if and only if G is connected. Let the eigenvalues of L be $0 = \rho_0 \leq \rho_1 \leq \cdots \leq \rho_{n-1}$. It is easy to see that for regular graphs, $\rho_1 = \lambda_1 - \lambda_2$. This is the so-called *eigenvalue gap* of G. Applied to L, the Courant-Fisher theorem says that

$$\rho_1(G) = \min_{\mathbf{x} \perp \mathbf{j}} \frac{\mathbf{x}^t L \mathbf{x}}{\|\mathbf{x}\|^2}.$$

CHAPTER 3

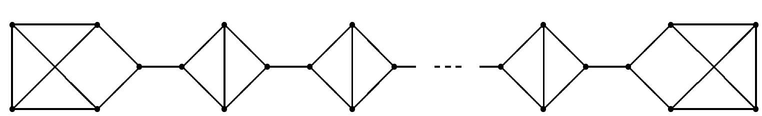
TRIVALENT GRAPHS WITH MINIMUM EIGENVALUE GAP

3.1 Introduction

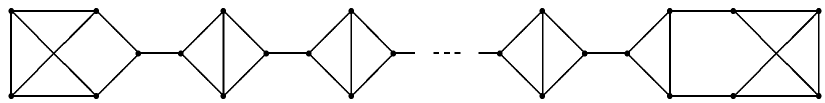
In 1976, Bussemaker, Čobeljić, Cvetković, and Seidel ([19], see also [20]) enumerated all connected trivalent graphs with at most 14 vertices. They ordered the graphs lexicographically by their eigenvalues. The ordering is interesting in that certain combinatorial properties change gradually (e.g. diameter, connectivity, girth). Graphs whose second largest eigenvalue is large, tend to be long, path-like; they have large diameter, small girth, and many cut-edges. Moving down the list, as the second eigenvalue decreases, the diameter decreases and both connectivity and girth increase. Those for which the second eigenvalue is smallest are very compact, they have small diameter, large girth, and high connectivity.

For connected graphs G, we define $\rho_1 = \lambda_1 - \lambda_2$ to be the *eigenvalue gap* of G. The eigenvalue gap was first investigated by Fiedler in 1973, who called it the *algebraic connectivity* of G (see [46]). Fiedler and others have shown a direct correlation between the gap and various graph parameters describing the strength of the interconnections in G (see page 9). Their results give little information when ρ_1 is minimum. In this chapter, we consider this case and determine the unique extremal graphs.

According to Bussemaker et al., the connected trivalent graphs with minimum eigenvalue gap for $n = 10$, 12, and 14 coincide with the graphs pictured below. These pictures suggest a general pattern. We define the graph Γ_n as:



whenever $n \equiv 2 \pmod 4$, and



whenever $n \equiv 0 \pmod 4$.

The main result of this chapter confirms the natural conjecture suggested by the experimental results of Bussemaker et al.:

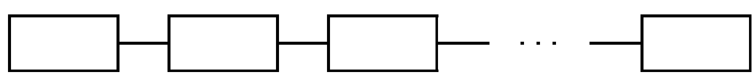
Theorem 3.1 *For (even) $n \geq 10$, the graph Γ_n is the unique connected trivalent graph with minimum eigenvalue gap.*

In Section 3.6 we show that Γ_n is the connected trivalent graph on n vertices with maximum diameter.

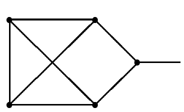
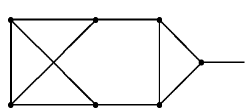
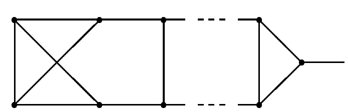
3.2 Outline of the proof

Some preliminary definitions are required.

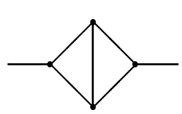
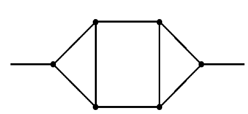
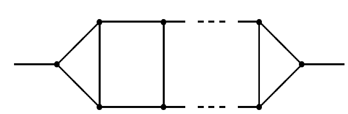
Definition 3.1 A trivalent graph is said to be *path-like* if it has the form:



where each end block is one of the following:

 or  or 

(the right-hand end block is the mirror image of one of the blocks shown) and each middle block is one of the following:

 or  or 

We will call end blocks with 5 vertices and middle blocks with 4 vertices *small*, end blocks with 7 vertices and middle blocks with 6 vertices *medium*, and all others *large*.

It will be convenient to consider the Laplacian $L = L_G$ rather than the adjacency matrix A_G. The Laplacian of G is defined as $L_G = D_G - A_G$, where A_G is the adjacency matrix and D_G is the diagonal matrix whose (i,i) entry is the degree of the vertex i. L is singular, as $L\mathbf{j} = \mathbf{0}$. Moreover, L is positive semidefinite and has the following interpretation for graphs: $\mathbf{x}^t L \mathbf{x} = \sum_{i \sim j} (x_i - x_j)^2$. It follows that L has rank $n-1$ if and only if G is connected. Let the eigenvalues of L be $0 = \rho_0 \leq \rho_1 \leq \cdots \leq \rho_{n-1}$. It is easy to see that for regular graphs, $\rho_1 = \lambda_1 - \lambda_2$, as defined earlier.

By the Courant-Fisher theorem, it follows that

$$\rho_1 = \min_{\mathbf{x} \perp \mathbf{j}} \frac{\mathbf{x}^t L_G \mathbf{x}}{\|\mathbf{x}\|^2}.$$

We will make use of this fact extensively.

The proof of Theorem 3.1 is in three parts. In Section 3.3 we show that if G is a connected trivalent graph with minimum eigenvalue gap, then G must be path-like, with no large blocks. In Section 3.4 we then show that G can only have small blocks in the middle. This finishes our proof when $n \equiv 0 \pmod 4$, as Γ_n is the unique graph with this property. If $n \equiv 2 \pmod 4$, then we are left with two choices, either Γ_n, or the path-like graph Π_n which has two medium end blocks and only small middle blocks. In Section 3.5 we show that Γ_n has smaller eigenvalue gap than Π_n.

All three parts are proved using similar methods. We let G be a connected trivalent graph on n vertices with minimum gap ρ_1, and let $\mathbf{x}$ be an eigenvector for $\rho_1(G)$. We assume that G is not in the required form, and then demonstrate a new graph H of the desired form, i.e., path-like without large blocks, and then show that the quadratic form given by H evaluated at $\mathbf{x}$ is not larger than $\rho_1(G)$, showing that $\rho_1(H)$ is at most $\rho_1(G)$, and in fact that if $G \neq H$ that it is strictly less than $\rho_1(G)$, contradicting the minimality of $\rho_1(G)$.

In the first part, we do this entirely by local methods. We assume that G is not path-like, and define a sequence of graphs $G = G_0, G_1, \ldots, G_n$ obtained from G by moving edges to put G into path-like form. The graph G_i is path-like for the first i vertices. At each step, we show that if G_i is path-like only for the first i vertices and not the $(i+1)$st, then we can rewire G_i to get G_{i+1} which is trivalent and connected, and whose eigenvalue gap is no larger than G_i's. We bound the eigenvalue gap above using the Rayleigh quotient, using the vector $\mathbf{x}$. We choose the rewiring carefully so that (assuming that $\|\mathbf{x}\| = 1$):

$$\rho_1(G) = \mathbf{x}^t L_{G_0} \mathbf{x} \geq \mathbf{x}^t L_{G_1} \mathbf{x} \geq \cdots \geq \mathbf{x}^t L_{G_n} \mathbf{x} \geq \rho_1(G_n).$$

When we are finished, we have a path-like graph with no large blocks.

We then show that these rewirings are not reversible, i.e., that if G_n is a path-like graph with no large blocks, then any rewiring of the type we did (reversing our steps) would increase the eigenvalue gap, hence

$$\rho_1(G) > \rho_1(G_n),$$

a contradiction.

We then show that G can only have small blocks in the middle. The method here is semi-local. We "move" the bigger blocks towards the outside ends. Given a graph G with a medium block among the middle blocks, close to the "center", we produce a graph H which has no medium blocks so close to the center. Given a positive eigenvector $\mathbf{x}$ of $\rho_1(G)$, we make a local change to $\mathbf{x}$ and then a global shift to produce a vector $\mathbf{y}$ such that

$$\rho_1(G) = \mathbf{x}^t L_G \mathbf{x} > \mathbf{y}^t L_H \mathbf{y} / \|\mathbf{y}\|^2.$$

The shift is to ensure $\mathbf{y} \perp \mathbf{j}$ so that the right-hand side of the above equation is an upper bound for $\rho_1(H)$. We may then repeat this process of moving the medium blocks from the middle towards the outside. Any large block may be immediately collapsed into two smaller ones. After this step, there are only small blocks in the middle. If $n \equiv 0 \pmod 4$, then we must end up with Γ_n, and we are done, as we cannot have medium blocks at both ends by the value of n.

We now come to part three of the proof, which we only arrive at for $n \equiv 2 \pmod 4$ (and $n \geq 14$). For these values of n, we are left with two possible graphs and need only to determine which has smaller eigenvalue gap. This involves a very delicate eigenvalue estimate. From an eigenvector for Π_n, the other candidate, we construct a vector such that the Rayleigh quotient for L_Γ is smaller than $\rho_1(H_n)$. Surprisingly, this is the most tedious part of the entire proof.

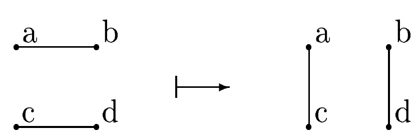
3.3 Path-like structure

In this section, we will show that if G has minimum eigenvalue gap, then G must be path-like. We restate the claim here.

Lemma 3.2 *Let G be a connected trivalent graph on n vertices $(n \geq 10)$, such that among all connected trivalent graphs on n vertices, G has minimum eigenvalue gap. Then G is path-like.*

We make one more elementary definition and then outline the proof of the proposition. As we mentioned in the previous section, we will prove this by rewiring the graph. The following definition describes how we will achieve that.

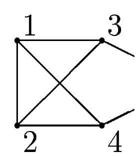
Definition 3.2 An *elementary switch* in a graph is a switching of parallel edges: let $a \sim b$ and $c \sim d$ in G, $a \not\sim c$, $b \not\sim d$ (here $\sim$ and $\not\sim$ denote adjacency and non-adjacency in G), then the elementary switch: SWITCH(a, b, c, d) removes the edges $\{a, b\}$ and $\{c, d\}$ and replaces them with the edges $\{a, c\}$ and $\{b, d\}$.



We will use only elementary switches to rewire G to put it in path-like form, choosing the four vertices carefully so that G remains connected and during the switches the eigenvalue gap never increases. We will then show that any elementary switch on a path-like graph either leaves it path-like or strictly increases the eigenvalue gap. We may then concluded that if G has minimum gap, it must be path-like.

Let $\mathbf{x}$ be an eigenvector for ρ_1, considered as a weighting on the vertices; for $v \in V$ we write x_v for the weight of vertex v. We assume the vertex set is $[n] = \{1, 2, \ldots, n\}$ and that the vertices are numbered so that $x_1 \geq x_2 \geq \cdots \geq x_n$. We call this a *proper labeling* of the vertices (with respect to $\mathbf{x}$).

We can now clarify the rewiring. With respect to a proper labeling, we show that we can rewire to get vertex 1 adjacent to vertices 2, 3, and 4. We can then rewire to get 2 adjacent to 3 and 4. This now looks like:



We show that we can continue in this way, getting a path-like graph, with the labels increasing from left to right. The trick is not to disconnect the graph while we are rewiring, and not to increase the eigenvalue gap. We ensure that these do not happen by choosing our switch carefully. We have the following lemma which aids in not increasing the eigenvalue gap.

Lemma 3.3 *Let G be a trivalent graph and $\mathbf{x}$ be an eigenvector for ρ_1. If there are vertices a, b, c, d in G such that $a \sim b, c \sim d, a \not\sim c, b \not\sim d, x_a \geq x_d$, and $x_c \geq x_b$, then* SWITCH(a, b, c, d) *does not increase the eigenvalue gap. If both of the inequalities are strict, then the gap strictly decreases.*

Proof: We may assume that $\|\mathbf{x}\| = 1$, then $\rho_1 = \mathbf{x}^t L\mathbf{x}$. Let L' be the Laplacian matrix of the graph after the rewiring. In light of the Rayleigh quotient, it suffices to show that

$$\mathbf{x}^t L'\mathbf{x} \leq \mathbf{x}^t L\mathbf{x}.$$

This follows immediately from

$$\begin{aligned}\mathbf{x}^t L\mathbf{x} - \mathbf{x}^t L'\mathbf{x} = \mathbf{x}^t(L' - L)\mathbf{x} &= 2x_a x_c + 2x_b x_d - 2x_a x_b - 2x_c x_d \\ &= 2(x_a - x_d)(x_c - x_b) \geq 0.\end{aligned}$$

□

We have the following lemma to help with keeping the graph connected during rewiring:

Lemma 3.4 *Let G be a connected trivalent graph on $[n]$ with minimum gap ρ_1, properly labeled with respect to an eigenvector $\mathbf{x}$ of ρ_1. Assume that $G \setminus [r]$ is disconnected and that each of its components has an edge which is not a cut edge. Then we may rewire the graph using elementary switches to connect $G \setminus [r]$, not changing ρ_1.*

Proof: It suffices to prove the lemma when $G \setminus [r]$ has two connected components H and K. We will prove the lemma by contradiction. Assume that we cannot rewire the graph to accomplish our goal. Let $\{u_1, u_2\}$ be a non-cut edge in H and $\{v_1, v_2\}$ a non-cut edge in K. Because these edges are not cut edges, both SWITCH(u_1, u_2, v_1, v_2) and SWITCH(u_1, u_2, v_2, v_1) would leave G and $G \setminus [r]$ connected, so it must be the case that these switches increase ρ_1. Based on the previous lemma, this only happens if the weights of one pair are both strictly greater than those of the other pair. We may assume that $x_{u_1}, x_{u_2} > x_{v_1}, x_{v_2}$. Let w be an element in $[r]$ adjacent to K and let $(v_1, v_2, v_3, \ldots, v_t)$ be a shortest path in G, $v_t = w$ (we may possibly need to switch the roles of v_1 and v_2). For $1 \leq i < t$, SWITCH(u_1, u_2, v_i, v_{i+1}) and SWITCH(u_1, u_2, v_{i+1}, v_i) would connect H and K, leaving the graph connected, so by induction, $x_{u_1}, x_{u_2} > x_{v_1}, x_{v_2}, \ldots, x_{v_t} = x_w$, but this is a contradiction, as $x_w \geq x_v$ for all $v \in H$. □

3.3.1 Rewiring to get a path-like graph

Assume that G is a connected trivalent graph on n vertices, $n \geq 10$. We further assume that among all connected trivalent graphs on n vertices, G has minimum eigenvalue gap, and that G is properly labeled. During the rewiring, we will denote G by G_k to indicate that the first k vertices are in path-like form.

Getting G_4

Connecting 1 to 2. If $1 \not\sim 2$ then there is a shortest path $(1, i_1, \ldots, i_r, 2)$ from 1 to 2. Let k be a neighbor of 1 such that $k \neq i_1$ and $k \not\sim i_r$, then we may apply SWITCH$(1, k, 2, i_r)$, not increasing the eigenvalue gap and leaving 1 adjacent to 2 and G connected.

Connecting 1 to 3. If $1 \not\sim 3$ then let $k \neq 2$ be a neighbor of 1. By a simple counting argument, each connected component of $G \setminus \{1\}$ contains a cycle. We may therefore use Lemma 3.4 to assume that $G \setminus \{1\}$ is connected. Let $(k, i_1, \ldots, i_r, 3)$ be a shortest path from k to 3 not passing through 1. Let ℓ be a neighbor of 3 so that $\ell \neq i_r$ and $\ell \not\sim i_r$, then SWITCH$(1, k, 3, \ell)$.

Connecting 1 to 4. (This is identical to the previous rewiring.) If $1 \not\sim 4$ then let k be the third neighbor of 1. We may assume (by Lemma 3.4), that $G \setminus \{1\}$ is connected. Let $(k, i_1, \ldots, i_r, 4)$ be a shortest path from k to 4 not passing through 1. Let ℓ be a neighbor of 4 so that $\ell \neq i_r$ and $\ell \not\sim i_r$, then SWITCH$(1, k, 4, \ell)$.

Connecting 2 to 3. We may assume that $G \setminus \{1\}$ is connected. Let $(2, i_1, \ldots, i_r, 3)$ be a shortest path in $G \setminus \{1\}$. Let k be the third neighbor of 2 and ℓ the third neighbor of 3. If $r = 2$, $k \sim i_2$, and $i_1 \sim \ell$, then k cannot be adjacent to ℓ because $G \setminus \{1\}$ is connected, so SWITCH$(2, k, 3, \ell)$ connects 2 to 3, as required. Otherwise, either $k \not\sim i_r$ and SWITCH$(2, k, 3, i_r)$, or $i_1 \not\sim \ell$ and SWITCH$(2, i_1, 3, \ell)$.

Connecting 2 to 4. If there is a vertex k adjacent to 2, 3, and 4, let ℓ be third neighbor of 4, then $k \not\sim \ell$ and SWITCH$(2, k, 4, \ell)$. Otherwise, we may assume by Lemma 2 that $G \setminus [4]$ is connected. Let k be the third neighbor of 2, ℓ the third neighbor of 3, and let u and v be the two other neighbors of 4. If $3 \sim 4$ then SWITCH$(2, k, 4, 3)$. Otherwise, if $k \neq u$ and $k \not\sim u$, then apply SWITCH$(2, k, 4, u)$. If one of these relations does not hold, try the same for v instead of u. If the same relations hold for v, try to get $3 \sim 4$ by considering 3 instead of 2 and looking at u and v; then SWITCH$(2, k, 4, 3)$ will work. If none of these are allowed, then $G \setminus [4]$ has a connected component consisting of just $\{k, \ell, u, v\}$, this set having 2 or 4 points depending on the equalities, and being disconnected from the rest of the graph. This contradicts the fact that $G \setminus [4]$ is connected (in fact, in this case G has a connected component with 6 or 8 vertices, contradicting the fact that G is connected with at least 10 vertices).

General Steps

We now introduce general steps that deal with the remaining vertices. We assume at this point that the graph G has the desired connections among the vertices $[r]$, i.e. we have G_r. The next three sets of general steps show how to rewire G_r to get either G_{r+1} or G_{r+2}.

When r is odd. Based on our construction, we only arrive at this case when $r \sim r-2$ and $r \sim r-1$, so there is only one edge leaving the first r vertices, and it leaves from r. We need to connect r to $r+1$. Let k be the third neighbor of r and ℓ be a neighbor of $r+1$ the furthest possible from r and SWITCH$(r, k, r+1, \ell)$. This gives us G_{r+1}.

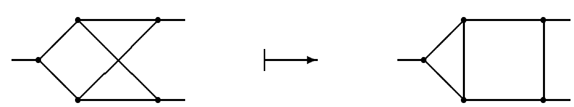
When r is even After rewiring the first $r = 2k$ vertices, there are two edges connecting these vertices to the rest of the graph. By our rewiring, they come either both from r, or one from r and the other from $r-1$. We treat these separately. First, let us consider the case where they both come from r.

Step 1. Connect r to $r+1$. Let k be the neighbor of r closest to $r+1$ and let ℓ be the neighbor of $r+1$ furthest from r. SWITCH$(r, k, r+1, \ell)$.

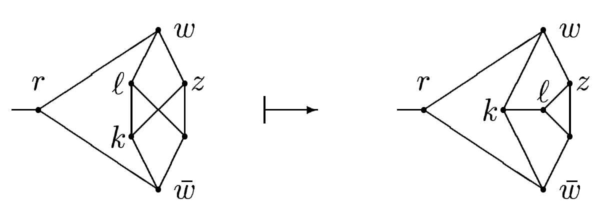
Step 2. Connect r to $r+2$. We may assume that $G \setminus [r+1]$ is connected. Let k be the third neighbor of r. Let ℓ be the neighbor of $r+2$ furthest from k in $G \setminus [r]$. SWITCH$(r, k, r+2, \ell)$. This does not disconnect because there is a path from k to one of the other neighbors of $r+2$ not using the two removed edges.

Step 3. Connect $r+1$ to $r+2$. We may assume that $G \setminus [r+2]$ is connected. There are four cases to consider:

CASE I: $r+1$ and $r+2$ share all three neighbors. Call the neighbors k and ℓ. If $k \sim \ell$, then $n = r+4$ and we are done as this is G_n. Otherwise, SWITCH$(r+1, k, r+2, \ell)$. This leaves G_{r+2}. (See picture below.)



CASE II: $\text{dist}_{G\setminus[r]}(r+1, r+2) = 3$ and both neighbors of $r+1$ and $r+2$ are adjacent to each other (then $n = r+6$). Let k be the smallest among the remaining vertices (i.e. $k = r+3$), so x_k is largest among the remaining vertices. Let ℓ, z be the two neighbors of k and let $w = r+1$ or $r+2$, whichever is adjacent to ℓ and z, and call the other $\bar{w}$. Then SWITCH(w, ℓ, k, z) reduces the graph to case III. (See picture below.)



CASE III: $\text{dist}_{G\setminus[r]}(r+1, r+2) = 2$. If we arrive at this case then $r+1$ and $r+2$ share one neighbor (because of CASE I). Call this neighbor k and let ℓ and z be the other neighbors of $r+1$ and $r+2$ respectively. Then either $k \not\sim \ell$ and SWITCH$(r+1, \ell, r+2, k)$, or $k \not\sim z$ and SWITCH$(r+1, k, r+2, z)$. This leaves G_{r+2}.

CASE IV: Let k and ℓ be neighbors of $r+1$ and $r+2$ respectively, such that $k \not\sim \ell$ and one of them is on a path from $r+1$ to $r+2$. SWITCH$(r+1, k, r+2, \ell)$.

This completes the case when both edges come from r.

We now treat the case when the two edges leaving the first r vertices are from r and $r-1$. We note that if we arrive at this case, then $r \sim r-1$.

Step 1. Connect $r-1$ to $r+1$. We may assume that $G \setminus [r]$ is connected and hence there is a path from $r-1$ to $r+1$ not passing through r. Let k be the third neighbor of $r-1$ and let ℓ be the neighbor of $r+1$ furthest from $r-1$ in $G_r \setminus \{r\}$. SWITCH$(r-1, k, r+1, \ell)$. If it is also the case that $r \sim r+1$, then this is G_{r+1} and skip the following steps.

Step 2. Connect r to $r+2$. This is the same as step 2 above.

Step 3. Connect $r+1$ to $r+2$. This is the same as for step 3 above.

3.3.2 The weights are strictly decreasing

In the previous section we rewired the graph to put it in path-like form with the weights given by $\mathbf{x}$ non-increasing from left to right (for the proper labeling we considered). Assume that the graph is drawn horizontally like the original example in the definition of path-like, with the vertices numbered 1 to n, increasing from left to right. Further, assume that the weights of the vertices given by an eigenvector $\mathbf{x}$ of ρ_1 are non-increasing from left to right. We will show that these weights are in fact strictly decreasing from left to right. We may assume that vertices with the same vertical position as there is a graph automorphism interchanging them (a set of points are in the said to have the same *vertical position* if they lie on the same vertical line – for vertices other than 1 and 2, this is equivalent to saying that vertices at the same distance from 1 are in the same vertical position). Assume that there are two adjacent vertices in different vertical positions with the same weight. If this is the case, then we can find two such vertices c and d (c to the left of d) so that the a left-most neighbor of c, call it a, has greater weight than a right-most neighbor of d, call this f. Let b and e be the other neighbors of c and d, respectively. It is possible that some of these coincide, but here are some important observations: a cannot be to the right of c, f cannot be to the left of d, b cannot be to the right of d, and e cannot be to the left of c. Summarizing what we know about the weights, we have $x_a > x_f$ and $x_a \geq x_b \geq x_c = x_d \geq x_e \geq x_f$. We show that for some $\epsilon > 0$, we may increase x_c by ϵ and decrease x_d by ϵ (keeping the vector perpendicular to $\mathbf{j}$) to decrease the Rayleigh quotient, thus showing that the eigenvalue gap was not minimum, and hence arriving at a contradiction. We assume that $\|\mathbf{x}\| = 1$, so for the new vector, the Rayleigh quotient is

$$\frac{\lambda_2 + 2\epsilon(x_a + x_b + x_d - x_c - x_e - x_f - \epsilon)}{1 + 2\epsilon(x_c - x_d + \epsilon)},$$

which is greater than λ_2 if

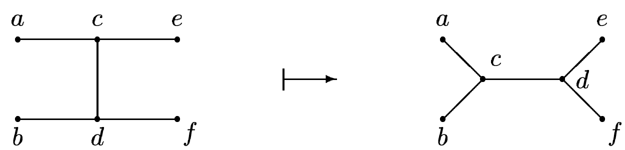
$$x_a + x_b - x_e - x_f > (\lambda_2 + 1)\epsilon.$$

The left hand side is greater than zero, so choosing an ε small enough, we arrive ar the desired contradiction.

3.3.3 Collapsing large blocks

We have now shown that we may rewire G to make it path-like without increasing the eigenvalue gap. In order to show that G must have been path-like to begin with, we need to get rid of large blocks.

We can collapse any block that is large (see page 21). By applying SWITCH($r+1, r+3, r+2, r+4$) as often as possible to G (to vertices of the form in the diagram below), we are left with a graph which has end blocks and middle blocks of the first two types (see page 20). By the previous section, we see that the the eigenvector for the resulting graph must have strictly decreasing coordinates (left-to-right) and such a switch would strictly decrease ρ_1.



To complete the proof that G must be path-like, it suffices to show that any elementary switch on a path-like graph which does not result in a path-like graph must increase the Rayleigh quotient.

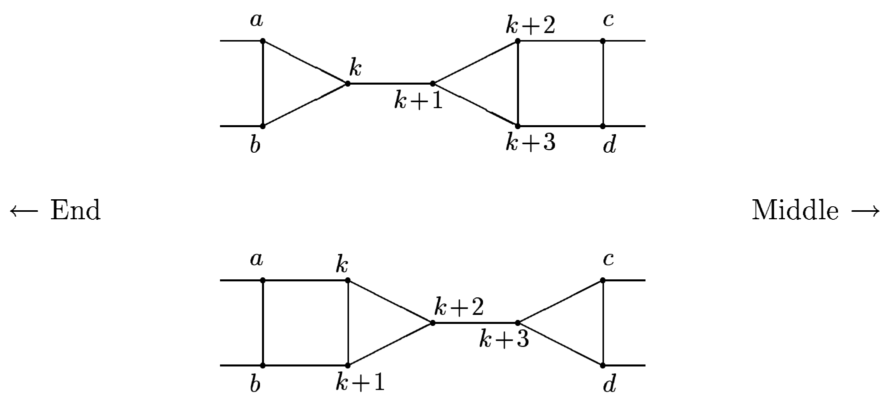
If we apply SWITCH(a, b, c, d) to rewire without decreasing the Rayleigh quotient, we must find four vertices a, b, c, d such that $a \sim b$, $c \sim d$, $a \not\sim c$, $b \not\sim d$, SWITCH(a, b, c, d) does not disconnect G, and $x_a \geq x_d$, $x_c \geq x_b$. In a path-like graph labeled so that the coordinates of $\mathbf{x}$ are strictly decreasing from left to right, these four vertices only exist when a and b are in the same vertical position, c and d are in the same vertical position, $a \sim d$, and $b \sim c$. In this case, rewiring leaves a graph isomorphic to the original. This completes the proof that G must be path-like.

3.4 Only small blocks occur in the middle

We know from the previous section that G must be path-like, and in fact that only small and medium blocks may occur. We will now prove:

Lemma 3.5 *If G is a connected trivalent graph on n ($n \geq 10$) vertices, then G has only small blocks in the middle.*

The idea of "pushing" medium blocks towards the outside which we previously alluded to is illustrated in the following picture:



The block containing vertices c and d becomes smaller, and the block containing vertices a and b becomes bigger. This type of rewiring cannot be accomplished by the operation SWITCH used in the previous section. For the Rayleigh quotient to decrease, we need to alter the vector.

If G is a path-like graph with a medium block in the middle, then the following lemma may be applied to either the eigenvector $\mathbf{x}$ or the eigenvector $-\mathbf{x}$ to move the "extra" edge outward, decreasing the eigenvalue, and contradicting minimality.

Lemma 3.6 *Let G be reduced path-like graph on n vertices ($n \geq 10$), with a medium block as diagrammed above in the upper part of the figure. Let $\mathbf{x}$ be an eigenvector and assume that $x_k > x_{k+1} > x_{k+2} \geq 0$ (otherwise use $-\mathbf{x}$). Then the eigenvalue gap of the graph obtained by performing this "push" is smaller than that of G.*

Proof: We show this by demonstrating a vector $\mathbf{y} = (y_1, y_2, \ldots, y_n)$ perpendicular to the $\mathbf{j}$ vector which gives a smaller value in the Rayleigh quotient than the smallest positive eigenvalue of the original graph. This shows that the smallest positive eigenvalue associated with the new graph is smaller than that of the original graph.

Let G be the original graph, and let the medium block be labeled as in the upper part of the diagram. Let H be the new graph with the local change ("push") given above. To define the new vector $\mathbf{y}$, we change only two coordinates of $\mathbf{x}$ and then shift the entire vector to keep it perpendicular to $\mathbf{j}$.

$$y_i = \begin{cases} x_i - \delta & \text{if } i \leq k \text{ or } i \geq k+3, \\ x_k - \delta & \text{if } i = k+1, \\ x_k + x_{k+2} - x_{k+1} - \delta & \text{if } i = k+2. \end{cases} \tag{3.1}$$

where $\delta = 2(x_k - x_{k+1})/n$ ensures that $\sum y_i = 0$, i.e., that $\mathbf{y}$ is perpendicular to $\mathbf{j}$. We may assume that the vector $\mathbf{x}$ has norm 1 and then the smallest positive eigenvector of G, $\rho_1(G)$, is given by

$$\rho_1 = \sum_{i \sim j} (x_i - x_j)^2.$$

The Rayleigh quotient for the graph H and vector $\mathbf{y}$ is

$$\text{Rayleigh quotient} = \frac{\sum_{i \sim j} (y_i - y_j)^2}{\|\mathbf{y}\|^2} = \frac{\rho_1(G)}{\|\mathbf{y}\|^2}.$$

We only need to show that $\|\mathbf{y}\| > 1$.

$$\begin{aligned} \sum y_i^2 &= \sum (x_i - \delta)^2 - (x_{k+1} - \delta)^2 - (x_{k+2} - \delta)^2 \\ &\quad + (x_k - \delta)^2 + (x_k + x_{k+2} - x_{k+1} - \delta)^2 \\ &= \sum x_i^2 - 2\delta \sum x_i + n\delta^2 + (x_k - x_{k+1})(2x_k + 2x_{k+2} - 4\delta) \\ &= 1 + \frac{4}{n}(x_k - x_{k+1})^2 + (x_k - x_{k+1})(2x_k + 2x_{k+2} - \frac{8}{n}(x_k - x_{k+1})) \end{aligned}$$

We need to show that this is greater than 1, hence that

$$\frac{4}{n}(x_k - x_{k+1})^2 + (x_k - x_{k+1})(2x_k + 2x_{k+2} - \frac{8}{n}(x_k - x_{k+1})) > 0$$

or using that $x_k - x_{k+1} > 0$ and dividing through, we need to show that

$$\frac{4}{n}(x_k - x_{k+1}) + (2x_k + 2x_{k+2} - \frac{8}{n}(x_k - x_{k+1})) > 0$$

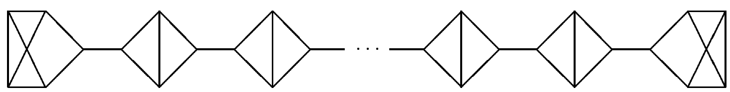
or equivalently

$$x_k + x_{k+2} > \frac{2}{n}(x_k - x_{k+1})$$

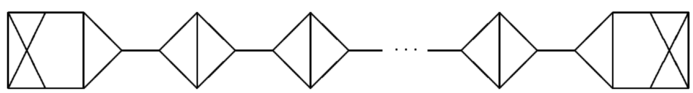
which is clearly true, as we assumed that $x_k > x_{k+1} > x_{k+2} \geq 0$ and $n \geq 10$. This completes the proof of Lemma 3.6 and hence of Lemma 3.5 too. □

3.5 Choosing the optimum between two candidates

We have now shown that G is path-like, has small or medium blocks on the ends, and only small blocks in the middle. If $n \equiv 0 \pmod 4$, then G must be the unique graph Γ_n. If $n \equiv 2 \pmod 4$, then we are left with two candidates for the minimum gap. Either the graph has a medium block at each end, or it has all small blocks. The graphs are drawn here:



Γ_n



Π_n

The graph Γ_n has diameter $(3n-10)/4$, while Π_n has diameter $(3n-14)/4$. Intuitively we would expect the graph with larger diameter to have the smaller eigenvalue ρ_1. The next lemma confirms that this is indeed true, which will complete the proof of Theorem 3.1.

Lemma 3.7 *Let $n \equiv 2 \pmod 4$ and $n \geq 14$. For this n, $\rho_1(L_{\Gamma_n}) < \rho_1(\Pi_n)$.*

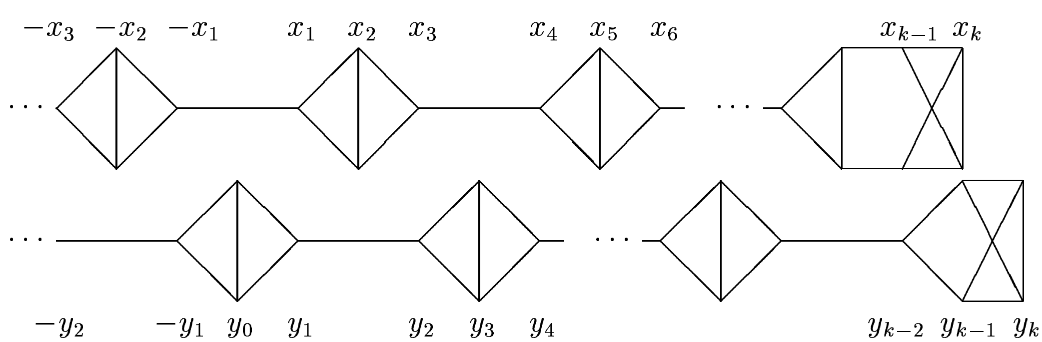
The idea of the proof is simple: we modify an eigenvector of Π_n to get a new vector, still perpendicular to $\mathbf{j}$. We then show that the Rayleigh quotient for Γ_n with the newly defined vector is less than the eigenvalue of Π_n, thus showing that the eigenvalue of Γ_n is less than the eigenvalue of Π_n. The implementation of this idea, however, is very delicate. There are two different cases to consider for when the diameter of Γ_n is even and when it is odd. The proofs are very similar, but each requires separate analysis.

3.5.1 $n \equiv 2 \pmod 8$

Definition of $\mathbf{x}$ and $\mathbf{y}$.

We will exploit the symmetry of Γ_n and Π_n to represent the eigenvector vector of Π_n and the vector for Π_n. The coordinates of the eigenvector for $\rho_1(\Pi_n)$ is a weighting of the vertices that depends only on the vertical position of the vertex, with the graph drawn as we have drawn it. Because the graph has as an automorphism the reflection about the central vertical axis, weights of vertices interchanged by this reflection are negative of each other. Thus we may specify the eigenvector by a vector $\mathbf{x}$ having one coordinate for each vertical position, counting from the middle. If there is a vertex on this axis, we start our labeling of $\mathbf{x}$ with 0, and note that by symmetry its value is 0; if an edge is in the middle, we start our labeling with subscript 1.

Because $n \equiv 2 \pmod 8$, in this case we start our labeling with 1. The following figure shows one half of the graph and establishes the nomenclature. From the vector $\mathbf{x}$, we define a vector $\mathbf{y}$ in a similar way for the graph Γ_n. Note that for Γ_n, the labeling starts with 0.



The components of $\mathbf{y}$ are defined in the following way:

$$
\begin{array}{llll}
y_0 = 0, & y_1 = x_1, & & \\
y_2 = x_3, & y_3 = \dfrac{x_3 + x_4}{2 - \rho_1}, & y_4 = x_4, & \\
y_5 = x_6, & y_6 = \dfrac{x_6 + x_7}{2 - \rho_1}, & y_7 = x_7, & \dots, \\
y_{k-5} = x_{k-4}, & y_{k-4} = \dfrac{x_{k-4} + x_{k-3}}{2 - \rho_1}, & y_{k-3} = x_{k-3}, & \\
y_{k-2} = x_{k-1}, & y_{k-1} = 2x_{k-1} - x_{k-2}, & y_k = x_k + x_{k-1} - x_{k-2}. &
\end{array}
$$

Since $\mathbf{x}$ is an eigenvector for $\rho_1(\Pi_n)$, we may assume $0 < x_1 < x_2 < \cdots < x_k$. Correspondingly, $0 = y_0 < y_1 < y_2 < \cdots < y_k$.

The vectors $\mathbf{x}$ and $\mathbf{y}$ will be tacitly thought of as the n dimensional vectors which they represent, and we will write

$$
\frac{\mathbf{x}^t L_H \mathbf{x}}{\|\mathbf{x}\|^2} \quad \text{and} \quad \frac{\mathbf{y}^t L_G \mathbf{y}}{\|\mathbf{y}\|^2}.
$$

We will estimate the numerator and the denominator of these Rayleigh quotients separately, all in terms of x_1, x_{k-1}, and ρ_1, and finally show that

$$
\frac{\mathbf{y}^t A_{\Gamma_n} \mathbf{y}}{\|\mathbf{y}\|^2} < \frac{\mathbf{x}^t A_{\Pi_n} \mathbf{x}}{\|\mathbf{x}\|^2} = \rho_1(\Pi_n),
$$

which shows that $\rho_1(\Gamma_n) < \rho_1(\Pi_n)$, completing the proof.

Relationships among the coordinates.

First we establish a few relationships among the coordinates of $\mathbf{x}$, using the fact that it is an eigenvector. All of these arise from the eigenvalue equation $L\mathbf{y} = \rho_1 \mathbf{y}$ (again here for the vector arising from $\mathbf{y}$)

We can write x_2 in terms of x_1, x_3, and ρ_1 from the eigenvalue equation $-x_1 + 2x_2 - x_3 = \rho_1 x_2$. We do the same for $x_5, \dots, x_{k-2}$.

$$
x_2 = \frac{x_1 + x_3}{2 - \rho_1}, \quad x_5 = \frac{x_4 + x_6}{2 - \rho_1}, \quad \dots, \quad x_{k-2} = \frac{x_{k-3} + x_{k-1}}{2 - \rho_1}. \tag{3.2}
$$

We may write x_3 in terms of x_1 and x_4 by solving the eigenvalue equations:

$$-x_1 + 2x_2 - x_3 = \rho_1 x_4 \qquad \text{and} \qquad -2x_2 + 3x_3 - x_4 = \rho_1 x_5. \tag{3.3}$$

Their solution yields

$$x_3 = \frac{2x_1 + (2-\rho_1)x_4}{(4-\rho_1)(1-\rho_1)}$$

for which we will use the inequalities

$$x_3 > \frac{(2-\rho_1)(x_1 + x_4)}{(4-\rho_1)(1-\rho_1)} \tag{3.4}$$

and

$$x_3 < \frac{2(x_1 + x_4)}{(4-\rho_1)(1-\rho_1)}, \tag{3.5}$$

which hold as long as $0 < \rho_1 < 1$. Corresponding inequalities hold for $x_6, \ldots, x_{k-4}$.

We can write the values on the ends of both graphs in terms of ρ_1 and x_{k-1}. Consider the eigenvalue equations:

$$-x_{k-2} + 3x_{k-1} - 2x_k = \rho_1 x_{k-1} \qquad \text{and} \qquad -2x_{k-1} + 2x_k = \rho_1 x_k.$$

Solving these as well as substituting in the definitions of y_{k-1} and y_k gives

$$x_{k-2} = \frac{2 - 5\rho_1 + \rho_1^2}{2-\rho_1} x_{k-1}, \qquad x_k = \frac{2}{2-\rho_1} x_{k-1}, \tag{3.6}$$

$$y_{k-1} = \frac{2 + 3\rho_1 - \rho_1^2}{2-\rho_1} x_{k-1}, \qquad y_k = \frac{2 + 4\rho_1 - \rho_1^2}{2-\rho_1} x_{k-1}. \tag{3.7}$$

Additionally using the equation centered around x_{k-2} and substituting the above values, we may write

$$x_{k-3} = -x_{k-1} + (2-\rho_1)x_{k-2} = (1 - 5\rho_1 + \rho_1^2)x_{k-1}. \tag{3.8}$$

Estimating the Norm.

We will write $\|\mathbf{y}\|$ in terms of $\|\mathbf{x}\|$, x_1, x_{k-1}, and ρ_1. The norms of $\mathbf{x}$ and $\mathbf{y}$ are

$$\|\mathbf{x}\|^2 = 2(x_1^2 + 2x_2^2 + x_3^2 + x_4^2 + 2x_5^2 + \cdots + x_{k-3}^2 + 2x_{k-2}^2 + 2x_{k-1}^2) + 2x_{k-1}^2 + 4k_k^2,$$
$$\|\mathbf{y}\|^2 = 2(y_0^2 + y_1^2 + y_2^2 + 2y_3^2 + y_4^2 + \cdots + 2y_{k-4}^2 + y_{k-3}^2 + y_{k-2}^2) + 4y_{k-1}^2 + 4y_k^2.$$

Their difference is

$$\|\mathbf{y}\|^2 - \|\mathbf{x}\|^2 = 4(-x_2^2 + y_3^2 - x_5^2 + \cdots + y_{k-4}^2 - x_{k-2}^2) + (4y_{k-1}^2 + 4y_k^2 - 2x_{k-1}^2 - 4x_k^2). \tag{3.9}$$

Call the two summands S_1 and S_2, respectively. First we consider S_1. Substituting the definitions (3.2) of y_3, y_6, …, y_{k-4}, most of the squares cancel, giving:

$$\begin{aligned} S_1 &= 4(-x_2^2 + y_3^2 - x_5^2 + \cdots + y_{k-4}^2 - x_{k-2}^2) \\ &= \frac{4}{(2-\rho_1)^2}\Big(-(x_1+x_3)^2 + (x_3+x_4)^2 - \cdots + (x_{k-4}+x_{k-3})^2 - (x_{k-3}+x_{k-1})^2\Big) \\ &= \frac{4}{(2-\rho_1)^2}\Big(-x_1^2 + 2x_3(x_4 - x_1) + \cdots + 2x_{k-4}(x_{k-3} - x_{k-6}) - 2x_{k-3}x_{k-1} - x_{k-1}^2\Big). \end{aligned}$$

We may now insert the bounds for x_3 in terms of x_1 and x_4, and the similar bounds for x_6, …, and x_{k-4} to give a bound for S_1 from below. The bound gives a telescopic sum, where all the middle terms cancel out. We also write x_{k-3} in terms of x_{k-1} from above. We have:

$$\begin{aligned} S_1 &= \frac{4}{(2-\rho_1)^2}\Big(-x_1^2 - 2x_1x_3 + 2x_4(x_3 - x_6) + \cdots + 2x_{k-3}(x_{k-1} - x_{k-4}) - x_{k-1}^2\Big) \\ &> \frac{4}{(2-\rho_1)^2}\Bigg[-x_1^2 - 2x_1x_3 + \frac{4}{(4-\rho_1)(1-\rho_1)}\Big((x_3+x_6)(x_3-x_6) + \\ &\qquad + (x_6+x_9)(x_6-x_9) + \cdots + (x_{k-4}+x_{k-1})(x_{k-4}-x_{k-1})\Big) - x_{k-1}^2\Bigg] \\ &> \frac{4}{(2-\rho_1)^2}\Bigg[-x_1^2 - 2x_1x_3 - x_{k-1}^2 + \frac{4}{(4-\rho_1)(1-\rho_1)}\Big(x_3^2 - x_{k-1}^2\Big)\Bigg] \\ &> \frac{1}{\Delta}\Big((32 - 52\rho_1 + 28\rho_1^2 - 4\rho_1^3)x_1^2 + (-32 + 40\rho_1 - 4\rho_1^2)x_{k-1}^2\Big). \end{aligned}$$

Here we let $\Delta = (2-\rho_1)^2(4-\rho_1)(1-\rho_1)$ to make things simpler.

We now consider S_2. Using the equations found above, we may write everything in terms of ρ_1 and x_{k-1}. We have:

$$\begin{aligned} S_2 &= \frac{1}{(2-\rho_1)^2}\Big(4(2+3\rho_1-\rho_1^2)^2+4(2+4\rho_1-\rho_1^2)^2-2(2-\rho_1)^2-4(2)^2\Big)\,x_{k-1}^2 \\ &= \frac{1}{\Delta}(32+248\rho_1-328\rho_1^2-86\rho_1^3+198\rho_1^4-72\rho_1^5+8\rho_1^6)\,x_{k-1}^2. \end{aligned}$$

We may then bound the norm of $\mathbf{y}$ by:

$$\begin{aligned} \|\mathbf{y}\|^2 = \|\mathbf{x}\|^2 + S_1 + S_2 > \|\mathbf{x}\|^2 + \frac{1}{\Delta}(32-52\rho_1+28\rho_1^2-4\rho_1^3)\,x_1^2 + \\ + \frac{1}{\Delta}(288\rho_1-332\rho_1^2-86\rho_1^3+198\rho_1^4-72\rho_1^5+8\rho_1^6)\,x_{k-1}^2. \end{aligned}$$

A Bound for $\mathbf{y}^t L'\mathbf{y}$.

Here we wish to find an upper bound for $\mathbf{y}^t L_H \mathbf{y}$ in terms of $\mathbf{x}^t L_G \mathbf{x}$, x_1, x_{k-1}, and ρ_1.

We have:

$$\begin{aligned} \mathbf{x}^t L\mathbf{x} = 2\Big(&2(x_1)^2+2(x_2-x_1)^2+2(x_3-x_2)^2+(x_4-x_3)^2+\cdots+ \\ &+2(x_{k-5}-x_{k-6})^2+2(x_{k-4}-x_{k-5})^2+(x_{k-3}-x_{k-4})^2 \\ &+2(x_{k-2}-x_{k-3})^2+2(x_{k-1}-x_{k-2})^2+4(x_k-x_{k-1})^2\Big) \\ \mathbf{y}^t L'\mathbf{y} = 2\Big(&2(y_1)^2+(y_2-y_1)^2+2(y_3-y_2)^2+2(y_4-y_3)^2+\cdots+ \\ &+(y_{k-5}-y_{k-6})^2+2(y_{k-4}-y_{k-5})^2+2(y_{k-3}-y_{k-4})^2 \\ &+(y_{k-2}-y_{k-3})^2+2(y_{k-1}-y_{k-2})^2+4(y_k-y_{k-1})^2\Big). \end{aligned}$$

Notice that the contribution at the very center of each is the same, as is the contribution of the last two terms of each. Subtracting, we get:

$$\begin{aligned}
\mathbf{y}^t L' \mathbf{y} - \mathbf{x}^t L \mathbf{x} =& 2\Big((y_2 - y_1)^2 + 2(y_3 - y_2)^2 + 2(y_4 - y_3)^2 - \\
& \qquad - 2(x_2 - x_1)^2 - 2(x_3 - x_2)^2 - (x_4 - x_3)^2 \Big) + \cdots + \\
& + 2\Big((y_{k-5} - y_{k-6})^2 + 2(y_{k-4} - y_{k-5})^2 + 2(y_{k-3} - y_{k-4})^2 - \\
& \qquad - 2(x_{k-5} - x_{k-6})^2 - 2(x_{k-4} - x_{k-5})^2 - (x_{k-3} - x_{k-4})^2 \Big) \\
& + 2\Big((y_{k-2} - y_{k-3})^2 + 2(y_{k-1} - y_{k-2})^2 + 4(y_k - y_{k-1})^2 - \\
& \qquad - 2(x_{k-2} - x_{k-3})^2 - 2(x_{k-1} - x_{k-2})^2 - 4(x_k - x_{k-1})^2 \Big).
\end{aligned}$$

Let the two parts of this be T_1, the part contained on the first four lines, and T_2 the part from the ends, contained on the last two lines.

First we investigate T_1. Comparing the contributions between x_1 and x_4 with those from y_1 to y_4, using the substitutions we found above, we have:

$$\begin{aligned}
&(y_2 - y_1)^2 + 2(y_3 - y_2)^2 + 2(y_4 - y_3)^2 - \\
&\qquad - 2(x_2 - x_1)^2 - 2(x_3 - x_2)^2 - (x_4 - x_3)^2 = \\
&\qquad\qquad = \frac{\rho_1^2}{(2 - \rho_1)^2} (x_4 - x_1)(x_1 + 2x_3 + x_4).
\end{aligned}$$

We have similar equations for the other terms, giving:

$$\begin{aligned}
T_1 &= \frac{\rho_1}{(2 - \rho_1)^2} \Big[(x_4 - x_1)(x_1 + 2x_3 + x_4) + (x_7 - x_4)(x_4 + 2x_6 + x_7) + \cdots + \\
&\qquad + (x_{k-3} - x_{k-6})(x_{k-6} + 2x_{k-4} + x_{k-3}) \Big] \\
&= \frac{\rho_1}{(2 - \rho_1)^2} \Big[x_{k-3}^2 - x_1^2 + 2x_3(x_4 - x_1) + 2x_6(x_7 - x_4) + \cdots + \\
&\qquad + 2x_{k-4}(x_{k-3} - x_{k-6}) \Big].
\end{aligned}$$

Substituting the bounds for x_3, x_6, $\dots$, we have:

$$\begin{aligned} T_1 &< \frac{\rho_1^2}{(2-\rho_1)^2}\Big[x_{k-3}^2 - x_1^2 + \frac{4}{(4-\rho_1)(1-\rho_1)}\Big((x_1+x_4)(x_4-x_1) + \\ &\qquad + (x_4+x_7)(x_7-x_4) + \dots + (x_{k-6}+x_{k-3})(x_{k-3}-x_{k-6})\Big)\Big] \\ &< \frac{\rho_1^2(8-5\rho_1+\rho_1^2)}{\Delta}(x_{k-3}^2 - x_1^2). \end{aligned}$$

Writing x_{k-3} in terms of ρ_1 and x_{k-1} from above, we have:

$$\begin{aligned} T_1 < \frac{\rho_1^2}{\Delta}\Big[&(-8+5\rho_1-\rho_1^2)x_1^2 + \\ &+ (8 - 85\rho_1 + 267\rho_1^2 - 225\rho_1^3 + 85\rho_1^4 - 15\rho_1^5 + \rho_1^6)x_{k-1}^2\Big]. \end{aligned}$$

We now consider T_2. For both Γ_n and Π_n, the last two terms are equal, hence they cancel and we are left with:

$$\begin{aligned} T_2 &= \Big((y_{k-2}-y_{k-3})^2 - 2(x_{k-2}-x_{k-1})^2\Big) \\ &= \Big((x_{k-1}-x_{k-3})^2 - 2(x_{k-2}-x_{k-1})^2\Big). \end{aligned}$$

Using the substitutions already mentioned, we can write all of this in terms of x_{k-1} and ρ_1:

$$T_2 = \frac{\rho_1^2}{\Delta}(272 - 836\rho_1 + 956\rho_1^2 - 515\rho_1^3 + 141\rho_1^4 - 19\rho_1^5 + \rho_1^6)x_{k-1}^2.$$

We may now combine these to get the desired bound:

$$\begin{aligned} \mathbf{y}^t L'\mathbf{y} = \mathbf{x}^t L\mathbf{x} + T_1 + T_2 < \mathbf{x}^t L\mathbf{x} + \frac{\rho_1^2}{\Delta}\Big[&(-8+5\rho_1-\rho_1^2)x_1 + \\ &+ (280 - 921\rho_1 + 1233\rho_1^2 - 740\rho_1^3 + 226\rho_1^4 - 37\rho_1^5 + 2\rho_1^6)x_{k-1}^2\Big]. \end{aligned}$$

The Rayleigh Quotient.

Now comes the easy part. We combine inequalities (3.16) and (3.17).

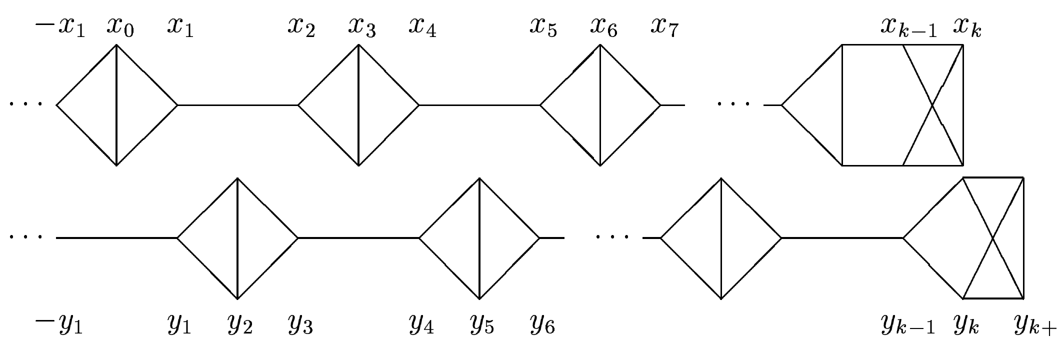
$$\begin{aligned}\frac{\mathbf{y}^t L'\mathbf{y}}{\|\mathbf{y}\|^2} &= \frac{\mathbf{x}^t L\mathbf{x} + T_1 + T_2}{\|\mathbf{x}\|^2 + S_1 + S_2} \\ &< \rho_1 \frac{\|\mathbf{x}\|^2\Delta + \rho_1(280 - 921\rho_1 + \cdots)x_{k-1}^2 + \rho_1(-8 + 5\rho_1 + \cdots)x_1^2}{\|\mathbf{x}\|^2\Delta + \rho_1(288 - 332\rho_1 + \cdots)x_{k-1}^2 + (32 - 52\rho_1 + \cdots)x_1^2} \\ &< \rho_1.\end{aligned}$$

This last inequality certainly holds whenever $0.1 > \rho_1 > 0$. The smallest possible graph considered here is $n = 18$, and already $n = 18$, $\rho_1(\Pi_n) < 0.05$, so this is always valid. □

3.5.2 $n \equiv 6 \pmod 8$

Definition of $\mathbf{x}$ and $\mathbf{y}$.

This section is very similar to the previous one. As above, we exploit the symmetry. $\mathbf{x}$ is an eigenvector for $\rho_1(\Pi_n)$ as above, only now we have a component x_0 and no y_0, by the symmetry.



We define the components of $\mathbf{y}$ as

$$\begin{array}{llll} y_1 = x_1, & y_2 = \dfrac{x_1 + x_2}{2 - \rho_1}, & y_3 = x_2, & \\ y_4 = x_4, & y_5 = \dfrac{x_4 + x_5}{2 - \rho_1}, & y_6 = x_5, & \ldots, \\ y_{k-1} = x_{k-1} & y_k = 2x_{k-1} - x_{k-2}, & y_{k+1} = x_k + x_{k-1} - x_{k-2}. & \end{array} \tag{3.10}$$

Estimating the Norm.

The norms of $\mathbf{x}$ and $\mathbf{y}$ are

$$\begin{aligned} \|x\|^2 &= 2(x_1^2 + x_2^2 + 2x_3^2 + x_4^2 + \cdots + x_{k-3}^2 + 2x_{k-2}^2 + 2x_{k-1}^2 + 2x_k^2), \\ \|y\|^2 &= 2(y_1^2 + 2y_2^2 + y_3^2 + y_4^2 + \cdots + y_{k-2}^2 + y_{k-1}^2 + 2y_k^2 + 2y_{k+1}^2). \end{aligned}$$

The difference is

$$\|y\|^2 - \|x\|^2 = 4(y_2^2 - x_3^2 + y_5^2 - x_6^2 + \cdots + y_{k-3}^2 - x_{k-2}^2) - 2x_{k-1}^2 - 4x_k^2 + 4y_k^2 + 4y_{k+1}^2. \tag{3.11}$$

Solving the eigenvalue equations

$$\begin{aligned} -x_{k-2} + 3x_{k-1} - 2x_k &= \rho_1 x_{k-1} \\ -2x_{k-1} + 2x_k &= \rho_1 x_k \end{aligned}$$

for x_{k-2} and x_k, we may express all end components of the vectors in terms of ρ_1 and x_{k-1}:

$$\begin{aligned} x_{k-2} &= \frac{2 - 5\rho_1 + \rho_1^2}{2 - \rho_1} x_{k-1} \\ x_k &= \frac{2}{2 - \rho_1} x_{k-1} \\ y_k &= \frac{2 + 3\rho_1 - \rho_1^2}{2 - \rho_1} x_{k-1} \\ y_{k+1} &= \frac{2 + 4\rho_1 - \rho_1^2}{2 - \rho_1} x_{k-1}. \end{aligned}$$

Then the last terms in expression (3.11) are

$$-2x_{k-1}^2 - 4x_k^2 + 4y_k^2 + 4y_{k+1}^2 = \frac{2(4 + 60\rho_1 + 33\rho_1^2 - 28\rho_1^3 + 4\rho_1^4)}{(2-\rho_1)^2} x_{k-1}^2$$

For $0 < \rho_1 < 1$ certainly $33\rho_1^2 - 28\rho_1^3 + 4\rho_1^4 > 0$. Thus, dropping these terms yields a lower bound,

$$-2x_{k-1}^2 - 4x_k^2 + 4y_k^2 + 4y_{k+1}^2 > \frac{8(1 + 15\rho_1)}{(2-\rho_1)^2} x_{k-1}^2. \tag{3.12}$$

To deal with the remaining terms on the right side of equation (3.11), we make x_3 explicit in the eigenvalue equation $-x_2 + 2x_3 - x_4 = \rho_1 x_3$, and accordingly, $x_6, \ldots, x_{k-2}$.

$$x_3 = \frac{x_2 + x_4}{2 - \rho_1}, \; x_6 = \frac{x_5 + x_7}{2 - \rho_1}, \; \cdots, \; x_{k-2} = \frac{x_{k-3} + x_{k-1}}{2 - \rho_1}. \tag{3.13}$$

Then, substituting the definitions (3.10) of $y_2, y_5, \ldots, y_{k-3}$, most of the squares cancel,

$$\begin{aligned} &4(y_2^2 - x_3^2 + y_5^2 - x_6^2 + \cdots + y_{k-3}^2 - x_{k-2}^2) = \\ &= \frac{4}{(2-\rho_1)^2}\left((x_1 + x_2)^2 - (x_2 + x_4)^2 + (x_4 + x_5)^2 - \cdots - (x_{k-3} + x_{k-1})^2\right) \\ &= \frac{4}{(2-\rho_1)^2}\left(x_1^2 + 2x_2(x_1 - x_4) + 2x_5(x_4 - x_7) + \cdots + 2x_{k-3}(x_{k-4} - x_{k-1}) - x_{k-1}^2\right). \end{aligned} \tag{3.14}$$

Eliminating x_2 and x_3 from the eigenvalue equations

$$\begin{aligned} -x_1 + 3x_2 - 2x_3 &= \rho_1 x_2 \\ -x_2 + 2x_3 - x_4 &= \rho_1 x_3 \end{aligned}$$

yields

$$x_2 = \frac{(2-\rho_1)x_1 + 2x_4}{(4-\rho_1)(1-\rho_1)} < \frac{2(x_1 + x_4)}{(4-\rho_1)(1-\rho_1)}$$

where the inequality holds as long as $0 < \rho_1 < 1$. Corresponding inequalities hold for $x_5, \ldots, x_{k-3}$. Note that the differences $(x_1 - x_4), (x_4 - x_7), \ldots, (x_{k-4} - x_{k-1})$ are all negative. Using these bounds for $x_2, x_5, \ldots, x_{k-3}$ into equation (3.14), we obtain a lower bound. The sum is telescopic. We have:

$$\begin{aligned}
&4(y_2^2 - x_3^2 + y_5^2 - x_6^2 + \cdots + y_{k-3}^2 - x_{k-2}^2) \\
> \; & \frac{4}{(2-\rho_1)^2}\left[x_1^2 + \frac{4}{(4-\rho_1)(1-\rho_1)}\Big((x_1+x_4)(x_1-x_4)\right. \\
+ \; & \left.(x_4+x_7)(x_4-x_7) + \cdots + (x_{k-4}+x_{k-1})(x_{k-4}-x_{k-1})\Big) - x_{k-1}^2\right] \\
= \; & \frac{4(8-5\rho_1+\rho_1^2)}{(2-\rho_1)^2(4-\rho_1)(1-\rho_1)}(x_1^2 - x_{k-1}^2). \qquad (3.15)
\end{aligned}$$

Dropping x_1 in the last factor does no harm to the inequality. Combined with inequality (3.12) we get in the end

$$\|y\|^2 - \|x\|^2 > \frac{4\rho_1(115-149\rho_1+30\rho_1^2)}{(2-\rho_1)^2(4-\rho_1)(1-\rho_1)}x_{k-1}^2 > \frac{\rho_1(115-149\rho_1)}{(2-\rho_1)^2}x_{k-1}^2. \qquad (3.16)$$

A Bound for $\mathbf{y}^t L'\mathbf{y}$.

The contributions to $\mathbf{x}^t L\mathbf{x}$ from the four edges between $-x_1$ and x_1 in Γ_n are equal to the contribution in $\mathbf{y}^t L'\mathbf{y}$ from the edge between $-y_1$ and y_1 in Π_n.

Comparing the contributions between x_1 and x_4 with those from y_1 to y_4, we write

$$\delta = 2(y_1-y_2)^2 + 2(y_2-y_3)^2 + (y_3-y_4)^2 - (x_1-x_2)^2 - 2(x_2-x_3)^2 - 2(x_3-x_4)^2.$$

Inserting from equations (3.10) and (3.13) brings

$$\delta = \frac{-\rho_1^2}{(2-\rho_1)^2}(x_4-x_1)(x_1+2x_2+x_4) < 0.$$

In the same way all other edges between x_4 and x_{k-1} may be compared. Edges between x_{k-1} and x_k contribute as much as edges between y_k and y_{k+1}. The only exception are the edges between y_{k-1} and y_k and their mirror images on the other end of Π_n, which are not counterbalanced by edges in Γ_n. Their contribution is

$$4(y_{k-1}-y_k)^2 = \frac{4\rho_1^2(4-\rho_1)^2}{(2-\rho_1)^2}x_{k-1}^2.$$

Now for the difference of the quadratic forms, we have the bound:

$$\mathbf{y}^t L' \mathbf{y} - \mathbf{x}^t L \mathbf{x} < \frac{4\rho_1^2(4-\rho_1)^2}{(2-\rho_1)^2} x_{k-1}^2 < \frac{64\rho_1^2}{(2-\rho_1)^2} x_{k-1}^2 \tag{3.17}$$

The Rayleigh Quotient.

Now comes the easy part. We combine the inequalities (3.16) and (3.17).

$$\begin{aligned} \frac{\mathbf{y}^t L' \mathbf{y}}{\|\mathbf{y}\|^2} &< \frac{\mathbf{x}^t L \mathbf{x} + \frac{64\rho_1^2}{(2-\rho_1)^2} x_{k-1}^2}{\|\mathbf{x}\|^2 + \frac{\rho_1(115-149\rho_1)}{(2-\rho_1)^2} x_{k-1}^2} \\ &= \rho_1 \frac{(2-\rho_1)^2\|\mathbf{x}\|^2 + 64\rho_1 x_{k-1}^2}{(2-\rho_1)^2\|\mathbf{x}\|^2 + \rho_1(115-149\rho_1) x_{k-1}^2} < \rho_1. \end{aligned}$$

The last inequality holds as long as $115 - 149\rho_1 > 64$ and $\rho_1 > 0$. The smallest possible graph considered here is for $n = 14$, and already $\rho_1 \approx 0.12709$; for larger n the eigenvalues will be smaller. □

3.6 The graph Γ_n has maximum diameter

In this section, we make the following observation:

Proposition 3.8 *Among all connected trivalent graphs on n vertices, Γ_n has maximum diameter. For $n \equiv 2 \pmod 4$, it is the unique graph with maximum diameter.*

Proof: Let G have diameter d and let $D = (v_0, \ldots, v_d)$ be a diameter (a walk of length d). Then there cannot be another edge between two vertices of D. Every vertex has degree 3, and therefore there are $d+3$ edges leaving D. The vertex v_0 must have two distinct neighbors, neither of which is adjacent to v_3, as this would contradict D being a diameter, and both of which must be of distance at most d from v_d. We apply the same argument at the other end. The vertices $v_3, \ldots, v_{d-3}$ have collectively $d-6$ edges leaving D, thus they determine at least $(d-6)/3$ vertices not on D. Together this is

$$\lceil d + 4 + (d-6)/3 \rceil \le n.$$

Rearranging, we get

$$d \leq \lfloor 3(n-2)/4 \rfloor .$$

These are tight for Γ_n, for all n. To determine for which graphs equality holds, we can draw a diameter horizontally, draw one edge pointing up from each vertex (two out of the ends) and connect them in such a way that ends get identified in threes, the two from each end do not get identified, and ends do not get identified that would shorten the diameter. There is a unique way to do this if $n \equiv 2 \pmod 4$, and for $n \equiv 0 \pmod 4$, we get precisely all path-like graphs with all but one block of smallest size, the remaining block being of medium size. Thus there are $(n-4)/4$ blocks and $\lceil (n-4)/8 \rceil$ different graphs with maximum diameter. $\square$

CHAPTER 4

SPECTRAL EXTREMA FOR EXCLUDED SUBGRAPHS

4.1 Introduction

Many classical results in extremal graph theory study the maximum number of edges $ex(n, \mathcal{H})$ among all graphs G on n vertices which do not contain any of the graphs $H \in \mathcal{H}$ as a subgraph. In this chapter we consider a spectral analogue of $ex(n, \mathcal{H})$, namely we ask for the maximum spectral radius $spex(n, \mathcal{H})$ of graphs G on n vertices, over the same set of graphs. (If $\mathcal{H} = \{H\}$, we write $ex(n, H)$ and $spex(n, H)$ for $ex(n, \mathcal{H})$ and $spex(n, \mathcal{H})$, respectively.) Spectral results are stronger than the classical results: from the fact that the average degree satisfies the inequality $d_{\text{ave}}(G) \leq \lambda_1(G)$, we see that $spex(n, \mathcal{H})$ is an upper bound for the extremal average degree $2 \cdot ex(n, \mathcal{H})/n$, or equivalently that $n \cdot spex(n, \mathcal{H})/2$ is an upper bound for $ex(n, \mathcal{H})$. We define the *spectral density* to be $\lambda_1(G)/n$, and remark that this is an upper bound for the density of G (recall that the density of a graph with n vertices and m edges is $m/\binom{n}{2}$).

We consider two fundamental families of excluded subgraphs $\mathcal{H}$: the first is when $\mathcal{H}$ consists of the complete graph K_t; the second when $\mathcal{H}$ consists of the complete bipartite graph $K_{s,t}$. In both of these cases, the asymptotic bounds we get for $n \cdot spex(n, \mathcal{H})/2$ are the same as those for $ex(n, \mathcal{H})$. In general, it is not the case that the spectral radius of a graph and its average degree are the same; the spectral radius can be of a larger order of magnitude than its average degree. For example. if $\mathcal{H}$ consists of P_3, the path of length 3 alone, it is easy to see that $2 \cdot ex(n, P_3)/n = 2$. yet $spex(n, P_3) = \sqrt{n-1}$. We will that graphs with the *Hereditarily Bounded Property* $P_{t,r}$ discussed is Section 4.6 constitute another example.

In 1941, Paul Turán [85] determined the exact value of $ex(n, K_{t+1})$. He found that the unique extremal graph is the t-partite graph $T(n,t)$ whose t color classes have size $\lceil n/t \rceil$ or $\lfloor n/t \rfloor$. Edges connect all pairs of vertices belonging to different color classes. The density of $T(n,t)$ is asymptotically $1 - 1/t$. In fact the number of edges is never more than $(1-1/t)\binom{n}{2}$.

Wilf proved a spectral version of Turán's result, showing that the density bound given by Turán's theorem holds the spectral density as well:

Theorem 4.1 (Wilf [89]) *Let G be a graph on n vertices not containing K_{t+1} as a subgraph, then $\lambda_1(G) \leq (1 - 1/t)n$*

We establish the following spectral version of Turán's theorem, tightening Wilf's result and determining the extremal graphs.

Theorem 4.2 (Spectral Turán theorem) *Let G be a graph with n vertices not containing K_{t+1} as a subgraph. Then*

$$\lambda_1(G) \leq \lambda_1(T(n,t)).$$

Equality holds if and only if G is the Turán graph $K(n,t)$.

(Our result coincides with Wilf's bound if and only if $t|n$.)

Nosal proved a more general result for the case $t = 2$:

Theorem 4.3 (Nosal [76]) *If G is a triangle-free graph with m edges, then*

$$\lambda_1 \leq \sqrt{m}.$$

Using Mantel's theorem that a triangle-free graph G can have at most $\lfloor n^2/4 \rfloor$ edges (this is Turán's theorem for $t = 2$), we see that

$$\lambda_1(G) \leq \sqrt{\lfloor n^2/4 \rfloor} = \lambda_1(T(n,2)).$$

Erdős-Stone [45] and Erdős-Simonovits [42] generalized Turán's theorem to any non-bipartite excluded subgraph H, and in fact to any set $\mathcal{H}$ of non-bipartite excluded subgraphs. They found that the asymptotic density of the graphs not containing any graph $H \in \mathcal{H}$ as a subgraph depends only on the smallest chromatic number among graphs $H \in \mathcal{H}$. Let $\mathcal{H}$ be a set of graphs, and let $\psi(\mathcal{H})$ denote the *subchromatic number* of $\mathcal{H}$, one less than the minimum chromatic number of graphs in $\mathcal{H}$. They proved:

Theorem 4.4 (Erdős-Stone-Simonovits theorem)

$$\lim_{n\to\infty} ex(n,\mathcal{H})/\binom{n}{2} = 1 - 1/\psi(\mathcal{H}).$$

If $\mathcal{H}$ contains a bipartite graph, then the extremal graphs have 0 density, a fact which also follows from the Kővári-Sós-Turán theorem below.

We show that the density upper bound of Erdős-Stone-Simonovits remains valid asymptotically as a spectral density upper bound. This result strengthens the Erdős-Stone-Simonovits theorem. We state our result.

Theorem 4.5 (Spectral Erdős-Stone-Simonovits theorem)

$$\lim_{n\to\infty} spex(n,\mathcal{H})/n = 1 - 1/\psi(\mathcal{H}).$$

A bipartite analogue to the problem considered by Turán was posed by Zarankiewicz in 1951 [90]. He asked for $ex(n, K_{s,t})$ (he actually only asked for $n \leq 6$). The problem has become known as the *Zarankiewicz problem.* In 1954, Kővári, Sós, and Turán gave an upper bound for $ex(n, K_{s,t})$. They showed that

Theorem 4.6 (Kővári-Sós-Turán [64]) *Let G be a graph on n vertices not containing $K_{s,t}$ as a subgraph. Then*

$$2 \cdot |E(G)| \leq (t-1)^{1/s} n^{1-1/s}.$$

There is no simple extremal graph as in the case of Turán's theorem, and it is still an open problem for $s = t$ greater than 3, whether or not this is the correct order of magnitude. It is conjectured that this bound is asymptotically correct for all s and t.

We prove the following spectral version of Theorem 4.6:

Theorem 4.7 (Spectral Kővári-Sós-Turán theorem) *If G is a graph on n vertices, not containing $K_{s,t}$ as a subgraph, then*

$$\lambda_1(G) \leq ((t-1)^{1/s} + o(1))n^{1-1/s}.$$

Our bound is stronger than the Kővári-Sós-Turán bound and is of the correct order of magnitude and also asymptotically correct whenever this is true for Theorem 4.6.

Erdős [39] and Simonovits [79] independently showed that Turán's theorem is stable in the following sense: if G is a graph with clique number t having almost as many edges as the Turán graph $T(n,t)$, then by removing only a few edges from G, it can be made a subgraph of $T(n,t)$. We prove the following spectral version of this result for $t = 2$ and 3.

Theorem 4.8 (Spectral stability theorem) *For all $\varepsilon > 0$ and for $t = 2$ or 3, there exists a constant $c = c(t)$, such that for all graphs G on n vertices not containing K_{t+1} as a subgraph, if G has spectral radius satisfying*

$$\lambda_1(G) \geq (1 - 1/t)n(1-\varepsilon),$$

then removing at most $c \cdot \varepsilon \cdot n^2$ edges can make G t-partite and removing at most $c \cdot \sqrt{\varepsilon} \cdot n^2$ edges can make G a subgraph of the Turán graph $T(n,t)$.

Our last investigation targets graphs with *hereditarily bounded average* degree. Let $t \in \mathbb{N}$ and $r \geq -\binom{t+1}{2}$. We consider graphs G which have the *Hereditarily Bounded Property* $P_{t,r}$:

$$|E(H)| \leq t \cdot |V(H)| + r, \qquad \forall H \leq G,\ |V(H)| \geq t. \qquad (P_{t,r})$$

If the set $\mathcal{H}_{t,r}$ consists of all graphs K on at least t vertices for which $|E(K) > t \cdot |E(K)| + r$, then graphs with the Property $P_{t,r}$ are exactly those which do not contain elements of $\mathcal{H}$ as a subgraph. Notice that $ex(n, \mathcal{H}) = tn + r$, whereas the graph $K_{t,n-t}$ has the Property $P_{t,0}$ and has spectral radius $\sqrt{tn - t^2}$.

The trivial upper bound on λ_1 is

$$\lambda_1 \leq \sqrt{2m} \leq \sqrt{tn + r},$$

which can be improved a little using a result of Hong [59] to give:

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

We show that for graphs with hereditarily bounded degree, the coefficient of $\sqrt{n}$ can be significantly improved.

Theorem 4.9 *Let $t \in \mathbb{N}$ and $r \geq -\binom{t+1}{2}$. If G is a graph on n vertices with the Hereditarily Bounded Property $P_{t,r}$, then*

$$\lambda_1(G) \leq (t-1)/2 + \sqrt{(t+1)t + 2r} + \sqrt{tn},$$

and asymptotically,

$$\lambda_1(G) \leq (t-1)/2 + \sqrt{tn} + o(1).$$

The asymptotic bound is tight.

We also show that the unique extremal graph for $r = -\binom{t+1}{2}$ is the graph having t vertices of degree $n-1$, all others of degree t (if $n \leq t$, then this is just K_n).

As a consequence of this result, we obtain the following bounds for graphs embeddable on arbitrary surfaces.

Corollary 4.10 *Let G be a graph embeddable on a fixed surface of Euler characteristic χ. Then*

$$\lambda_1(G) < 1 + \sqrt{6(2-\chi)} + \sqrt{3n},$$

and asymptotically,

$$\lambda_1(G) < 1 + \sqrt{3n} + o(1).$$

This improves upon previous bounds for all surfaces obtained by Hong [60].

4.2 Zarankiewicz problem

We establish the following spectral analogue of the Kővári-Sós-Turán theorem:

Theorem 4.7 (Spectral Kővári-Sós-Turán theorem) *If G is a graph on n vertices, not containing $K_{s,t}$ as a subgraph, then*

$$\lambda_1(G) \leq ((t-1)^{1/s} + o(1))n^{1-1/s}.$$

4.2.1 Preliminary definitions

First, we consider an easy case which illustrates the idea of the proof.

Proposition 4.11 *If G is C_4-free, then $\lambda_1 \leq \sqrt{2(n-1)}$.*

Proof: Let $D = (D_{ii})$ be the diagonal matrix of degrees of G, I the $n \times n$ identity matrix, and J the $n \times n$ matrix of all 1's. Notice that the (i,j) entry of A^2 is the number of common neighbors of i and j (if $i = j$, then it is just the degree). We have $A^2 \leq D + (J - I)$, where the inequality is coordinate-wise. It follows that:

$$\lambda_1^2 = \lambda_1(A^2) \leq \lambda_1(D) + \lambda_1(J - I) \leq (n-1) + (n-1). \qquad \square$$

By a more careful estimate of $\lambda_1(A^2)$ we can obtain $\sqrt{n-1}$ as an upper bound. We will use a more careful analysis in the general case below.

We use the following notation (for $W \subset \{1, \ldots, n\}$ and $\mathbf{x} = (x_1, \ldots, x_n)^t \in \mathbb{R}^n$):

$$S_W := \sum_{i \in W} x_i,$$
$$S_W^r := \Big(\sum_{i \in W} x_i \Big)^r,$$
$$P_W(r) := \sum_{i \in W} x_i^r.$$

Omission of W indicates the entire set itself.

We now establish some lemmas we will need. The proofs of the first two are straightforward; we refer the reader to [65].

Lemma 4.12 *For r a positive integer and $W \subset \{1, \dots, n\}$, we have*

$$\Big(\sum_{i\in W} x_i\Big)^r \le |W|^{r-1} \sum_{i\in W} x_i^r, \quad i.e., \quad S_W^r \le |W|^{r-1} P_W(r).$$

Lemma 4.13 *Let $\mathbf{x}$ be a nonnegative vector, and a and b nonnegative real numbers. Then*

$$\Big(\sum_{i\in W} x_i^a\Big)\Big(\sum_{i\in W} x_i^b\Big) \le |W| \sum_{i\in W} x_i^{a+b}, \quad i.e., \quad P_W(a)P_W(b) \le |W| P_W(a+b).$$

We will need the Kövári-Sós-Turán upper bound on the maximum number of edges in a $K_{s,t}$-free graph to obtain the following:

Lemma 4.14 *Let G be a graph on n vertices not containing $K_{s,t}$. G has at most $(t-1)^{1/s} n^{1-1/2s}$ vertices of degree at least $n^{1-1/2s}$.*

Proof: If G had more than this many vertices of this degree, then it would have more than $(t-1)^{1/s} n^{1-1/s}/2$ edges, more than are allowed by Theorem 4.6. □

We will also need the following inequality:

Lemma 4.15 *Let X and Y be disjoint subsets of $\{1, \dots, n\}$. Further, let a and b be positive integers and set $s = a + b$. Then*

$$\Big(\sum_{i\in X} x_i^a\Big)\Big(\sum_{i\in Y} x_i^b\Big) \le |X|^{a/s} |Y|^{b/s} \sum_{i\in X\cup Y} x_i^s,$$

i.e.,

$$P_X(a)P_Y(b) \le |X|^{b/s} |Y|^{a/s} P(s).$$

Proof: This follows easily from Hölder's inequality, which in our case implies that

$$P_X(a) \le |X|^{b/s} P_X(s).$$

4.2.2 $K_{2,t}$-free graphs

We start by considering the case $s = 2$, namely the case of graphs not containing the complete bipartite graph $K_{2,t}$ as a subgraph. We will pay special attention to the error term. In the next section we will consider the case $s > 2$ and we will not be concerned with lower-order terms.

We prove the following theorem:

Theorem 4.16

$$spex(n, K_{2,t}) < \Big((t-1)^{1/2} + o(1)\Big)n^{1/2}.$$

Proof: We will actually prove that

$$spex(n, K_{2,t}) < (t-1)^{1/2}n^{1/2} + \frac{1}{2^{3/4}}(t-1)^{1/4}n^{1/4} + \frac{1}{2^{1/2}}.$$

We let G be a graph on n vertices not containing $K_{s,t}$, and let $\mathbf{x}$ be a nonnegative eigenvector for $\lambda_1(G)$. The theorem follows by bounding the expression $\lambda_1^2 \sum_i x_i^2$. We may rewrite this as:

$$\lambda_1^2 \sum_i x_i^2 = \sum_i (\lambda_1 x_i)^2 = \sum_i \Big(\sum_{j\sim i} x_j\Big)^2 = \sum_i d_i x_i^2 + \sum_{i\neq j} d_{ij} x_i x_j \tag{4.1}$$

where d_i is the degree of vertex i and d_{ij} is the number of common neighbors of i and j. To simplify the notation a little, we will use $P = \sum_i x_i^2$ and $P_X = P_X(2) = \sum_{i\in X} x_i^2$. We can immediately get a reasonable bound on this using only the fact that $d_i < n$ and $d_{ij} < t-1$, by virtue of the fact that G does not contain $K_{2,t}$. Using Lemma 4.13 we may immediately conclude:

$$\lambda_1^2 P = \sum_i d_i x_i^2 + \sum_{i\neq j} d_{ij} x_i x_j < nP + (t-1)nP < tnP,$$

implying that $\lambda_1 < t^{1/2}n^{1/2}$. (This is analogous to Proposition 4.11.) To correct the constant to $(t-1)^{1/2}$, we need to examine the two terms a little more carefully.

We will partition the vertices of G into a set U of vertices with high degree and a set of vertices with low degree, and split our terms up into multiple parts.

Let $D = \Big(2(t-1)n\Big)^{1/2}$ and $U = \{x \in V : d(x) > D\}$ and $W = V \setminus U$. We then claim that U cannot be too big.

Claim 4.1 $|U| \le \left(2n/(t-1)\right)^{1/2}$.

To prove the claim, let $u = |U|$ and assume that G is labeled so that $U = \{1, \dots, u\}$. Let $N_i \subset [n]$ be the set of neighbors of i, then the family of sets $\{N_1, \dots, N_u\}$ has the property that any two members intersect in at most $(t-1)$ points. Thus the union of any k sets must contain at least $D + (D-t) + \cdots + (D - (k-1)\,t)$ elements, whenever $k \le (2n/t)^{1/2}$. Thus the family of sets cannot have $(2n/t)^{1/2}$ members as

$$\left(2(2tn)^{1/2} - ((2n/t)^{1/2} - 1)\,t\right)\frac{(2n/t)^{1/2}}{2} > n. \qquad \square$$

Now armed with the maximum number of vertices with large degree, we may complete the proof. We split the first summation on the right-hand side of (4.1) into two parts

$$\begin{aligned}\sum_i d_i x_i^2 &\le nP_U + DP_W \\ &\le nP_U + 2^{1/2}(t-1)^{1/2}n^{1/2}P_W,\end{aligned}$$

where the first term is the dominant term. Now, using the fact that $d_{ij} \le t-1$, the second summation becomes:

$$\begin{aligned}\sum_{i\neq j} d_{ij}x_ix_j &\le (t-1)\sum_{i,j\in U} x_ix_j + (t-1)\sum_{i,j\in V} x_ix_j + 2(t-1)S_US_V \\ &\le (t-1)uP_W + (t-1)nP_U + 2(t-1)\sqrt{unP_U(2)P_W(2)} \\ &\le (t-1)nP_W + 2^{1/2}(t-1)^{1/2}n^{1/2}P_U + (t-1)\sqrt{un}P \\ &\le (t-1)nP_W + 2^{1/2}(t-1)^{1/2}n^{1/2}P_U + 2^{1/4}(t-1)^{3/4}n^{3/4}P,\end{aligned}$$

where the first term here is also the dominant term. We are now done if we ignore terms of lower order, as $nP_U + (t-1)nP_W \le (t-1)nP$ and all other terms are of lower order. However, by further analysis, we may determine the error more precisely:

$$\begin{aligned}\lambda_1^2 P &\le (t-1)nP + \sqrt{2(t-1)n}P + 2^{1/4}(t-1)^{3/4}n^{3/4}P \\ &\le \left((t-1)^{1/2}n^{1/2} + \frac{1}{2^{3/4}}(t-1)^{1/4}n^{1/4} + \frac{1}{\sqrt{2}}\right)^2 P.\end{aligned}$$

Thus we have shown that $\lambda_1 < (t-1)^{1/2}n^{1/2} + O(t^{1/4}n^{1/4})$. □

4.2.3 $K_{s,t}$-free graphs

Theorem 4.17

$$spex(n, K_{s,t}) < ((t-1)^{1/s} + o(1))n^{1-1/s}.$$

Proof: We restrict ourselves to the case $s > 2$, as the case $s = 2$ is just Theorem 4.16.

$$\begin{aligned}\lambda_1^s P(s) &= \sum_{i=1}^{n}(\lambda_1 x_i)^s = \sum_{i=1}^{n}\Big(\sum_{j\sim i} x_j\Big)^s \\ &\leq \sum_{i_1=1}^{n}\cdots\sum_{i_s=1}^{n} d(i_1,\ldots,i_s)x_{i_1}\cdots x_{i_s}\end{aligned}$$

where $d(i_1,\ldots,i_s)$ is the number of common neighbors of the s (not necessarily distinct) vertices $i_1,\ldots,i_s$. If the vertices are distinct, this is at most $t-1$, otherwise it can be at most n. We will show that we need only consider the case when the s-tuple $(i_1,\ldots,i_s)$ is distinct, showing that

$$\sum_{i_1=1}^{n}\cdots\sum_{i_s=1}^{n} d(i_1,\ldots,i_s)x_{i_1}\cdots x_{i_s} \leq ((t-1)+o(1))n^{s-1}P(s), \tag{4.2}$$

and thus completing the proof of the theorem.

We break the sum up into two parts. The first part is all summands for which the s-tuple consists of s distinct vertices, and we call this $\sum_{\text{distinct}}$. For these s-tuples, the number of common neighbors is at most t and this sum may be bounded above by

$$\sum_{\text{distinct}} \leq (t-1)\sum_{i_1=1}^{n}\cdots\sum_{i_s=1}^{n} x_{i_1}\cdots x_{i_s} \leq (t-1)n^{s-1}P(s),$$

by Lemma 4.12. The part which remains we call $\sum_{\text{non-distinct}}$. This may be bounded above by

$$\sum_{\text{non-distinct}} \leq \binom{s}{2}\sum_{i_1=1}^{n}\cdots\sum_{i_{s-2}=1}^{n}\sum_{j=1}^{n} d(i_1,\ldots,i_{s-2},j)x_{i_1}\cdots x_{i_{s-2}}x_j^2.$$

This is clear because if the s-tuple is not distinct, there is at least one equality, and this can happen in $\binom{s}{2}$ ways. We will show this is $o(n^{s-1})$, thus completing the proof.

Let U be the set of vertices with degree at least $D = n^{1-1/2s}$, and let V be the set of remaining vertices. By Lemma 4.14, we see that $|U| \le (t-1)^{1/s} n^{1-1/2s}$. We now split each of the sums up into parts corresponding to U and V, and then use the fact that if at least one vertex is from V, then the number of common neighbors can be at most D. Hence the sum is bounded above by

$$\sum_{i_1=1}^{n} \cdots \sum_{i_{s-2}=1}^{n} x_{i_1} \cdots x_{i_{s-2}} \sum_{j=1}^{n} x_j^2 \le D S^{s-2} P(2) + n S_U^{s-2} P_U(2).$$

The first term is bounded by

$$D S^{s-2} P \le D n^{s-2} P(s) = o(n^{s-1}) P(s).$$

The second term, consisting of all elements from U, is bounded by

$$n S_U^{s-2} P_U(2) \le n u^{s-2} P_U(s) \le o(n^{s-1}) P(s).$$

This completes the proof of the theorem. □

4.3 Turán's theorem

We restate and prove our spectral analogue of Turán's theorem

Theorem 4.2 (Spectral Turán theorem) *Let G be a graph with n vertices not containing K_{t+1} as a subgraph. Then*

$$\lambda_1(G) \le \lambda_1(T(n,t)).$$

Equality holds if and only if G is the Turán graph $K(n,t)$.

We will first prove the theorem, then we derive some consequences.

4.3.1 Proof of the spectral Turán theorem

We adapt Zykov's proof of Turán's theorem [91] (see also [80]). He showed that if G does not contain K_{t+1} as a subgraph, then there is a t-partite graph H with at least as many edges as G. He used the idea of symmetrizing: two vertices in G are called *symmetric* if they have the same set of neighbors. Symmetrizing a vertex v to a vertex u means to remove all edges from u and to add all edges between u and vertices adjacent to v. If G does not contain K_{t+1}, then after symmetrizing, the new graph H also does not contain K_{t+1}. Zykov showed that it is possible to symmetrize successively to produce a graph H in such a way that H is t-partite and H has no fewer edges than G.[1] Turán's theorem then follows by an easy analysis of complete t-partite graphs.

Let $\mathbf{x}$ be a nonnegative vector associating a weight x_i to each vertex i. We show that it is possible to symmetrize to obtain a t-partite graph H without decreasing the quadratic form at $\mathbf{x}$, i.e.,

$$\mathbf{x}^t A_H \mathbf{x} \geq \mathbf{x}^t A_G \mathbf{x}.$$

Our Spectral Turán theorem will then follow by analyzing the complete t-partite graphs (Lemma 4.19).

Let $N_G(v)$ be the set of neighbors of v in G, and $w_G(v) = \sum_{i \in N_G(v)} x_i$ be the weighted sum of the neighbors of vertex v. We will prove the following lemma, similar to the approach of Zykov, with the observation of Erdős (see footnote on this page):

Lemma 4.18 *Let G be a graph not containing K_{t+1} as a subgraph, and let $\mathbf{x}$ be a positive vector. Then there exists a complete t-partite graph H that dominates G with respect to the weighted sum of neighbors in the sense that $w_H(i) \geq w_G(i)$, for all $i \in V$, and*

$$\mathbf{x}^t A_H \mathbf{x} \geq \mathbf{x}^t A_G \mathbf{x}.$$

Equality holds if and only if $G \cong H$.

[1] Zykov's proof was rediscovered by Erdős [40] (see also [12], Theorem 7.8), who made the additional observation that H degree-dominates G, i.e., $d_H(i) \geq d_G(i)$, for all $i \in V$.

The special case of $\mathbf{x} = \mathbf{j}$, implying $d_i = w_G(i)$ and $\mathbf{x}^t A_G \mathbf{x} = 2 \cdot |E(G)|$, can be interpreted as Zykov's proof of Turán's theorem.

Proof of Lemma 4.18: The second claim of the theorem follows immediately from the first. Indeed, $\mathbf{x}^t A_G \mathbf{x} = \sum_i x_i w_G(i)$.

We prove the lemma by induction. For $t = 1$ it is trivial.

Let $t > 1$, and assume the lemma is true for all $t' < t$. Let v_0 be a vertex such that $w_G(v)$ is maximum. Let V_0 be the set of neighbors of v_0, and let $V_1 = V \setminus V_0$. Symmetrize all non-neighbors of v_0 to v_0. Call this graph K. The graph K dominates G with respect to the weighted sum of neighbors. Indeed,

$$\forall\, u \in V_0: \quad N_G(u) \subseteq N_K(u), \quad \text{which implies} \quad w_K(u) \geq w_G(u); \tag{4.3}$$

and for $u \in V_1$, we have: $w_K(u) = w_K(v_0) = w_G(v_0) \geq w_G(u)$.

Let G_0 be the subgraph of K induced by V_0 (V_0 also induces G_0 in G, as the edges in V_0 are unchanged). G_0 does not have K_t as a subgraph, otherwise with v_0 the graph G would contain K_{t+1}. Thus by induction there is a complete $(t-1)$-partite graph H_0 on vertex set V_0 for which $w_{H_0}(i) \geq w_{G_0}(i)$ for all $i \in V_0$. Let H be the complete t-partite graph on vertex set $V_0 \cup V_1$, formed by adjoining all vertices of V_0 to all vertices of V_1. (H is similarly obtained from K by replacing the edges given by G_0 with the edges from H_0.)

The graph H satisfies the conclusion of the lemma:

$$w_H(u) = w_K(u) = w_K(v_0) = w_G(v_0) \geq x_G(u), \quad \text{for} \quad u \in V_1,$$

and letting $w(V_1) := \sum_{i \in V_1} x_i$, as have

$$w_H(u) = w_{H_0}(u) + w(V_1) \geq w_{G_0}(u) + w(V_1) \geq w_G(u), \quad \text{for} \quad u \in V_0.$$

If equality occurs, then equality occurs in every inequality, in particular in (4.3), which implies that all vertices of V_0 are adjacent to all vertices of V_1 in G. Hence equality holds for G_0, and we are done by induction. □

By applying the lemma to an eigenvector of $\lambda_1(G)$, we remark that the lemma implies that

$$\lambda_1(G) \leq \lambda_1(H),$$

and equality holds if and only if G is a complete t-partite graph.

We now analyze the complete t-partite graphs.

Lemma 4.19 *Let G be a complete t-partite graph on n vertices. Then $\lambda_1(G) \leq \lambda_1(T(n,t))$ and equality holds if and only if G is the Turán graph $T(n,t)$).*

Proof: It is easily verified (cf. [29], §2.6) that the characteristic polynomial of G is

$$\lambda^{n-k}\left(1 - \sum_{i=1}^{k} \frac{n_i}{\lambda + n_i}\right) \prod_{i=1}^{k} (\lambda + n_j),$$

and hence λ_1 is the unique positive root of

$$1 - \sum_{i=1}^{k} \frac{n_i}{\lambda + n_i}.$$

Consider the function:

$$F(\delta, \lambda) = \frac{n_1 - \delta}{\lambda + n_1 - \delta} + \sum_{i=2}^{k-1} \frac{n_i}{\lambda + n_i} + \frac{n_k + \delta}{\lambda + n_k + \delta}.$$

Notice that $F(0, \lambda_1) = 0$. Computing the derivative with respect to δ, we have:

$$F_\delta(\delta, \lambda) = \frac{\lambda}{(\lambda + n_1 - \delta)^2} - \frac{\lambda}{(\lambda + n_k + \delta)^2}$$

which is negative for $\lambda > 0$ and $0 < \delta < (n_1 - n_k)/2$. We conclude that if $n_1 \geq n_k + 2$, then decreasing the size of the largest set by 1 and increasing the size of the smallest set by 1 increases the spectral radius. Thus the Turán graph is the unique extremal graph, as it is the only t-partite graph with largest and smallest sets differing in size by at most 1. $\square$

4.3.2 Consequences

We now determine the spectral radius of $T(n,t)$ and show that Theorem 4.2 implies Turán's theorem. We will prove the following:

Proposition 4.20 *If G is a graph on n vertices having spectral radius satisfying $\lambda_1(G) \le \lambda_1(T(n,t))$, then $|E(G)| \le |E(T(n,t))|$.*

Note that we do not make any assumptions on the clique number of G. The following corollary is then immediate:

Corollary 4.21 *Theorem 4.2 implies the edge bound of Turán's theorem.*

The proof of Proposition 4.20 is straightforward, yet a bit tedious. We calculate the spectral radius of the Turán graph. The spectral radius of a graph gives the bound $\lfloor \lambda_1 n/2 \rfloor$ on the number of edges. We show that this is equal to the number of edges in the Turán graph, completing the proof.

We will use the notation $n = kt + r$, $0 \le r < t$ throughout.

An easy calculation shows that

$$|E(T(n,t))| = \binom{r}{2}(k+1)^2 + \binom{t-r}{2}k^2 + r(t-r)k(k+1). \tag{4.4}$$

There are only two orbits of the vertices under the automorphism group of $T(n,r)$, and hence the eigenvector associated to $\lambda_1(G)$ has only two distinct components. Thus λ_1 is the largest eigenvalue of the matrix:

$$\begin{pmatrix} (r-1)(k+1) & (t-r)k \\ r(k+1) & (t-r-1)k \end{pmatrix}.$$

Solving, we have

$$\lambda_1(T(n,t)) = \frac{1}{2}\left(kt + r - 2k - 1 + \sqrt{k^2t^2 + 2ktr + 2kt - 4kr + r^2 - 2r + 1}\right).$$

If G is any graph with clique number at most t, then Theorem 4.2 and the bound $|E(G)| \le \lfloor n\lambda_1(G)/2 \rfloor$ gives the following bound on the number of edges:

$$|E(G)| \le \left\lfloor \frac{n}{4}\left(kt + r - 2k - 1 + \sqrt{k^2t^2 + 2ktr + 2kt - 4kr + r^2 - 2r + 1}\right)\right\rfloor. \tag{4.5}$$

We will show that the bounds given in (4.4) and (4.5) are equal for all n and t. We may assume that $r > 0$, as for $r = 0$ the two quantities are equal without taking the integer part. Let $\delta = n\lambda_1(T(n,t))/2 - |E(T(n,t))|$, i.e.

$$\begin{aligned}\delta = \frac{1}{4}(kt+r)(kt+r-2k-1) &+ \\ &+ \frac{1}{4}(kt+r)\sqrt{(kt+r-1-2k)^2 - 4k(k+1)(t-1)} - \\ &- \frac{1}{2}r(r-1)(k+1)^2 - \frac{1}{2}(t-r)(t-r-1)k^2 - r(t-r)k(k+1).\end{aligned}$$

We need to show that $\lfloor \delta \rfloor = 0$, i.e. that $\delta < 1$. Solving for the radical we get

$$\begin{aligned}\delta + \frac{1}{4}k^2t^2 + \frac{1}{2}krt + \frac{1}{4}kt - \frac{1}{2}kr + \frac{1}{4}r^2 - \frac{1}{4}r &= \\ &= \frac{1}{4}(kt+r)\sqrt{(kt+r-1-2k)^2 + 4k(k+1)(t-1)}\end{aligned}$$

and then squaring, simplifying, and moving everything to the left we have

$$\delta^2 + \frac{1}{2}(k^2t^2 + 2ktr + kt - 2kr + r^2 - r)\delta - \frac{1}{4}k(k+1)r(t-r) = 0.$$

Let the expression on the left be $f(\delta)$. We see that

$$f(0) = -\frac{1}{4}k(k+1)r(t-r) \leq 0.$$

(Equality holds only when $r = 0$.) Additionally, we have

$$f(1) = \frac{1}{4}(2k^2t^2 - k^2rt + 3ktr + 2kt + k^2r^2 + kr^2 - 4kr + 2r^2 - 2r + 4) > 0.$$

This shows that $f(\delta)$ has one positive root, and that it is strictly less than 1. This completes the proof of the proposition. $\square$

4.4 Erdős-Stone-Simonovits Theorem

We restate and prove our result for arbitrary families of excluded graphs.

Theorem 4.22 (Spectral Erdős-Stone-Simonovits Theorem) *Let $\mathcal{H}$ be a set of graphs such that* $\min_{H \in \mathcal{H}} \chi(H) = t + 1$. *Then*

$$\lim_{n \to \infty} spex(n, \mathcal{H})/n = 1 - 1/t.$$

The Turán graph $T(n,t)$ has chromatic number t and therefore does not contain H. On the other hand,

$$\lim_{n \to \infty} \lambda_1(T(n,t))/n = 1 - 1/t.$$

This implies

$$\limsup_{n \to \infty} spex(n, H)/n \geq 1 - 1/t.$$

We need to prove the reverse inequality for lim inf. We reformulate this statement, which constitutes the nontrivial part of our spectral version of the Erdős-Stone-Simonovits theorem.

Theorem 4.23 *Let H be a graph of chromatic number $\chi(H) = t+1$. Then for every $\xi > 0$ there exists $N = N(H, \xi)$ such that every graph G with $n \geq N$ vertices not containing H as a subgraph satisfies*

$$\lambda_1(G)/n \leq 1 - 1/t + \xi.$$

For a graph L and a positive integer r, we define the graph $L(r)$ by replacing each vertex of L by r independent vertices, and replacing each edge of L by a complete bipartite graph between the corresponding r-tuples. ($L(r)$ is the *lexicographic product* of L with $\overline{K_r}$. Cf. e.g. [5], page 1466.)

Following Erdős-Simonovits [42] we note that it suffices to prove Theorem 4.23 for the case $H = K_{t+1}(r)$, r and t fixed. Indeed, for any H let r be the maximum size of an independent set of H and let $t = \chi(H) - 1$. Obviously, H is a subgraph of $K_{t+1}(r)$.

The proof of Theorem 4.23 relies on Szemerédi's powerful uniformity lemma. Before stating this lemma, we need some definitions.

Let U and W be disjoint subsets of $V(G)$. Let $e(U,W)$ be the number of edges between the sets U and W. Define the *density* of the pair (U,W) to be[2]

$$d(U,W) = \frac{e(U,W)}{|U||W|}.$$

We say that the pair (U,W) is (ε,δ)-*uniform* if for all pairs of sets $U' \subseteq U$, $W' \subseteq W$ satisfying $|U'| \geq \delta|U|$ and $|W'| \geq \delta|W|$ we have $|d(U,W) - d(U',W')| < \varepsilon$.

We may now state Szemerédi's result.

Theorem 4.24 (Szemerédi's Uniformity Lemma [83]) *Given $\varepsilon > 0$ and an integer m, there is an $M = M(\varepsilon, m)$ such that the vertex set of every graph with n vertices, $n \geq m$, can be partitioned into classes $V_0, \ldots, V_k$, where $m \leq k \leq M$, such that $|V_0| \leq \varepsilon n$, $|V_1| = |V_2| = \cdots = |V_k|$, and all but at most $\varepsilon\binom{k}{2}$ of the pairs (V_i, V_j), $1 \leq i < j \leq k$ are $(\varepsilon,\varepsilon)$-uniform.*

Proof of Theorem 4.23: First we describe the idea informally. We consider a Szemerédi partition of $V(G)$ into k blocks, for some $k > t$ (k will not depend on n). We then remove all edges from within the blocks themselves, obtaining a k-partite graph, and removing also those edges lying between pairs of blocks that are not $(\varepsilon,\varepsilon)$-uniform, for some ε larger than some threshold. In this way, all the remaining edges are between vertices of different color classes, and if there is at least one edge between two color classes U and W, then $d(U,W)$ is above the predetermined threshold and the pair (U,W), is $(\varepsilon,\varepsilon)$-uniform. Call this resulting graph Γ.

We will need a technical lemma (of independent interest) which states that under certain conditions, if Γ contains a K_{t+1}, then Γ contains a $K_{t+1}(r)$, and hence so does G. Thus Γ cannot contain K_{t+1} and we may apply (Theorem 4.1) to bound its spectral radius. We use Lemma 2.3, item (iii), to show that the edges we removed cannot contribute much to the spectral radius.

[2]The reader should beware that in this section we are using d to denote density rather than degree. These are, however, easily distinguished from each other by the number of arguments.

The main work of our proof is contained in the following technical lemma. (A similar lemma, with a stronger condition and a stronger conclusion, appears in [24].)

Lemma 4.25 *Given $k, r, \tau, \varepsilon, \delta$ such that $\varepsilon < \tau/4^k$ and $\delta < (\tau - 2^k\varepsilon)^{kr}$, there exists an $R = R(k, r, \tau, \varepsilon, \delta)$ such that the following holds. If Γ is a graph on the vertex set $\{1, \ldots, k\}$, G is a k-partite graph on disjoint sets $V_1, \ldots, V_k$, each set of size at least N, and for all $\{i, j\} \in E(\Gamma)$, the pair (V_i, V_j) is (ε, δ)-uniform with density at least τ, then $\Gamma(r) \subseteq G$.*

Proof: Without loss of generality we may assume that Γ is complete. Indeed, if Γ is not complete, let G' be the graph obtained from G by adding all edges between V_i and V_j whenever $\{i, j\} \in E(\overline{\Gamma})$ and apply the lemma to find $K_t(r)$ in G'. This $K_t(r)$ contains the desired $\Gamma(r)$ in G.

We will actually prove the lemma under the following slightly weaker condition on δ:

$$\delta < (\tau - \varepsilon)^r(\tau - 3\varepsilon)^r \cdots (\tau - (2^k - 1)\varepsilon)^r. \tag{4.6}$$

Before we proceed with the proof, we make two more definitions. Let G be a graph, S a subset of the vertices of G, and x a vertex of G. Let $N_S(x)$ is the set of vertices in S adjacent to x. If X is a set of vertices, then $N_S(X) = \cap_{x \in X} N_S(x)$.

The proof is by induction on k. For $k = 1$, the lemma is true with

$$R(1, r, \tau, \varepsilon, \delta) = r.$$

We assume that the lemma is true for $k = t$ (with the weaker condition (4.6) for δ), and prove it for the case $k = t + 1$.

Let $k = t + 1$, and assume that r, ε, δ, τ, are given, and that they satisfy the hypotheses of the lemma (again, for the weaker condition on δ). We further assume that G is given on sets $V_1, \ldots, V_{t+1}$ such that (V_i, V_j) is (ε, δ)-uniform with density at least τ, and all sets have size at least M, where

$$M = \max\Big\{r/(1-\delta)^r, N\Big(t, r, \tau - \varepsilon, 2\varepsilon, \delta/(\tau - \varepsilon)^r\Big)/(\tau - \varepsilon)^r\Big\}.$$

We will find $X = \{x_1, \ldots, x_r\} \subseteq V_{t+1}$, such that if $V_i' \subseteq N_{V_i}(X)$, for $i = 1, \ldots, t$, then the conditions of the lemma are met for the graph G' induced on the sets $V_1', \ldots, V_t'$. Then set X together with the $K_t(r)$ from the inductive step is the desired $K_{t+1}(r)$.

Let $U = V_{t+1}$. Within U, we will find a set of large size such that all elements have large degree in each of the V_i. From this set we choose x_1. We then restrict to the neighbors of x_1, and repeat the procedure, finding an x_2, etc.

Defining the degree of a vertex x in a set S to be $d_S(x) = |\{y \in S : x \sim y\}|$, we let $U^1 = \{y \in U : d_{V_1}(x) \geq (\tau - \varepsilon)|V_1|\}$ and $\overline{U^1} = U \setminus U^1$. Notice that

$$d(\overline{U^1}, V_1) < \frac{|\overline{U^1}|(\tau - \varepsilon)|V_1|}{|\overline{U^1}||V_1|} = \tau - \varepsilon$$

which is a contradiction of (ε, δ)-uniformity of (U, V_1) whenever $|\overline{U^1}| > \delta|U|$. Thus we have shown

Fact 4.1 $|U^1| \geq (1 - \delta)|U|$.

For $i = 2, \ldots, t$, let $U^i = \{y \in U^{i-1} : d_{V_i}(x) \geq (\tau - \varepsilon)|V_{i+1}|\}$. As above, we have

Fact 4.2 $|U^i| \geq (1 - \delta)|U^{i-1}|$ for $i = 2, \ldots, t$.

We now choose $x_1 \in U^t$ arbitrarily. (We note that that U^t has size some constant fraction of the size of U, and has at least r vertices by our initial assumption on M.)

We let $V_i^1 = N_{V_i}(x_1)$ and repeat the process with the V_i^1's and the same U. Let U_1^j be the successive subsets of U obtained for the sets V_i^1; choose $x_2 \in U_1^r$ different from x_1. We repeat this r times in all, finding $x_1 \ldots, x_r$, getting sets $V_i' = V_i^r$, where $V_i^r \subseteq \cdots \subseteq V_i^1 \subseteq V_i$ and $V_i^r = N_{V_i}(\{x_1, \ldots, x_r\})$. (Again, we can always find these r vertices by the initial assumption on M.) By our methods, we have $|V_i^{j+1}| \geq (\tau - \varepsilon)|V_i|$

for each j and hence $|V_i'| > (\tau - \varepsilon)^r |V_i|$. The sets $V_1', \ldots, V_t'$ are (ε', δ')-uniform with density at least τ' for

$$\begin{aligned}|V_i'| &> (\tau - \varepsilon)^r |V_i|,\\ \varepsilon' &= 2\varepsilon,\\ \delta' &= \frac{\delta}{(\tau - \varepsilon)^r},\\ \tau' &= \tau - \varepsilon.\end{aligned}$$

We only need to show that these new values satisfy the hypotheses of the lemma for $k = t$.

It is immediate that $\varepsilon' < \tau/2^t$, as

$$\varepsilon < \frac{\tau}{4^{t+1}} = \frac{\tau' + \varepsilon}{4^{t+1}}$$

hence $\varepsilon < \tau'/(4^{t+1} - 1)$ and we conclude

$$\varepsilon' = 2\varepsilon < 2 \cdot \frac{\tau'}{4^{t+1} - 1} < \frac{\tau'}{4^t}.$$

The second hypothesis is also straightforward:

$$\begin{aligned}\delta' = \frac{\delta}{(\tau - \varepsilon)^r} &< \frac{(\tau - \varepsilon)^r (\tau - 3\varepsilon)^r \cdots (\tau - (2^{t+1} - 1)\varepsilon)^r}{(\tau - \varepsilon)^r}\\ &= (\tau - 3\varepsilon)^r \cdots (\tau - (2^{t+1} - 1)\varepsilon)^r\\ &= (\tau' - \varepsilon')^r (\tau' - 3\varepsilon')^r \cdots (\tau' - (2^t - 1)\varepsilon')^r\end{aligned}$$

Thus we may choose

$$R(t + 1, r, \tau, \varepsilon, \delta) = \frac{1}{(\tau - \varepsilon)^r} R(t, r, \tau', \varepsilon', \delta')$$

and the lemma is true by induction. □

Proof of Theorem 4.22. Let $H = K_{t+1}(r)$. It remains to show that for every $\xi > 0$ there exists an $R(t, r, \xi)$ such that $\mathit{spex}(n, K_{t+1}(r)) < (1 - 1/t + \xi)n$.

We use Lemma 4.25. Given r, t, ξ, let τ, ε, and δ be arbitrary positive constants satisfying $\tau < \xi^2/3$, $\varepsilon < \tau/4^t$, and $\delta < (\tau - 2^t\varepsilon)^{tr}$. Let G be a graph on $n > R = R(t, r, \tau, \varepsilon, \delta)$ vertices not containing $K_{t+1}(r)$ as a subgraph. Set $m = \min\{\lceil 1/\tau \rceil, t\}$ and take a Szemerédi partition of G into ℓ parts, where $m < \ell < M(m, \varepsilon)$. Remove all edges with an end in the one set of smaller size (at most εn^2 edges), remove edges from within sets (at most n^2/k edges), from between pairs of sets that are not ε-uniform (at most εn^2 edges), and from between pairs of sets that have density less than τ (at most τn^2 edges). Thus we have removed at most $(2\varepsilon + \tau)n^2 \leq \xi^2 n^2/2$ edges. Call the resulting graph Γ.

Γ does not contain K_{t+1}, because if it did, then by Lemma 4.25 it and hence G would contain $K_{t+1}(\Gamma)$. By Wilf's theorem (Theorem 4.1) it follows that

$$\lambda_1(\Gamma) \leq (1 - 1/t)n.$$

Moreover, since we deleted at most $\xi^2 n^2/2$ edges, we conclude by Lemma 2.3, item (iii), that

$$\lambda_1(G) \leq \lambda_1(\Gamma) + \xi n \leq (1 - 1/t + \xi)n. \qquad \square$$

4.5 Stability of the Spectral Turán theorem

We now consider graphs that do not contain K_{t+1} as a subgraph and have spectral radius close to that of the extremal graph $T(n, t)$. We will prove the following result concerning the stability of the extremal graphs.

Theorem 4.8 (Spectral stability theorem) *For all $\varepsilon > 0$ and for $t = 2$ or 3, there exist constants $c_1 = c_1(t)$ and $c_2 = c_2(t)$, such that for all graphs G on n vertices not containing K_{t+1} as a subgraph, if G has spectral radius satisfying*

$$\lambda_1(G) \geq (1 - 1/t)n(1 - \varepsilon),$$

then: (i) removing at most $c_1\varepsilon n^2$ edges can make G t-partite; (ii) removing at most $c_2\varepsilon^{1/2}n^2$ edges can make G a subgraph of the Turán graph $T(n, t)$.

We remark that item (ii) follows from item (i) by a straighforward analysis of t-partite graphs (Proposition 4.30).

We will first present a proof of the case $t = 2$, as this proof is remarkably simple. We will then discuss a technique that could be applied to the general case. We apply this technique to prove the theorem for the case $t = 3$.

4.5.1 Triangle-free graphs

We prove the following theorem, representing the nontrivial part of Theorem 4.8 for $t = 2$.

Theorem 4.26 *For every $\varepsilon > 0$, if G is a triangle-free graph and $\lambda_1(G) \geq \frac{1}{2}n(1-\varepsilon)$, then G is at most εn^2 edges away from being bipartite.*

Proof: Let $\mathbf{x}$ be a nonnegative eigenvector for $\lambda_1(G)$ and assume that G is labelled so that vertex 1 has maximum weight, i.e., x_1 is maximum, and among the neighbors of 1, x_2 is maximum. We donte by d_i the degree of vertex i. From the eigenvalue equations at vertices 1 and 2, the following inequalities hold:

$$\lambda_1 x_1 = \sum_{i\sim 1} x_i \;\leq\; d_1 x_2 \;\leq\; d_1 x_1, \tag{4.7}$$

$$\lambda_1 x_2 = \sum_{i\sim 2} x_i \;\leq\; d_2 x_1. \tag{4.8}$$

Multiplying these two together and simplifying, we have:

$$\lambda_1 \leq \sqrt{d_1 d_2} \leq (d_1 + d_2)/2. \tag{4.9}$$

It follows from (4.9) that there are at most εn vertices not adjacent to either 1 or 2; call this set B. Removing all edges adjacent to a vertex in B, i.e., at most εn^2 edges, leaves a bipartite graph with bipartition given by 1 and 2. $\square$

4.5.2 General method

Our general method uses *lexicographical cliques.* Let $\mathbf{x}$ be an eigenvector for G and let $(v_1, \ldots, v_r)$ be a clique; the clique is *lexicographic* if: v_1 is a vertex with maximum weight given by $\mathbf{x}$ among vertices of G; v_i is a vertex of maximum weight among common neighbors of $v_1, \ldots, v_{i-1}$, for $i = 2, \ldots, r$; the clique is *lexicographically maximal* if there is no lexicographic clique on $r+1$ vertices containing $\{v_1, \ldots, v_r\}$, i.e., the vertices $v_1, \ldots, v_r$ have no common neighbor.

We make the following observation, which is a slight strengthening of our Spectral Turán theorem (Theorem 4.2).

Proposition 4.27 *Let G be a graph on n vertices not containing K_{t+1} as a subgraph. Let $\mathbf{x}$ be a nonnegative eigenvector for $\lambda_1(G)$, and let $\{v_1, \ldots, v_r\}$ be a lexicographically maximal clique. Then $\lambda_1(G) \leq \lambda_1(T(n,r))$.*

Proof: We mimic the proof of Theorem 4.2. Let V_i be the set of all vertices adjacent to $v_1, \ldots, v_{i-1}, v_{i+1}, \ldots, v_t$, for $i = 1, \ldots, t$. For $i = 1, \ldots, r-1$, let U_i be the set of vertices not adjacent to v_i, and not adjacent to at least one of $v_{i+1}, \ldots, v_r$. We then symmetrize all vertices in U_i to v_i to create an r-partite graph G_0. We claim that this does not decrease the quadratic form at $\mathbf{x}$. As in Section 4.3, we write $\mathbf{x}^t A \mathbf{x} = \sum_v x_v w(v)$, where $w(v) = \sum_{i \sim v} x_i$. For $v \in V_i \cup U_i$ we have

$$w_G(v) \leq w_G(i) \leq w_{G_0}(i),$$

the second inequality follows from the fact that $N_G(i) \subseteq N_{G_0}(i)$, the first follows because $\{1, \ldots, i\}$ is as a lexicographic clique. Thus

$$\lambda_1(G) \leq \lambda_1(G_0) \leq \lambda_1(T(n,r)). \qquad \square$$

It follows from this proposition that if $\lambda_1(G) > (1 - 1/t)n(1 - \varepsilon)$ and $\varepsilon < 1/t^2$, then any lexicographically maximal clique has size at least t.

Let $\{v_1, \ldots, v_t\}$ be a lexicographically maximal clique. Let V_i be the set of all vertices adjacent to $v_1, \ldots, v_{i-1}, v_{i+1}, \ldots, v_t$, for $i = 1, \ldots, t$. The sets V_i induce a

t-partite graph G_0. Call the set of remaining vertices B. Removing all edges with an end in B leaves a t-partite graph. Our general idea is to show that B can never be too large, given that λ_1 is large. This holds for $t = 2$, as we showed above. For $t = 3$, we show that it also holds, but does not seem to follow easily as it did for $t = 2$.

For a lexicographically maximal clique $\{v_1, \ldots, v_t\}$, and all $1 \leq r \leq t$, we examine the eigenvalue equations at the first r vertices:

$$\lambda_1(x_1 + \cdots + x_r) = \sum_{i \sim 1} x_i + \cdots + \sum_{i \sim r} x_i.$$

The following lemma will help in working with the equation above.

Lemma 4.28 *Let $x_1 \geq \cdots \geq x_n \geq 0$, and assume λ is a number satisfying*

$$\lambda(a_1 + \cdots + a_n) \leq a_1 x_1 + \cdots + a_n x_n.$$

It then follows that

$$\lambda \leq \max\left\{a_1, \frac{a_1 + a_2}{2}, \ldots, \frac{a_1 + \cdots + a_n}{n}\right\}.$$

Proof: The proof uses a technique called *Abel rearrangement.* For convenience, define $x_{n+1} = 0$. Setting $M = \max\{a_1, (a_1+a_2)/2, \ldots, (a_1+\cdots+a_n)/n\}$, we have $a_1+\cdots+a_k \leq k \cdot M$ for all k. The conclusion follows immediately from rewriting the sum:

$$\begin{aligned}
\lambda(a_1 + \cdots + a_n) &\leq a_1 x_1 + \cdots + a_n x_n \\
&= \sum_{i=1}^{n} (a_1 + \cdots + a_i)(x_i - x_{i+1}) \\
&\leq \sum_{i=1}^{n} iM(x_i - x_{i+1}) \\
&= M(x_1 + \cdots + x_n)
\end{aligned}$$

□

4.5.3 t-partite graphs

We mentioned above that the second claim of Theorem 4.8 follows from the first with an analysis of t-partite graphs. We first show that if a t-partite graph has one of its color classes too large, then the spectral radius is small.

Lemma 4.29 *Let G be a complete t-partite graph on n vertices, and assume that one color class has size $n_1 = (1/t + \delta)n$, for some $\delta > 0$. Then*

$$\lambda_1(G) \leq (1 - 1/t)n(1 - \delta^2/t).$$

Proof: It follows from the arguments in the proof of Lemma 4.19 in Section 4.3 that for n_1 fixed in a complete t-partite graph, the spectral radius is maximum for all other color classes having equal size. We may assume all $t-1$ other classes have size $n_2 = \cdots = n_t = (1/t - \delta/(t-1))n$ and get equal weight. Thus the spectral radius is bounded above by the largest eigenvalue of the 2×2 matrix

$$\begin{pmatrix} 0 & (t-1)(1/t - \delta/(t-1))n \\ (1/t + \delta)n & (t-2)(1/t - \delta/(t-1))n \end{pmatrix}.$$

Let $f(\lambda)$ be the characteristic polynomial of this matrix. This is a quadratic with one positve root. The proposition is then proved by showing that the positive root is to the left of $(1-1/t)n(1-1/t)\delta^2$, i.e., that $f((1-1/t)n(1-1/t)\delta^2) > 0$. We have:

$$f((1-1/t)n(1-\delta^2/t)) = \frac{\delta^2 n^2}{t^4}\Big(t^4 - t^3 + t^2 - 3t^3\delta + 2t^2\delta + t^2\delta^2 + \delta^2\Big),$$

which is greater than 0 for all $t \geq 1$ and $0 < \delta < 1$, as required. □

We may now use this to show that in Theorem 4.8 that (ii) implies (i).

Proposition 4.30 *Let G be a graph on n vertices not containing K_{t+1} as a subgraph satisfying $\lambda_1(G) > (1-1/t)n(1-\varepsilon)$. Let $\mathbf{x}$ be a nonnegative eigenvector for $\lambda_1(G)$ and let $\{v_1, \ldots v_t\}$ be a lexicographically maximal clique. Assume that there are at most δn vertices not adjacent to $t-1$ vertices of the lexicographically maximal clique. Then removing at most $(\delta + t^{3/2}\varepsilon^{1/2})n$ vertices, i.e., at most $(\delta + t^{3/2}\varepsilon^{1/2})n^2$ edges, G can be made a subgraph of Turán's graph $T(n,t)$.*

Proof: Let B be the set of at most δn vertices not adjacent to $t-1$ vertices of the clicue $\{v_1, \ldots, v_t\}$. Let G_0 be the t-partite graph obtained from G by symmetrizing with respect to $\{1, \ldots, t\}$ in the same way as in the proof of Proposition 4.27, in this case only changing the adjacencies of vertices in B. We have

$$\lambda_1(G_0) \geq \lambda_1(G) \geq (1 - 1/t)n(1 - \varepsilon).$$

Proposition 4.30 then shows that no color class in G_0 can be larger than $(1/t + \sqrt{t\varepsilon})n$. Thus removing at most $\sqrt{t\varepsilon}n$ vertices from each color class of G_0, and the vertices B, we transform G into a subgraph of Turán's graph. □

4.5.4 Graphs not containing K_4

Here we prove the following theorem:

Theorem 4.31 *For every $\varepsilon > 0$ there is a c such that every G on n vertices not containing K_4 as a subgraph and satisfying*

$$\lambda_1(G) \geq \frac{2}{3}n(1 - \varepsilon) \tag{4.10}$$

is at most $c\varepsilon n^2$ edges away from a t-partite graph.

Proof: We will actually show that the t-partite graph given by a lexicographically maximal clique (the vertices of this are all vertices of G adjacent to $t-1$ vertices of the clique) contains at least $n(1 - c\varepsilon)$ vertices, proving the theorem.

We prove the theorem for $c = 20$. For convenience, let $\delta = 20\varepsilon$.

The proof is by contradiction. Let G have vertex set $\{1, \ldots, n\}$ and assume it is labeled so that $(1, 2, 3)$ is a lexicographically maximal clique with respect to a nonnegative eigenvector $\mathbf{x}$. (If there is no lexicographically-maximal 3-clique, then by Proposition 4.27, we would already have a contradiction.)

We assume that our stronger claim is false, i.e., the set B of vertices adjacent to at most one vertex among $1, 2, 3$ has more than δn vertices. We will derive a series of conditions on G, eventially arriving at the contradiction $\lambda_1(G) < (1 - 1/3)n(1 - \varepsilon)$.

For $i = 1, 2, 3$, let B_i be the set of vertices adjacent to i only among $\{1, 2, 3\}$; let B_0 be the set adjacent to none of $\{1, 2, 3\}$; then $B = B_0 \dot\cup B_1 \dot\cup B_2 \dot\cup B_3$. Let $b_i = |B_i|$, and $b = |B| = b_0 + b_1 + b_2 + b_3$. Notice that $b = n - (d_{12} + d_{13} + d_{23})$, where d_{ij} denotes the number of common neighbors of vertices i and j. We have:

$$\lambda_1 x_1 \leq d_{12}x_3 + (d_1 - d_{12})x_2 = d_{12}x_3 + (d_{13} + b_1)x_2 \tag{4.11}$$

$$\lambda_1 x_2 \leq d_{12}x_3 + (d_2 - d_{12})x_1 = d_{12}x_3 + (d_{23} + b_2)x_1 \tag{4.12}$$

$$\lambda_1 x_3 \leq d_{13}x_2 + (d_3 - d_{13})x_1 = d_{12}x_3 + (d_{23} + b_3)x_1 \tag{4.13}$$

Proposition 4.32 *If $b \geq \delta n$, then*

$$d_1 + d_2 + d_3 \leq 2n - \frac{\delta}{2}n = 2n\left(1 - \frac{\delta}{4}\right).$$

Proof:

$$n - d_{ij} \leq (n - d_i) + (n - d_j) \Longrightarrow d_{ij} \geq d_i + d_j - n.$$

$$d_{12} + d_{13} + d_{23} \geq 2(d_1 + d_2 + d_3) - 3n.$$

$$\delta n \leq b = n - (d_{12} + d_{13} + d_{23}) \leq 4n - 2(d_1 + d_2 + d_3)$$

And hence

$$d_1 + d_2 + d_3 \leq 2n - \frac{\delta}{2}n = 2n\left(1 - \frac{\delta}{4}\right).$$ □

Condition 4.1 $d_1 + d_2 + d_3 < 2n(1 - \delta/4)$.

Proof: By the previous proposition, if this were not true, then $b < \delta n$, and removing all edges with an endpoint in B, i.e., at most δn^2, results in a 3-colorable graph determined by $\{1, 2, 3\}$. □

The following two conditions follow from (4.7) and (4.7).

Condition 4.2 $d_1 > (2n/3)(1 - \varepsilon)$.

Condition 4.3 $d_1 + d_2 > (4n/3)(1 - \varepsilon)$.

Considering only vertices 1 and 2, we have

$$n - d_{12} \leq 2n - (d_1 + d_2) < 2n - \frac{4n}{3}(1-\varepsilon) = \frac{2n}{3}(1+2\varepsilon).$$

The second inequality follows by Condition 4.3.

We will write down the first three eigenvalue equations together as:

$$\lambda_1(x_1 + x_2 + x_3) = \sum_{i\sim 1} x_i + \sum_{i\sim 2} x_i + \sum_{i\sim 3} x_i \leq a_1x_1 + a_2x_2 + a_3x_3,$$

where we bound each summand by the best x_i possible, $i = 1, 2, 3$, and a_i is the number of summands that get this bound. Notice that no x_i cannot appear in all three summations, as this would imply a K_4. We have:

$$\begin{aligned} a_1 &\leq 2(n - d_1) - (b_2 + b_3) \\ a_1 + a_2 &\leq 2(n - d_{12}) - b \\ a_1 + a_2 + a_3 &= d_1 + d_2 + d_3 \end{aligned}$$

It follow immediately from Lemma 4.28 that

Proposition 4.33 *For* λ_1*, we have*

$$\lambda_1 \leq \max\left\{a_1, \frac{a_1 + a_2}{2}, \frac{a_1 + a_2 + a_3}{3}\right\} \tag{4.14}$$

We will now examine all three of the terms individually. We would like to show that each is too small, i.e., implying that $\lambda_1 < (2/3)n(1-\varepsilon)$.

For the third term of (4.14), we have:

$$\frac{a_1 + a_2 + a_3}{3} = \frac{d_1 + d_2 + d_3}{3} \leq \frac{2n}{3}\left(1 - \frac{\delta}{4}\right) < \frac{2n}{3}(1-\varepsilon),$$

for all $\delta \geq 4\varepsilon$.

Using Condition 4.3, we see that

$$\begin{aligned} a_1 + a_2 &\leq 2(n - d_{12}) - b \leq \frac{4n}{3}(1+2\varepsilon)\delta n \\ \frac{a_1 + a_2}{2} &\leq \frac{2n}{3} - \left(\delta - \frac{8\varepsilon}{3}\right)n < \frac{2n}{3}(1-\varepsilon), \end{aligned}$$

for all $\delta \geq 10\varepsilon/3$.

In light of Proposition 4.33, we see that a_1 must be larger than $(2/3)n(1-\varepsilon)$. Thus we may assume:

Condition 4.4 $d_1 < \dfrac{2n}{3}(1+\varepsilon)$.

Proof: If not, we would have:

$$a_1 \leq 2(n-d_1) \leq 2\frac{n}{3}(1-2\varepsilon).$$ □

Condition 4.5 $b_2 + b_3 < \dfrac{7}{3}\varepsilon n$.

Proof: If not, we would have:

$$\begin{aligned} a_1 &\leq 2(n-d_1) - (b_2+b_3) \\ &< 2\Big(n - \frac{2n}{3}(1-\varepsilon)\Big) - \frac{7}{3}\varepsilon n \\ &= \frac{2n}{3} - \varepsilon n \end{aligned}$$ □

From these conditions, others follow:

Condition 4.6 $x_2 > x_1(1-2\varepsilon)$.

Proof: If $x_2 \leq x_1(1-2\varepsilon)$ then

$$\lambda_1 x_1 \leq d_1 x_2 \leq d_1(1-2\varepsilon)x_1$$

and hence

$$\begin{aligned} \lambda_1 &\leq d_1(1-2\varepsilon) \\ &< \frac{2n}{3}(1+\varepsilon)(1-2\varepsilon) \\ &< \frac{2n}{3}(1-\varepsilon), \end{aligned}$$

using Condition 4.4. □

Now comes the complicated part. It follows from $(4.11, 4.12, 4.13)$, that

$$\lambda_1 x_1^2 \leq d_{12}x_1x_3 + (d_1 - d_{12})x_1x_2 = d_{12}x_1x_3 + (b_1 + d_{13})$$
$$\lambda_1 x_2^2 \leq d_{12}x_2x_3 + (d_2 - d_{12})x_1x_2 = d_{12}x_2x_3 + (b_2 + d_{23})$$
$$\lambda_1 x_2x_3 \leq d_{13}x_2^2 + (d_3 - d_{13})x_1x_2 = d_{13}x_2^2 + (b_3 + d_{23})$$

Adding these three together, we have

$$\begin{aligned}
\lambda_1\Big(x_1^2 + &\frac{x_2^2 + x_2x_3}{2}\Big) \leq \\
&\leq x_1x_2\Big(b_1 + \frac{b_1+b_2}{2} + d_{13} + d_{23}\Big) + d_{12}x_1x_3 + \frac{1}{2}d_{12}x_2x_3 + \frac{1}{2}d_{13}x_2^2 \\
&= x_1x_2\Big(n - d_{12} - \frac{b_2+b_3}{2}\Big) + d_{12}x_1x_3 + \frac{1}{2}d_{12}x_2x_3 + \frac{1}{2}d_{13}x_2^2 \\
&= x_1x_2\Big(n - \frac{b_2+b_3}{2}\Big) - d_{12}x_1(x_2 - x_3) \\
&\qquad + \frac{1}{2}(d_{12} + d_{13})x_2^2 - \frac{1}{2}d_{12}x_2(x_2 - x_3) \\
&\leq x_1x_2\Big(n - \frac{B}{2}\Big) - d_{12}(x_2 - x_3)\Big(x_1 + \frac{x_2}{2}\Big)
\end{aligned}$$

and hence

$$\begin{aligned}
\lambda_1\Big(x_1^2 + x_2^2 - &\frac{1}{2}x_2(x_2 - x_3)\Big) \leq \\
&\leq x_1x_2\Big(n - \frac{b_2+b_3}{2}\Big) - \frac{b_1}{2}x_2^2 + \frac{d_1}{2}x_2^2 - (x_2 - x_3)d_{12}\Big(x_1 + \frac{x_2}{2}\Big)
\end{aligned}$$

Rearranging a little, we have

$$\begin{aligned}
\lambda_1(x_1^2 + x_2^2) &\leq x_1x_2\Big(n + \frac{d_1}{2}\frac{x_2}{x_1} - \frac{b_1}{2}\frac{x_2}{x_1} - \frac{b_2+b_3}{2}\Big) - \\
&\qquad - (x_2 - x_3)d_{12}(x_1 + x_2/2) + \lambda_1 x_2(x_2 - x_3)/2 \\
&\leq x_1x_2(n + \frac{d_1}{2} - (1 - 2\varepsilon)\frac{B}{2}\Big) - (x_2 - x_3)\Big(d_{12}\frac{3x_2}{2} - \frac{\lambda_1}{2}x_2\Big) \\
&= x_1x_2(n + \frac{d_1}{2} - (1 - 2\varepsilon)\frac{B}{2}\Big) - \frac{x_2 - x_3}{2} \cdot x_2(3d_{12} - \lambda_1)
\end{aligned}$$

Let $S = \frac{x_2 - x_3}{2} \cdot x_2(3d_{12} - \lambda_1)$, i.e., the last summand in the equation above. We may now make a very strong assumption on d_{12}.

Condition 4.7 $d_{12} < \frac{2}{9}n$.

Proof: Otherwise we would have $3d_{12} \geq 2n/3$, from which it follows that $S \geq 0$ and hence:

$$\lambda_1(x_1^2 + x_2^2) \leq x_1 x_2 \Big(n + \frac{d_1}{2} - (1 - 2\varepsilon)\frac{b}{2} \Big),$$

which implies

$$\lambda_1 \leq \frac{1}{2}\Big(n + \frac{d_1}{2} - (1 - 2\varepsilon)\frac{b}{2} \Big).$$

By Condition 4.4 we have

$$\begin{aligned} \lambda_1 &\leq \frac{1}{2}\Big(n + \frac{(2n/3)(1+\varepsilon)}{2} - (1 - 2\varepsilon)\frac{\delta n}{2} \Big) \\ &= \frac{2n}{3}\Big(1 - \frac{1}{8}(3\delta - 2\varepsilon + \delta\varepsilon/2) \Big) \\ &< \frac{2n}{3}(1 - \varepsilon). \end{aligned}$$

□

We now have

$$d_2 = d_{12} + (d_{23} + b_2) < \frac{5n}{9} + \frac{2\varepsilon}{3} \cdot n$$

and using Condition 4.6:

$$\lambda_1 x_2 \leq d_2 x_1 \leq d_2 x_2 (1 + 3\varepsilon)$$

and

$$\lambda_1 \leq d_2(a + 3\varepsilon) < \frac{5n}{9}(1 + c\varepsilon)(1 + 3\varepsilon) < \frac{2}{3}n(1 - \varepsilon)$$

This last inequality holds for $\varepsilon < 0.025$. If $\varepsilon \geq 0.025$, then G itself cannot have more that $\delta \cdot n^2 \geq n^2/2$ edges (we took $\delta = 20$), hence the result trivially follows.

Thus we have completed the proof of Theorem 4.31. □

4.6 Graphs with hereditarily bounded average degree

In this section we consider graphs with the *Hereditarily Bounded Property* $P_{t,r}$. A graph is said to have the *Hereditarily Bounded Property* $P_{t,r}$ if

$$|E(H)| \leq t \cdot |V(H)| + r, \qquad \forall H \leq G,\ |V(H)| \geq t. \tag{$P_{t,r}$}$$

For $r \geq 0$, we may safely omit the requirement that $|V(H)| \geq t+k$, as all graphs on fewer vertices trivially satisfy the condition. For negative r, the requirement on the size of $V(H)$ is important, as the inequality fails for subgraphs on few vertices; the term $t|E(H)| + r$ is negative. By defining k in the way we did, and having the requirement that $|V(H)| \geq t + k$ in the condition, we are considering all subgraphs for which the inequality makes sense.

The set of graphs satisfying Property $P_{t,r}$ can be easily interpreted in our language of forbidden subgraphs. Let $\mathcal{H}_{t,r}$ be the set of all graphs K on at least t vertices having more than $t \cdot |V(K)| + r$ edges, i.e., those with large average degree. Then graphs satisfying $P_{t,r}$ are exactly those which do not contain any graph in $\mathcal{H}$ as a subgraph.

We now restate our result:

Theorem 4.9 *Let $t \in \mathbb{N}$ and $r \geq -\binom{t+1}{2}$. If G is a graph on n vertices with property $P_{t,r}$, then*

$$\lambda_1(G) \leq (t-1)/2 + \sqrt{(t+1)t + 2r} + \sqrt{tn},$$

and asymptotically,

$$\lambda_1(G) \leq (t-1)/2 + \sqrt{tn} + o(1).$$

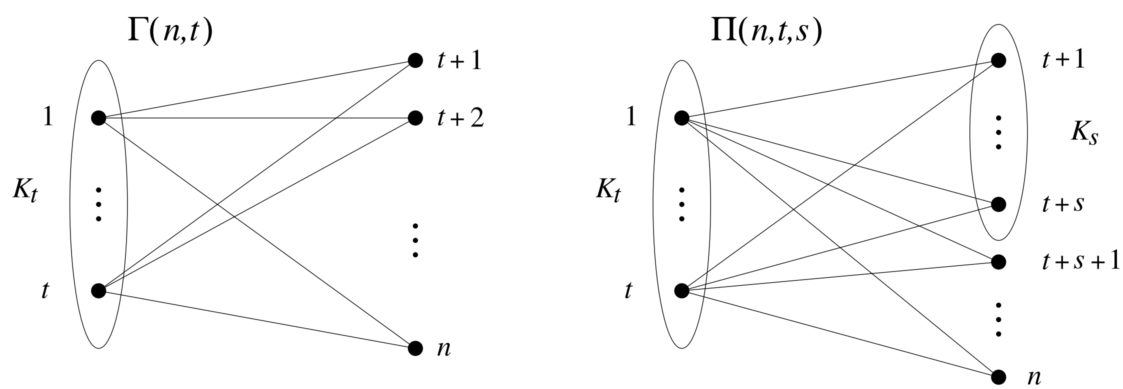
Furthermore, the asymptotic bound is tight.

Notice that if G_0 is a subgraph of G for which the edge bound is tight, then any other vertex of G can be adjacent to at most t vertices from G_0. The intuition is that if n is large, and G is a graph satisfying this property with maximum spectral radius, then most of the vertices are only adjacent to the t vertices that have maximum weight (given by an eigenvector). We will show that this intuition is correct.

4.6.1 Proof of the result

When discussing Property $P_{t,r}$, it will be convenient to set $s = \binom{t+1}{2} + r$, as the condition $r \geq -\binom{t+1}{2}$ can then be rephrased as $s \geq 0$, and as we will show, the extremal graphs will have the graph $\Gamma(n,t)$ defined in the next paragraph as a subgraph, with the addition of s edges.

Let $\Gamma(n,t)$ be the graph on vertex set $\{1, \ldots, n\}$, vertices $1, \ldots, t$ inducing a complete graph, and all other vertices adjacent to $\{1, \ldots, t\}$. If $n \leq t+1$, then $\Gamma(n,t)$ is just K_n. Notice that $\Gamma(n,t)$ has the property $P_{t,r}$ for all s. For $s = 0$, we will show that $\Gamma(n,t)$ is the unique extremal graph. For larger values of s, the extremal graphs will have $\Gamma(n,t)$ as a subgraph and have s additional edges.



Define $\Pi(n,t,s)$ to be the graph on vertex set $\{1, \ldots, n\}$, with $\Gamma(n,t)$ as a subgraph, and adding all edges between pairs of vertices in $\{t+1, \ldots, t+s\}$. If $n \leq t+s$, then $\Pi(n,t,s)$ is just K_n.

Let $\mathcal{S}(n,t,s)$ be the set of all graphs on n vertices having the property $P_{t,r}$, and let $\mathcal{S}_m(n,t,s)$ be its subset containing only those graphs with m edges. Define $\mathcal{Q}(n,t,s)$ to be the set of subgraphs H of $\Pi(n,t,s+1)$ with the property $P_{t,r}$, and having at most s edges among the vertices $\{t+1, \ldots, t+s+1\}$. Let $\mathcal{Q}_m(n,t,s)$ be its subset containing only those graphs with m edges.

The following theorem is a strengthening of Theorem 4.9 above. The strengthening is in the sense that we give a strong characterization of extremal graphs.

Theorem 4.34 *For all $G \in \mathcal{S}(n,t,s)$, there exists a graph $\Gamma \in \mathcal{Q}(n,t,s)$ for which*

$$\lambda_1(G) \leq \lambda_1(\Gamma).$$

The bounds given in Theorem 4.9 then follow immediately from estimates for $\lambda_1(\Pi(n,t,s+1))$. The fact that the bound given is asymptotically tight (within $o(1)$) follows from the value of $\lambda_1(\Gamma(n,t))$. We will calculate these below.

We remark that Brualdi and Solheid [18] proved this theorem for $t = 1$, and that Cvetković and Rowlinson [31] determined the extremal graphs for all s, and n large enough, confirming a conjecture of Brualdi and Solheid. The extremal graphs all have $\Gamma(n,1)$, the star, as a subgraph; for $s = 3$, the additional edges form a triangle, and for $s > 3$ (and n large enough), they form a star with center at $t+1$.

As in the proof of Theorem 4.2, we will show that for any vector $\mathbf{x}$, there is a graph in $\mathcal{Q}(n,t,s)$ whose quadtratic form at $\mathbf{x}$ is at least that of G's. The theorem above then follows by letting $\mathbf{x}$ be an eigenvector for $\lambda_1(G)$.

Theorem 4.35 *For every $\mathbf{x} \in \mathbb{R}^n$, $x_1 \geq \cdots \geq x_n \geq 0$, and for all $G \in \mathcal{S}_m(n,t,s)$, there is a graph $\Gamma \in \mathcal{Q}_m(n,t,s)$ for which*

$$\mathbf{x}^t A_G \mathbf{x} \leq \mathbf{x}^t A_\Gamma \mathbf{x}.$$

Proof: The proof is by induction on n. The theorem is clearly true for $n \leq t$. Assume $n > t$ and let G_0 be the graph obtained from G by deleting all d_n edges on vertex n and set $\mathbf{x}_0 = (x_1, \ldots, x_{n-1})^t$. Then by induction, there is a graph $\Gamma_0 \in \mathcal{Q}_{m-d_n}(n-1,t,s)$ for which

$$\mathbf{x}_0^t A_{G_0} \mathbf{x}_0 \leq \mathbf{x}_0^t A_{\Gamma_0} \mathbf{x}_0.$$

The contribution to the quadratic form of G of the d_n edges adjacent to n is bounded above by the contribution of edges from n to the first d_n vertices, i.e.,

$$\sum_{i \sim n} x_i x_n \leq (x_1 + \cdots + x_{d_n}) x_n.$$

Let Γ_1 be the graph Γ_0 with the addition of vertex n and the edges from n to the first d_n vertices. We have

$$\mathbf{x}^t A_G \mathbf{x} \leq \mathbf{x}^t A_{\Gamma_1} \mathbf{x}.$$

It is possible that Γ_1 does not have property $P_{t,r}$, but if it does, i.e., if $d_n \leq t$, then $\Gamma_1 \in \mathcal{Q}_m(n,t,s)$ and we are done. So we may assume that $d_n > t$.

Let F_1 be the set of edges from n to vertices $\{t+1, \ldots, d_n\}$. We will create the desired graph $\Gamma \in \mathcal{Q}_m(n,t,s)$ from Γ_1 by moving the edges in F_1. We do this in such a way that $\Gamma \in \mathcal{Q}_m(n,t,s)$, and so that

$$\mathbf{x}^t A_{\Gamma_1} \mathbf{x} \leq \mathbf{x}^t A_{\Gamma} \mathbf{x} \tag{4.15}$$

holds, thus proving the theorem. We will verify (4.15) edgewise, i.e., for each edge $\{i,n\}$ which we move to $\{j,k\}$, we do so in such a way that $j \leq i$ and $j < n$, so that $x_i x_n \leq x_j x_k$. We first replace any edge in F_1 by any edge missing in $\Gamma(n,t)$ missing from Γ_1. If we can replace all edges from F_1 in this way, we are done. Othwerwise, call the resulting graph Γ_2 and the set of remaining edges F_2.

The graph Γ_2 has $\Gamma(n,t)$ as a subgraph, so there are are at most s edges among the vertices $\{t+1, \ldots, n\}$, and these can all be moved to within the first $s+1$ of these vertices, in particular, all edges from F_2 can be replaced by edges $\{t+1, i\}$, where $i \leq t+s+1$. This new graph is Γ, for which the theorem holds.

All that remains is to check the bounds. We do this in the form of two lemmas.

Lemma 4.36 *The spectral radius of* $\Gamma(n,t)$ *is:*

$$\lambda_1(\Gamma(n,t)) = \frac{t - 1 + \sqrt{4tn - 3t^2 - 2t + 1}}{2} = \frac{t-1}{2} + \sqrt{tn} + o(1).$$

Proof: The value of $\lambda_1(\Gamma(n,t))$ is easily computed as there are only two vertex orbits under automorphisms and hence $\lambda_1(\Gamma(n,t))$ is the largest eigenvalue of

$$\begin{pmatrix} t-1 & n-t \\ t & 0 \end{pmatrix}.$$

□

Any graph $G \in \mathcal{Q}(n,t,s)$ having maximal $\lambda_1(G)$ we may bound above by writing it as the edge disjoint union of a graph with s edges (among the set S) and $\Gamma(n,t)$. Thus by Property 2.3 (iii), it follows that

$$\lambda_1(\Gamma) < (t-1)/2 + \sqrt{2s} + \sqrt{tn}. \tag{4.16}$$

To improve the error term, we consider the graph $\Pi(n, t, s+1)$. Γ is a subgraph of this, so its spectral radius is bounded above by the spectral radius of $\Pi(n, t, s+1)$. We compute the value of $\lambda_1(\Pi(n, t, s+1))$ in the following lemma:

Lemma 4.37 *The spectral radius of* $\Pi(n, t, s)$ *is:*

$$\lambda_1(\Pi(n, t, s+1)) = (t-1)/2 + \sqrt{tn} + o(1).$$

Proof: There are three vertex orbits under the automorphism group, hence three wieghts for the eigenvector, and $\lambda_1(\Pi(n, t, s+1))$ is the largest eigenvalue of

$$\begin{pmatrix} t-1 & s+1 & n-t-s-1 \\ t & s & 0 \\ t & 0 & 0 \end{pmatrix}$$

and hence the largest root of

$$F(\lambda) = \lambda^3 - (s+t-1)\lambda^2 - (tn - t^2 - st + s)\lambda + st(n-t-s-1).$$

To see that the largest root is not more than $\lambda_1(\Gamma(n, t)) + o(1)$, we may substitute $(t-1)/2 + \sqrt{tn}$ in for λ above. We have

$$F((t-1)/2+\sqrt{tn}) = \frac{1}{4}\left(3t^{5/2}+2t^{3/2}-t^{1/2}\right)n^{1/2}+\frac{1}{8}\left(3t^3-6st^2-t^2-12st-3t+2s+1\right).$$

This is bigger than zero for n large enough (s and t are fixed), which implies that $\lambda_1(\Pi(n, t, s+1)) < (t-1)/2 + \sqrt{tn}$, proving the claim. □

The proof of Theorem 4.9 is then complete by (4.16) and Lemma 4.37. □

4.6.2 Consequences and applications to graphs embeddable on surfaces

Corollary 4.38 *The graph $\Gamma(n,t)$ is the unique extremal graph for $s = 0$.*

Proof: Notice that for $s = 0$, there is a unique graph $\Gamma \in \mathcal{Q}(n,t,0)$. If $G \in \mathcal{S}(n,t,0)$ is any graph with extremal spectral radius λ_1, then for the eigenvector $\mathbf{x}$ of $\lambda_1(G)$, we have $\lambda_1(G) \leq \mathbf{x}^t A_{\Gamma(n,t)}\mathbf{x}$. The maximality of $\lambda_1(G)$ implies equality and hence that $\mathbf{x}$ is an eigenvector for $\Gamma(n,t)$. The eigenvector equation for $\Gamma(n,t)$ shows that the first t vertices must be adjacent to every other vertex, and hence that $G = \Gamma(n,t)$. □

We have some immediate corollaries. The first is due to Collatz and Sinogowitz [26] and to Lovász and Pelikán [68].

Corollary 4.39 *Let T be a tree, then $\lambda_1 \leq \sqrt{n-1}$, with equality if and only if T is the star.*

Proof: This follows from Corollary 4.38 and Lemma 4.36. □

By Euler's formula for graphs embeddable on surfaces (compact 2-dimensional manifolds), we have $|E(G)| \leq 3|V(G)| - 3\chi$, where χ is the Euler characteristic of the surface. This gives us

Corollary 4.10 *Let G be a graph embeddable on a surface of Euler characteristic χ. Then*

$$\lambda_1(G) < 1 + \sqrt{6(2-\chi)} + \sqrt{3n},$$

and asymptotically,

$$\lambda_1(G) < 1 + \sqrt{3n} + o(1),$$

where the $o(1)$ refers to $n \to \infty$ while χ is fixed.

For all surfaces other than the plane, our bound improves the coefficient of $\sqrt{n}$ in previous bounds given by Hong [60]. Hong showed the bound $c_1 + \sqrt{c_2 n}$, where $c_1 \geq 0$ and $c_2 \geq 3$ are constants depending only on χ, and for all surfaces other than the plane, $c_2 > 3$.

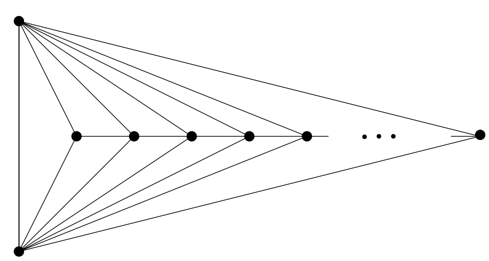
For planar graphs, we improve the best previous bound, but the improvement is negligible. Our result gives $1+\sqrt{3n}$, whereas previous bounds were $4+\sqrt{3n}$ given by Cao and Vince [21], improved to $2\sqrt{2}+\sqrt{3n}$ by Hong [60].

4.6.3 Addendum

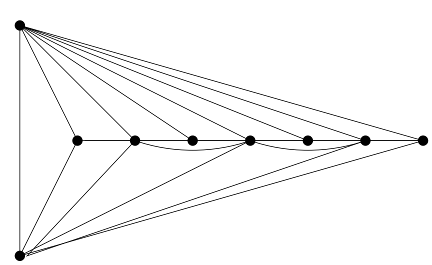
Since the writing of this chapter, Tom Hayes and I have improved upon Corollary 4.10, showing that if G is embeddable on a fixed surface Σ, then

$$\lambda_1(G) \leq \sqrt{2n} + c,$$

where c is a constant depending only upon the surface Σ. We have also shown that for n large enough, the extremal graphs have two vertices of degree $n-1$. This uniquely determines the extremal graph for the plane (for n large enough), confirming a conjecture of Cao and Vince [21] that the extremal graph is $P_2 \vee P_{n-2}$ pictured below.



Cao and Vince actually conjectured that the graph above has maximum spectral radius among all planar graphs on n vertices, for all n. We show that this is not true for small n, for example when $n = 8$, the graph below has larger spectral radius then Cao and Vince's graph.



CHAPTER 5

OPEN PROBLEMS

Here we list several open problems related to the work in this thesis.

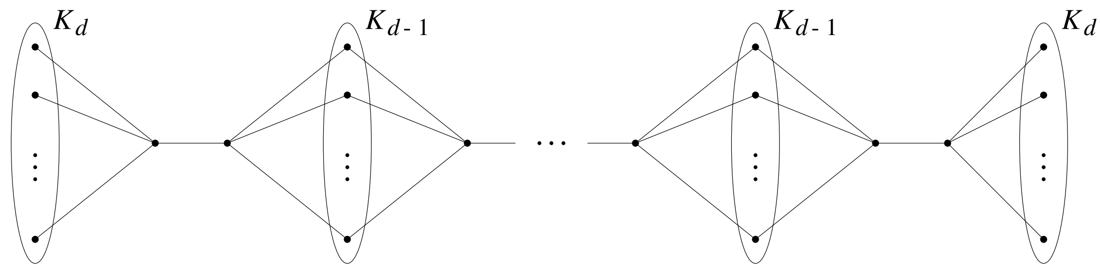
Connected graphs with minimum gap

Problem 5.1 If $n \equiv 0 \pmod 4$, then the trivalent graph with minimum gap has diameter $D = 3(n-4)/4$. There are $\lfloor (n-4)/8 \rfloor$ graphs with diameter D. Is it true that the graphs with maximal diameter have gap smaller than all others?

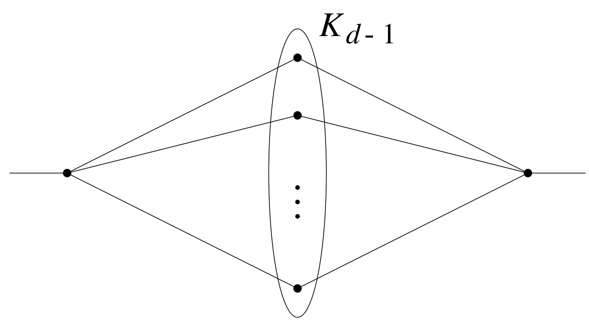
Problem 5.2 It seems quite natural to ask for a generalization of our result for connected d-regular graphs.

Bojan Mohar and I suggest another generalization for the problem: connected graphs of minimum degree d rather than d-regular graphs. We define ρ_1, the second smallest eigenvalue of the Laplacian matrix of G, to be the eigenvalue gap (ρ_1 is no longer equal to $\lambda_1 - \lambda_2$). ρ_1 increases with the addition of edges, and therefore one would expect most vertices to have degree d. (Unlike before, when the degree is odd, we may now consider any $n \in \mathbb{N}$, rather than just even n.) It is not immediately clear that an extremal graph will have cut edges, and indeed regular graphs of even degree cannot have cut edges.

Conjecture 5.1 *Assume $n \equiv 0 \pmod{d+1}$. Then the connected graph on n with minimum degree d having minimum eigenvalue gap ρ_1 is pictured below:*



Conjecture 5.2 *Let G be a connected graph on n vertices of minimum degree d having minimum eigenvalue gap $\rho_1(G)$ among all connected graphs on n vertices of minimum degree d. Then G is path-like, and except for some blocks near each end, all blocks occurring in the middle are of the form:*



Problems related to the Spectral Turán theorem

A generalization of Turán's theorem, conjectured by Erdős, and proved independently by Bollobás and Thomason [10] and Erdős and Sós [44] is given in the following theorem.

Theorem 5.3 (Bollobás, Thomason, Erdős, and Sós) *Let G be a graph on n vertices and assume that G has as many edges as the Turán graph $T(n,t)$. Then either $G \cong T(n,t)$, or there is a vertex v whose neighbors $N(v)$ induce a graph having more edges than $T(d_v, t-1)$.*

If G has more edges than the Turán graph, then Bondy [11] showed that the neighbors of any vertex v with maximum degree have more edges than the corresponding Turán graph $T(d_{\max}, t-1)$. His method uses a refinement of Zykov's proof. We conjecture that both of these results hold in the spectral case as well:

Conjecture 5.4 *Let G be a graph on n vertices and assume that $\lambda_1(G) \geq \lambda_1(T(n,t))$. Then either $G \cong T(n,t)$, or there is a vertex v whose neighbors $N(v)$ induce a graph G_0 satisfying $\lambda_1(G_0) \geq \lambda_1(T(|N(v)|, t-1))$. Furthermore, if $\lambda_1(G) > \lambda_1(T(n,t))$, then the conclusion holds for any vertex v having maximum weight given by a positive eigenvector for λ_1.*

In 1970, Nosal [76] showed that if a graph G does not contain a triangle, then $\lambda_1(G) \leq \sqrt{m}$. This implies our Spectral Turán Theorem for the case $t = 2$, by using Turán's theorem for the maximum number of edges. The theorem is stronger in the sense that for all triangle-free graphs it gives a bound on the spectral radius in terms of the number of edges.

Elphick [35] (see also [60]) proved the following result, where $\chi(G)$ is the chromatic number.

Theorem 5.5 *Let G be a graph with m edges and chromatic number $\chi(G)$. Then*

$$\lambda_1(G) \leq \sqrt{2m(1 - 1/\chi(G))}.$$

We conjecture that this bound holds with the clique number in place of the chromatic number:

Conjecture 5.6 *Let G be a graph having n vertices and m edges having clique number $\omega(G)$. Then*

$$\lambda_1(G) \leq \sqrt{2m(1 - 1/\omega(G))}.$$

We remark that for $\omega(G) = 2$ this is Nosal's theorem.

In fact, we make the following stronger conjecture, which, together with the theorem of Elphick, would imply the previous conjecture.

Conjecture 5.7 *Let G be a graph having n vertices and m edges not containing K_{t+1} as a subgraph, and let $\mathbf{x}$ be a positive vector. Then there is a t-partite graph H with n vertices and m edges, for which*

$$\mathbf{x}^t A_H \mathbf{x} \geq \mathbf{x}^t A_G \mathbf{x}.$$

Graphs with a prescribed number of edges

Far less work has been done on the minimum spectral radius under specified conditions, as compared to maximum spectral radius. Collatz and Sinogowitz [26] and Lovász and Pelikán [68] determined that among all trees on n vertices, the path is the unique graph with minimal spectral radius. We do not dare make a conjecture as to the exact graph for all m and n, yet we do make the following conjecture which would give quite a bit of structure to the extremal graphs.

Conjecture 5.8 *Let G be a graph on n vertices with m edges having minimum spectral radius. Let t be such that $|E(T(n,t-1)| < m \leq |E(T(n,t)|$. Then G is t-colorable.*

It is obvious that any regular graph with the required number of edges will have desired spectral radius, and that for $m = |E(T(n,t))|$, the "most regular" graph is the Turán graph, which is the unique t-colorable graph with n vertices and m edges.

Graphs with bounded average degree

We recall for $t \in \mathbb{N}$ and $r \geq -\frac{t+1}{2}$, that a graph G has the Hereditarily Bounded Property $P_{t,r}$ if $|E(H) \leq t \cdot |V(G)| + r$ for all subgraphs $H \leq G$ on at least t vertices (see Section 4.6). We remarked that Cvetković and Rowlinson [31] proved that for $t = 1$ and n sufficiently large, the extremal graph consists of a star and one vertex of degree $r + 2$. We conjecture that the structure of extremal graphs is similar, even for larger t:

Conjecture 5.9 *For all $t \in \mathbb{N}$ and $r \geq -\binom{t+1}{2}$, there is an N such that if G is a graph on $n > N$ vertices with the property $P_{t,r}$ and G has maximal spectral radius among all such graphs, then G is the unique graph having t vertices of degree $n-1$, and one vertex of degree $r + \binom{t+1}{2}$.*

We showed in Theorem 4.35 that G must have $\Gamma(n,t)$ as a subgraph (see page 81), and that it must have $r + \binom{t+1}{2}$ additional edges among the vertices $t+1, \ldots, t+s+1$. Our conjecture states that for n large enough, there is a unique extremal graph whose additional edges form a star.

Our next problem considers Property $P_{t,r}$, where t and r are not required to be integers. Our results show that:

$$\lambda_1(G) \leq c(s,t) + \sqrt{\lceil t \rceil n}\,.$$

Problem 5.3 Let $t, r \in \mathbb{R}$, $t > 0$ and $s \geq -\binom{\lfloor t+1 \rfloor}{2}$. Is it true that if G has Property $P_{t,r}$, then

$$\lambda_1(G) \leq c(s,t) + \sqrt{tn}\,?$$

Perhaps even this stronger statement may hold:

$$\lambda_1(G) \leq c(s,t) + \sqrt{\lfloor t \rfloor n}\,?$$

We may also ask for a generalization of this property, where the hereditary bound on the number of edges is not linear.

Problem 5.4 If for a graph G, $|E(H)| \leq c \cdot |V(H)|^2$ holds for all $H \leq G$, does it follow that $\lambda_1(G) \leq 2c \cdot |V(G)|$? What can be said if the exponent of 2 is replaced by some other constant less than 2?

We note that $\lambda_1(G) \leq \sqrt{2cn^2}$ is a trivial upper bound, and that $2c$ would be best possible, as seen by Wilf's theorem. If this question were true, then the Spectral Erdős-Stone-Simonovits theorem would follow from the Erdős-Stone-Simonovits theorem and Wilf's theorem would follow from Turán's theorem.

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