Beyond the classification theorem of Cameron, Goethals, Seidel, and Shult

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Abstract

In 1976, Cameron, Goethals, Seidel, and Shult classified all the graphs with smallest eigenvalue at least -2 by relating such graphs to root systems that occur in the classification of semisimple Lie algebras. In this paper, extending their beautiful theorem, we give a complete classification of all connected graphs with smallest eigenvalue in $(-\lambda^*, -2)$, where $\lambda^* = \rho^{1/2} + \rho^{-1/2} \approx 2.01980$, and ρ is the unique real root of $x^3 = x + 1$. Our result is the first classification of infinitely many connected graphs with their smallest eigenvalue in $(-\lambda, -2)$ for any constant $\lambda > 2$.

1 Introduction

A core problem in spectral graph theory is the characterization of graphs with limited eigenvalues. In this paper, by eigenvalues of a graph G, we specifically mean those associated with its adjacency matrix A_G. We focus on graphs with eigenvalues bounded from below, and we denote by $\mathcal{G}(\lambda)$ the family of graphs with smallest eigenvalue at least $-\lambda$. Since $\mathcal{G}(\lambda)$ is closed under disjoint union, it is enough to characterize the connected graphs in $\mathcal{G}(\lambda)$.

The well-known fact that all the line graphs have smallest eigenvalue at least -2 prompted a great deal of interest in the characterization of graphs in $\mathcal{G}(2)$. After Hoffman [7] constructed generalized line graphs, the interest deepened as it became apparent that generalized line graphs are not the only graphs in $\mathcal{G}(2)$. The ubiquitous Petersen graph, the Shrikhande graph, the Clebsch graphs, the Schläfli graph, and the three Chang graphs were among the first exceptional graphs to be identified. An important result in this direction is the complete enumeration of strongly regular graphs in $\mathcal{G}(2)$ by Seidel [15].

In 1976, the characterization of graphs in $\mathcal{G}(2)$ culminated in a beautiful theorem of Cameron, Goethals, Seidel, and Shult [3]. What is ingenious in their paper is the translation of the spectral

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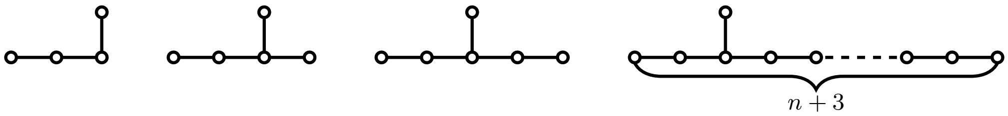

Figure 1: E_0, E_1, E_2 and E_n.

graph theoretic problem to one involving root systems, which have been used for the classification of semisimple Lie algebras. Cameron et al. proved that apart from the generalized line graphs, there are only finitely many other connected graphs in $\mathcal{G}(2)$, each of which is represented by a subset of the E_8 root system. We refer the reader to the monograph [6] for a comprehensive account of $\mathcal{G}(2)$.

Can we classify graphs with smallest eigenvalue beyond -2? In 1992, Bussemaker and Neumair [2, Theorem 2.5] determined the smallest $\lambda > 2$ such that $\mathcal{G}(\lambda) \setminus \mathcal{G}(2)$ consists of precisely one connected graph, which is E_6 defined in Figure 1. Recently, motivated by a discrete-geometric question on spherical two-distance sets in [11], Jiang and Polyanskii proved [10, Theorem 2.10] that the number of connected graphs in $\mathcal{G}(\lambda) \setminus \mathcal{G}(2)$ is finite for every $\lambda \in (2, \lambda^*)$. Here and throughout,

$$\lambda^* := \rho^{1/2} + \rho^{-1/2} \approx 2.0198008871,$$

where ρ is the unique real root of $x^3 = x + 1$. Despite its algebraic definition, the peculiar constant λ^* has a spectral graph theoretic interpretation.

Proposition 1 (Hoffman [8])**.** *For every $n \in \mathbb{N}$, define the graph E_n as in Figure 1. As $n \to \infty$, the largest eigenvalue of E_n increases to λ^*, or equivalently, the smallest eigenvalue of E_n decreases to $-\lambda^*$.* $\square$

The aforementioned finiteness result, together with Proposition 1, establishes λ^* as the smallest $\lambda > 2$ such that $\mathcal{G}(\lambda) \setminus \mathcal{G}(2)$ contains infinitely many connected graphs. Naturally, the authors of [10] raised the problem of finding all connected graphs in $\mathcal{G}(\lambda^*) \setminus \mathcal{G}(2)$.

We completely classify all connected graphs in $\mathcal{G}(\lambda^*) \setminus \mathcal{G}(2)$. We point out that the algebraic integer $-\lambda^*$ is not totally real, hence it cannot be a graph eigenvalue. As a result, $\mathcal{G}(\lambda^*) \setminus \mathcal{G}(2)$ consists precisely of graphs with smallest eigenvalue in the open interval $(-\lambda^*, -2)$.

In its weak form, our classification theorem says that every sufficiently large connected graph in $\mathcal{G}(\lambda^*) \setminus \mathcal{G}(2)$ looks more or less like the graph E_n for some sufficiently large $n \in \mathbb{N}$. To be more precise, we have the following characterization.

Definition 2 (Rooted graph and augmented path extension)**.** A *rooted graph* F_R is a graph F equipped with a nonempty subset R of vertices, which we refer to as *roots*, and are depicted by solid circles. Given a rooted graph F_R and $\ell \in \mathbb{N}$, the *augmented path extension* $(F_R, \ell,)$ of the rooted graph F_R is obtained from the disjoint union of F and the rooted graph by adding a path $v_0 \dots v_\ell$ of length ℓ, connecting v_0 to every vertex in R, and connecting v_ℓ to the two roots in . See Figure 2 for a schematic drawing.

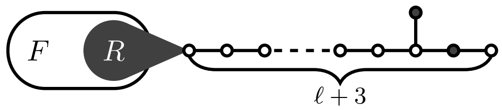

Figure 2: The augmented path extension $(F_R, \ell,)$.

Theorem 3. *There exists $N \in \mathbb{N}$ such that for every connected graph G on more than N vertices, if the smallest eigenvalue of G is in $(-\lambda^*, -2)$, then G is isomorphic to an augmented path extension of a rooted graph.*

We derive Theorem 3 using tools developed for forbidden subgraphs characterization in [10]. Since we rarely work with subgraphs that are not induced, we emphasize that *all subgraphs are induced* throughout this paper.

The first part of our classification theorem is an explicit enumeration of 794 classes of augmented path extensions in $\mathcal{G}(\lambda^*) \setminus \mathcal{G}(2)$. We state the first part qualitatively as follows.

Definition 4 (Single-rooted graph and its line graph)**.** A *single-rooted graph* H_r is a rooted graph H with one single root r. The *line graph* of a single-rooted graph H_r, denoted by $L(H_r)$, is the rooted graph F_R, where F is the line graph of H, and R is the set of edges incident to r in H.

Theorem 5. *There exists a finite family $\mathcal{F}$ of rooted graphs such that*

(a) every rooted graph in $\mathcal{F}$ is the line graph of a connected bipartite single-rooted graph,

(b) every connected augmented path extension with smallest eigenvalue in $(-\lambda^*, -2)$ is an augmented path extension of a rooted graph in $\mathcal{F}$, and

(c) for every rooted graph F_R in $\mathcal{F}$, there exists $\ell_0 \in \{0, \dots, 6\}$ such that the smallest eigenvalue of $(F_R, \ell,)$ is in $(-\lambda^*, -2)$ if and only if $\ell \geq \ell_0$.

A key ingredient in pinning down the augmented path extensions in $\mathcal{G}(\lambda^*) \setminus \mathcal{G}(2)$ is the following linear-algebraic lemma. This lemma simplifies the task of determining whether an augmented path extension belongs in $\mathcal{G}(\lambda^*)$ to a finite computation.

Lemma 6. *For every rooted graph F_R and $\ell \in \mathbb{N}$, the smallest eigenvalue of $(F_R, \ell,)$ is more than $-\lambda^*$ if and only if the same holds for $(F_R, 0,)$.*

The second part of our classification theorem is an explicit enumeration of connected graphs in $\mathcal{G}(\lambda^*) \setminus \mathcal{G}(2)$ that are not augmented path extensions.

Definition 7 (Maverick graph)**.** A *maverick graph* is a connected graph with smallest eigenvalue in $(-\lambda^*, -2)$ that is not an augmented path extension of any rooted graph.

Theorem 8. *There are a total of 4752 maverick graphs with the following statistics.*

order	*9*	*10*	*11*	*12*	*13*	*14*	*15*	*16*	*17*	*18*	*19*
#	*13*	*629*	*1304*	*1237*	*775*	*408*	*221*	*107*	*42*	*13*	*3*

As a consequence of Theorems 5 and 8, every relatively large graph in $\mathcal{G}(\lambda^*) \setminus \mathcal{G}(2)$ can be obtained from the line graph of a bipartite graph by adding a pedant edge.

Corollary 9. *For every connected graph G on at least 18 vertices, if the smallest eigenvalue of G is in $(-\lambda^*, -2)$, then there exists a unique leaf v of G such that $G - v$ is the line graph of a bipartite graph.*

Finally, we briefly explore graphs whose smallest eigenvalues are slightly beyond $-\lambda^*$. As it turns out, Theorem 3 generalizes, whereas Theorem 5 does not.

Theorem 10. *There exist $\lambda > \lambda^*$ and $N \in \mathbb{N}$ such that for every connected graph G on more than N vertices, if the smallest eigenvalue of G is in $(-\lambda, -2)$, then G is isomorphic to an augmented path extension of a rooted graph.*

Theorem 11. *For every $\lambda > \lambda^*$, finite family $\mathcal{F}$ of rooted graphs and $N \in \mathbb{N}$, there exists a connected graph G on more than N vertices such that the smallest eigenvalue of G is in $(-\lambda, -\lambda^*)$, and G is not an augmented path extension of any rooted graph in $\mathcal{F}$.*

The rest of the paper is organized as follows. In Section 2, we prove Theorem 3, in Section 3, we prove Lemma 6, and in Section 4, we prove Theorem 5. In Section 5, we explicitly describe the family $\mathcal{F}$ of rooted graphs in Theorem 5, and in Section 6, we enumerate the maverick graphs in Theorem 8. In Section 7, we explore a frequent pattern in maverick graphs, and we prove Corollary 9. In Section 8, we prove Theorems 10 and 11, and we end the paper with open problems in Section 9.

Part of our proofs are computer-assisted with validated numerics. We explain our computer-aided proofs and how anyone can reproduce them independently. To expedite the identification of computer-assisted proofs for readers, we employ a bespoke symbol 🖳 at the conclusion of each such proof. All our code is available as ancillary files in the arXiv version of this paper.

We deliberately craft our code without relying on third-party libraries, ensuring it can be adapted across different programming languages. This approach also offers the significant advantage that individuals interested in verifying our algorithms have the flexibility to use large language models to translate our code written in Ruby into their programming language of choice, providing a valuable starting point. It is important to note that while this translation serves as an efficient initial step, further human refinement may be necessary to ensure the code fully captures the nuances of our original implementations.

2 Forbidden subgraph characterization

The proof of Theorem 3 centers around the notion of *generalized line graphs* originally defined by Hoffman [7]. Although we do not need their definition, for concreteness we nevertheless state the

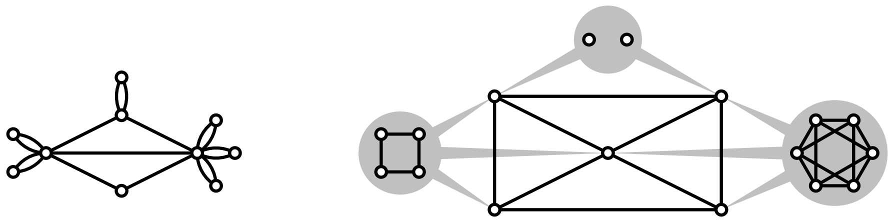

Figure 3: A graph $\hat{H}$ with petals and a schematic drawing of its line graph $L(\hat{H})$.

alternative definition from [5].

Definition 12 (Graph with petals and generalized line graph)**.** A *graph with petals* is a multigraph $\hat{H}$ obtained from a graph by adding pedant double edges. A *generalized line graph* $L(\hat{H})$ is the line graph of a graph $\hat{H}$ with petals where two vertices of $L(\hat{H})$ are adjacent if and only if the corresponding edges in $\hat{H}$ have exactly one vertex in common. See Figure 3 for a schematic drawing.

We need the following properties — just like line graphs, all the generalized line graphs are in $\mathcal{G}(2)$, and they have a finite forbidden subgraph characterization.

Theorem 13 (Theorem 2.1 of Hoffman [9])**.** *The smallest eigenvalue of a generalized line graph is at least* -2. $\square$

Theorem 14 (Cvetković, Doob, and Simić [4, 5], and Rao, Singhi, and Vijayan [13])**.** *There are 31 minimal forbidden subgraphs, one of which is* E_2 *defined in Figure 1, for the family* $\mathcal{D}_\infty$ *of generalized line graphs.* $\square$

To prove Theorem 3, the strategy is to forbid specific subgraphs, including all the minimal forbidden subgraphs for $\mathcal{D}_\infty$ except E_2, in every sufficiently large connected graph in $\mathcal{G}(\lambda^*) \setminus \mathcal{G}(2)$. To that end, we recall from [10] the following ways to extend a given graph.

Definition 15 (Path extension, clique extension, and path-clique extension)**.** Given a graph rooted graph F_R, $\ell \in \mathbb{N}$, and $m \in \mathbb{N}^+$,

(a) the *path extension* (F_R, ℓ) is obtained from F by adding a path $v_0 \dots v_\ell$ of length ℓ, and connecting v_0 to every vertex in R;[1]

(b) the *path-clique extension* (F_R, ℓ, K_m) is further obtained from (F_R, ℓ) by adding a clique of order m, and connecting every vertex in the clique to v_ℓ.

(c) the *clique extension* (F_R, K_m) is obtained from F by adding a clique of order m, and connecting every vertex in the clique to every vertex in R.

[1]The path of length 0 is simply a single vertex.

To forbid a subgraph F in every sufficiently large connected graph in $\mathcal{G}(\lambda)$, it is necessary that no sufficiently large path extension of F is in $\mathcal{G}(\lambda)$. This condition turns out to be sufficient when $\lambda \geq 2$. Hereafter, we denote the smallest eigenvalue of a graph G by $\lambda_1(G)$.

Lemma 16. *Suppose that F is a graph and $\lambda \geq 2$. If $\lim_{\ell\to\infty} \lambda_1(F_R, \ell) < -\lambda$ for every nonempty vertex subset R of F, then there exists $N \in \mathbb{N}$ such that F is never a subgraph of any connected graph on more than N vertices with smallest eigenvalue at least $-\lambda$.*

For the proof of Lemma 16, we need the following three results. The first two results automatically extend the inequality condition on path extensions to path-clique extensions and clique extensions.

Lemma 17 (Lemma 2.15 of Jiang and Polyanskii [10])**.** *For every rooted graph F_R and $\lambda \geq 2$, if $\lim_{\ell\to\infty} \lambda_1(F_R, \ell) < -\lambda$, then there exists $m \in \mathbb{N}^+$ such that $\lambda_1(F_R, \ell, K_m) < -\lambda$ for every $\ell \in \mathbb{N}$.* □

Lemma 18. *For every rooted graph F_R and $\lambda \geq 2$, if $\lim_{\ell\to\infty} \lambda_1(F_R, \ell) < -\lambda$, then there exists $m \in \mathbb{N}^+$ such that $\lambda_1(F_R, K_m) < -\lambda$.*

Proof. Pick $\ell \in \mathbb{N}^+$ such that $\lambda_1(F_R, \ell) < -\lambda$. Set $\lambda' := -\lambda_1(F_R, \ell)$. Let $v_0 \dots v_\ell$ be the path added to F to obtain (F_R, ℓ), where the vertex v_0 is connected to every vertex in R, and let $\boldsymbol{x}\colon V(F) \cup \{v_0, \dots, v_\ell\} \to \mathbb{R}$ be an eigenvector of (F_R, ℓ) associated with $-\lambda'$. We abuse notation and write x_i in place of x_{v_i} for $i \in \{0, \dots, \ell\}$. Define $\tilde{\boldsymbol{x}}\colon V(F) \cup V(K_m) \to \mathbb{R}$ by

$$\tilde{x}_v = \begin{cases} x_v & \text{if } v \in V(F); \\ x_0/m & \text{if } v \in V(K_m). \end{cases}$$

We claim that $\sum_{v\in V(F)} x_v^2 > 0$. Indeed, assume for the contradiction that $x_v = 0$ for $v \in V(F)$. Using $-\lambda' x_i = \sum_{u\sim v_i} x_u$ for $i \in \{0, \dots, \ell\}$, where the sum is taken over all vertices u that are adjacent to v_i in (F_R, ℓ), we obtain that

$$(A_P + \lambda' I) \begin{pmatrix} x_0 \\ \vdots \\ x_\ell \end{pmatrix} = \mathbf{0}$$

where P denotes the path $v_0 \dots v_\ell$. Since $\lambda_1(P) > -2 > -\lambda'$, the matrix $A_P + \lambda' I$ is positive definite, which contradicts with the assumption that $\boldsymbol{x}$ is a nonzero vector.

Because $\sum_{v\in V(F)} x_v^2 > 0$, clearly $\tilde{\boldsymbol{x}}$ is a nonzero vector. We compute

$$\tilde{\boldsymbol{x}}^\intercal \tilde{\boldsymbol{x}} = \sum_{v\in V(F)} x_v^2 + m(x_0/m)^2.$$

Moreover we can compute $\tilde{\boldsymbol{x}}^\intercal A_{(F_R,K_m)}\tilde{\boldsymbol{x}}$ as follows

$$\tilde{\boldsymbol{x}}^\intercal A_{(F_R,K_m)}\tilde{\boldsymbol{x}} = \sum_{u,v\in V(F_R,0):\, u\sim v} x_u x_v + m(m-1)(x_0/m)^2.$$

Since $\boldsymbol{x}$ is an eigenvector of (F_R,ℓ) associated with $-\lambda'$, we obtain that

$$\sum_{u,v\in V(F_R,0):\, u\sim v} x_u x_v + x_0x_1 = \sum_{v\in V(F_R,0)} x_v \sum_{u\sim v} x_u = -\lambda' \sum_{v\in V(F)} x_v^2 - \lambda' x_0^2.$$

Thus $\tilde{\boldsymbol{x}}^\intercal A_{(F_R,K_m)}\tilde{\boldsymbol{x}}$ can be simplified to

$$\tilde{\boldsymbol{x}}^\intercal A_{(F_R,K_m)}\tilde{\boldsymbol{x}} = -\lambda' \sum_{v\in V(F)} x_v^2 - \lambda' x_0^2 - x_0x_1 + m(m-1)(x_0/m)^2.$$

The Rayleigh principle says that $\lambda_1(F_R,K_m)$ is at most

$$\frac{-\lambda'\sum_{v\in V(F)} x_v^2 - \lambda' x_0^2 - x_0x_1 + m(m-1)(x_0/m)^2}{\sum_{v\in V(F)} x_v^2 + m(x_0/m)^2},$$

which, as $m\to\infty$, approaches

$$-\lambda' - \frac{(\lambda'-2)x_0^2 + x_0(x_0+x_1)}{\sum_{v\in V(F)} x_v^2}$$

Here we used the claim that the denominator in the limit is positive.

Recall that $\lambda' = -\lambda_1(F_R,\ell) > \lambda \geq 2$. It suffices to show that $x_0(x_0+x_1)\geq 0$. In fact, we prove inductively that $x_i(x_i+x_{i+1}) \geq 0$ for $i\in\{\ell-1,\dots,0\}$. The base case where $i=\ell-1$ follows immediately from $-\lambda' x_\ell = x_{\ell-1}$ and $\lambda'>2$. For the inductive step, using $-\lambda' x_{i+1} = x_i + x_{i+2}$ and $\lambda' > 2$, we obtain

$$\begin{aligned} x_{i+1}(x_{i+1}+x_{i+2}) = x_{i+1}(x_{i+1}-\lambda' x_{i+1} - x_i) &= -(\lambda'-2)x_{i+1}^2 - (x_i+x_{i+1})x_{i+1} \\ &\leq -(x_i+x_{i+1})x_{i+1} = -(x_i+x_{i+1})^2 + x_i(x_i+x_{i+1}) \leq x_i(x_i+x_{i+1}), \end{aligned}$$

which implies that $x_i(x_i+x_{i+1})\geq 0$ by the inductive hypothesis. □

The third result shows that forbidding a star and an extension family of F effectively forbids F itself in every sufficiently large connected graph. Denote by S_k the star on $k+1$ vertices.

Definition 19 (Extension family)**.** Given a graph F and $\ell, m\in\mathbb{N}^+$, the *extension family* $\mathcal{X}(F,\ell,m)$ of F consists of the path-extension (F_R,ℓ), the path-clique extension (F_R,ℓ_0,K_m), and the clique extension (F_R,K_m), where R ranges over the nonempty vertex subsets of F, and ℓ_0 ranges over $\{0,\dots,\ell-1\}$.

Lemma 20 (Lemma 2.6 of Jiang and Polyanskii [10])**.** *For every graph F and $k,\ell,m\in\mathbb{N}^+$, there exists $N\in\mathbb{N}$ such that for every connected graph G on more than N vertices, if no member in $\{S_k\}\cup\mathcal{X}(F,\ell,m)$ is a subgraph of G, then neither is F.* □

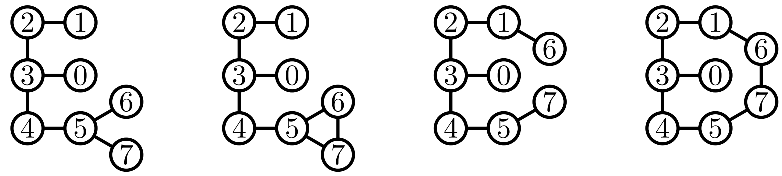

Figure 4: Four 8-vertex graphs F with two vertices v_6 and v_7 such that $F - \{v_6, v_7\}$ is isomorphic to E_2, and both $F - v_6$ and $F - v_7$ are isomorphic to E_3.

We now have all of the ingredients needed to establish Lemma 16.

Proof of Lemma 16. Choose $\ell \in \mathbb{N}^+$ such that $\lambda_1(F_R, \ell) < -\lambda$ for every nonempty $R \subseteq V(F)$. According to Lemmas 17 and 18, choose $m \in \mathbb{N}^+$ such that $\lambda_1(F_R, \ell_0, K_m) < -\lambda$ for every nonempty $R \subseteq V(F)$ and every $\ell_0 \in \mathbb{N}$, and $\lambda_1(F_R, K_m) < -\lambda$ for every nonempty $R \subseteq V(F)$.

Suppose that G is a graph with $\lambda_1(G) > -\lambda$. The choice of ℓ and m ensures that no member in $\mathcal{X}(F, \ell, m)$ is a subgraph of G. Furthermore, the star S_k, whose smallest eigenvalue is $-\sqrt{k}$, cannot be a subgraph of G for any $k \in \mathbb{N}^+$ satisfying $\sqrt{k} > \lambda$. Finally we apply Lemma 20 to obtain the desired $N \in \mathbb{N}$. $\square$

With Lemma 16 at our disposal, we return to forbidding certain subgraphs in every sufficiently large connected graph in $\mathcal{G}(\lambda^*) \setminus \mathcal{G}(2)$. The following computation ensures that E_2 occurs as a subgraph in every sufficiently large connected graph in $\mathcal{G}(\lambda^*) \setminus \mathcal{G}(2)$.

Lemma 21 (Lemma 2.14 of Jiang and Polyanskii [10])**.** *For every minimal forbidden subgraph F for the family $\mathcal{D}_\infty$ of generalized line graphs, if F is not isomorphic to E_2, then* $\lim_{\ell\to\infty} \lambda_1(F_R, \ell) < -\lambda^*$ *for every nonempty vertex subset R of F.* $\square$

In addition, we further forbid small supergraphs of E_2 through the following computation, which is proved under computer assistance in Appendix A.

Proposition 22. *For every connected graph F that contains E_2 as a subgraph, if F is a 7-vertex graph that is not isomorphic to E_3, or F is an 8-vertex graph in Figure 4, then* $\lim_{\ell\to\infty} \lambda_1(F_R, \ell) < -95/47$ *for every nonempty vertex subset R of F.*

Proof of Theorem 3. Combining Lemmas 16 and 21, we obtain $N_1 \in \mathbb{N}$ such that for every minimal forbidden subgraph F for $\mathcal{D}_\infty$, if F is not isomorphic to E_2, then F is not a subgraph of any connected graph on more than N_1 vertices with smallest eigenvalue more than $-\lambda^*$. Combining Lemma 16 and Proposition 22, we obtain $N_2 \in \mathbb{N}$ such that for every connected graph F that contains E_2 as a subgraph, if F is a 7-vertex graph that is not isomorphic to E_3, or F is an 8-vertex graph in Figure 4, then F is not a subgraph of any connected graph on more than N_2 vertices with smallest eigenvalue more than $-\lambda^*$. Here, we use the fact that $\lambda^* \approx 2.01980 < 2.02127 \approx 95/47$.

Suppose that G is a connected graph on more than $N := \max(N_1, N_2)$ vertices with smallest eigenvalue in $(-\lambda^*, -2)$. Observe from Theorem 13 that G is not a generalized line graph. Thus G

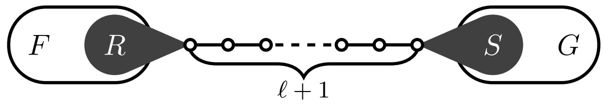

Figure 5: The path augmentation (F_R, ℓ, G_S).

contains a subgraph E that is a minimal forbidden subgraph for $\mathcal{D}_\infty$. The choice of N_1 forces E to be isomorphic to E_2. The choice of N_2 ensures that $G[V(E) \cup \{v\}]$ is isomorphic to E_3 for every vertex v at distance 1 from E in G, and moreover, such a vertex v is unique. In particular, G is an augmented path extension of a rooted graph. $\square$

3 The linear-algebraic lemma

We generalize Lemma 6 to a class of graphs that encapsulates both augmented path extensions and path-clique extensions.

Definition 23 (Path augmentation)**.** Given two rooted graphs F_R and G_S and $\ell \in \mathbb{N}$, the *path augmentation* (F_R, ℓ, G_S) of F_R and G_S is obtained from the disjoint union of F and G by adding a path $v_0 \dots v_\ell$ of length ℓ, connecting v_0 to every vertex in R, and connecting v_ℓ to every vertex in S. See Figure 5 for a schematic drawing.

Lemma 24. *Suppose that G_S is a rooted graph. If $\lambda = -\lim_{\ell\to\infty} \lambda_1(G_S, \ell)$, and $\lambda_1(G) > -\lambda$, then the following holds. For every rooted graph F_R and $\ell \in \mathbb{N}$, the smallest eigenvalue of (F_R, ℓ, G_S) is more than $-\lambda$ if and only if the same holds for $(F_R, 0, G_S)$.*

Proof of Lemma 6. Take $G_S =$ in Lemma 24, and observe that $(\,\cdot\,, \ell)$ is just E_ℓ. Lemma 6 follows immediately from Proposition 1. $\square$

To provide additional context for Lemma 24, we discuss the behavior of the smallest eigenvalue of the path augmentation (F_R, ℓ, G_S) as $\ell \to \infty$. The following result follows from [1, Proposition 3.5]. We provide a self-contained proof here.

Lemma 25. *For every rooted graphs F_R and G_S,*

$$\lim_{\ell\to\infty} \lambda_1(F_R, \ell, G_S) = \min\left(\lim_{\ell\to\infty} \lambda_1(F_R, \ell), \lim_{\ell\to\infty} \lambda_1(G_S, \ell)\right).$$

Proof. Set $\lambda_{F_R} = \lim_{\ell\to\infty} \lambda_1(F_R, \ell)$ and $\lambda_{G_S} = \lim_{\ell\to\infty} \lambda_1(G_S, \ell)$. Since both (F_R, ℓ) and (G_S, ℓ) are subgraphs of (F_R, ℓ, G_S), clearly $\limsup_{\ell\to\infty} \lambda_1(F_R, \ell, G_S) \le \min(\lambda_{F_R}, \lambda_{G_S})$.

To see the reverse, let $v_0 \dots v_\ell$ be the path added to the disjoint union of F and G to obtain (F_R, ℓ, G_S), and let $\boldsymbol{x}\colon V(F_R, \ell, G_S) \to \mathbb{R}$ be a unit eigenvector associated with $\lambda_1(F_R, \ell, G_S)$. We abuse notation and write x_i in place of x_{v_i}. Choose $k \in \{0, \ldots, \ell-1\}$ such that $x_k x_{k+1}$ reaches the minimum in absolute value. In particular, using the inequality $|x_i x_{i+1}| \le (x_i^2 + x_{i+1}^2)/2$, we obtain

$$|x_k x_{k+1}| \le \frac{1}{\ell}\sum_{i=0}^{\ell-1}|x_i x_{i+1}| \le \frac{1}{\ell}\sum_{i=0}^{\ell} x_i^2 \le \frac{1}{\ell}.$$

Notice that removing the edge $v_k v_{k+1}$ disconnects (F_R, ℓ, G_S) into subgraphs $F' := (F_R, k)$ and $G' := (G_S, \ell-k-1)$. Let $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ be the restrictions of $\boldsymbol{x}$ to $V(F')$ and $V(G')$ respectively. Finally, we bound the smallest eigenvalue of (F_R, ℓ, G_S) as follows:

$$\begin{aligned}\lambda_1(F_R, \ell, G_S) = \boldsymbol{x}^\intercal A_{(F_R,\ell,G_S)}\boldsymbol{x} = \boldsymbol{x}_1^\intercal A_{F'}\boldsymbol{x}_1 + 2x_k x_{k+1} + \\ + \boldsymbol{x}_2^\intercal A_{G'}\boldsymbol{x}_2 \ge \lambda_{F_R}\boldsymbol{x}_1^\intercal\boldsymbol{x}_1 - 2/\ell + \lambda_{G_S}\boldsymbol{x}_2^\intercal\boldsymbol{x}_2 \ge \min(\lambda_{F_R}, \lambda_{G_S}) - 2/\ell,\end{aligned}$$

which implies that $\liminf_{\ell\to\infty}\lambda_1(F_R, \ell, G_S) \ge \min(\lambda_{F_R}, \lambda_{G_S})$. $\square$

Example. Consider the two cases where $F_R \in \{$  ,  $\}$ and $G_S =$ . In both cases, because $\lim_{\ell\to\infty}\lambda_1(F_R,\ell) = -2$ and $\lim_{\ell\to\infty}\lambda_1(G_S,\ell) = -\lambda^*$, according to Lemma 25, $\lambda_1(F_R,\ell,G_S)$ approaches $-\lambda^*$ as $\ell\to\infty$. Interestingly, the smallest eigenvalue approaches $-\lambda^*$ in different ways — $\lambda_1($$, \ell,$ $)$ approaches $-\lambda^*$ from below, whereas $\lambda_1($$, \ell,$ $)$ approaches from above. Lemma 24 rules out other ways $\lambda_1(F_R,\ell,G_S)$ could approach its limit.

We devote the rest of the section to the proof of Lemma 24. Denote by $E_{v,v}$ the unit matrix where the (v,v)-entry with value 1 is the only nonzero entry. We first characterize $\lim_{\ell\to\infty}\lambda_1(G_S,\ell)$.

Lemma 26. *Suppose that G_S is a rooted graph. Let v_0 be the vertex in $V(G_S,0)\setminus V(G)$. If $\lambda = -\lim_{\ell\to\infty}\lambda_1(G_S,\ell)$, then the set of $x \ge 2$, for which the matrix*

$$A_{(G_S,0)} + xI - \left(x/2 - \sqrt{x^2/4-1}\right)E_{v_0,v_0} \tag{1}$$

is positive semidefinite, is equal to $[\lambda,\infty)$, and moreover, the above matrix is singular when $x = \lambda$.

Proof. Denote by P_ℓ the path of length ℓ. Since $\lim_{\ell\to\infty}\lambda_1(P_\ell) = -2$, clearly $\lambda \ge 2$. Let $x \ge 2$ be chosen later, and for every $n \in \mathbb{N}^+$, set $d_n := \det\bigl(A_{P_{n-1}} + xI\bigr)$. Use Laplace expansion, one can derive the linear recurrence $d_{n+2} = x d_{n+1} - d_n$ with the initial conditions $d_0 = 1$ and $d_1 = x$. It follows from the classical theory of linear recurrence that $\lim_{\ell\to\infty} d_{\ell-1}/d_\ell = x/2 - \sqrt{x^2/4-1}$.

Claim. For every $\ell \in \mathbb{N}^+$, the matrix $A_{(G_S,\ell)} + xI$ is positive semidefinite if and only if $A_{(G_S,0)} + xI - (d_{\ell-1}/d_\ell)E_{v_0,v_0}$ is positive semidefinite.

Proof of Claim. We partition the matrix $A_{(G_S,\ell)} + xI$ into the following blocks:

$$\begin{pmatrix} A_{(G_S,0)} + xI & B \\ B^\intercal & C \end{pmatrix},$$

Since $C = A_{P_{\ell-1}} + xI$, and $\lambda_1(P_{\ell-1}) > -2 \geq -x$, the block C is positive definite. Therefore, the above block matrix is positive semidefinite if and only if the Schur complement $A_{(G_S,0)} + xI - BC^{-1}B^\intercal$ of C is positive semidefinite. Let v_1 be the vertex in $V(G_S, 1) \setminus V(G_S, 0)$. Since the only nonzero entry of B is its (v_0, v_1) entry, the matrix $BC^{-1}B^\intercal$ simplifies to $(C^{-1})_{v_1,v_1} E_{v_0,v_0}$. Cramer's rule yields $(C^{-1})_{v_1,v_1} = \det C' / \det C$, where C' is obtained from C by removing the v_1-th row and column. To finish the proof of the claim, note that $\det C' = d_{\ell-1}$ and $\det C = d_\ell$. $\diamondsuit$

First, we consider the case where $x \geq \lambda$. The claim implies that $A_{(G_S,0)} + xI - (d_{\ell-1}/d_\ell)E_{v_0,v_0}$ is positive semidefinite. Sending ℓ to ∞, we know that the matrix in (1) is positive semidefinite when $x \geq \lambda$. Next, we consider the case where $x \in [2, \lambda)$. The claim implies that $A_{(G_S,0)} + xI - (d_{\ell-1}/d_\ell)E_{v_0,v_0}$ is not positive semidefinite for sufficiently large ℓ. Sending ℓ to ∞, we know that the matrix in (1) not is positive semidefinite when $x \in [2, \lambda)$. Finally, assume for the sake of contradiction that the matrix in (1) is positive definite when $x = \lambda$. We can then decrease x slightly so that the matrix in (1) is still positive definite, which yields a contradiction. $\square$

We adopt the convention that the path extension $(G_S, -1)$ is just the graph G.

Corollary 27. *Suppose that G_S is a rooted graph. If $\lambda = -\lim_{\ell\to\infty} \lambda_1(G_S, \ell)$, then for every $\ell \in \mathbb{N}$, the matrix*

$$A_{(G_S,\ell)} + \lambda I - \left(\lambda/2 - \sqrt{\lambda^2/4 - 1}\right) E_{v_\ell,v_\ell}$$

is singular, where v_ℓ is the vertex in $V(G_S, \ell) \setminus V(G_S, \ell - 1)$.

Proof. We prove by induction on ℓ. Lemma 26 implies the base case where $\ell = 0$. For the inductive step, suppose that $\ell \in \mathbb{N}^+$. Let r be the vertex in $V(G_S, \ell-1) \setminus V(G_S, \ell-2)$. Define the single-rooted graph H_r by $H = (G_S, \ell - 1)$. Note that $(H_r, m) = (G_S, \ell + m)$, and so $\lim_{m\to\infty} \lambda_1(H_r, m) = -\lambda$. Apply the base case to H_r, we know that $A_{(H_r,0)} + \lambda I - (\lambda/2 - \sqrt{\lambda^2/4 - 1})E_{v_\ell,v_\ell}$ is singular. $\square$

Now we obtain a simple matrix criterion to decide whether $\lambda_1(F_R, \ell, G_S) > \lim_{\ell\to\infty} \lambda_1(G_S, \ell)$, from which Lemma 24 follows immediately.

Lemma 28. *Suppose that G_S is a rooted graph. If $\lambda = -\lim_{\ell\to\infty} \lambda_1(G_S, \ell)$, and $\lambda_1(G) > -\lambda$, then the following holds. For every rooted graphs F_R and $\ell \in \mathbb{N}$, the smallest eigenvalue of the path augmentation (F_R, ℓ, G_S) is more than $-\lambda$ if and only if the matrix*

$$A_{(F_R,0)} + \lambda I - \left(\lambda/2 + \sqrt{\lambda^2/4 - 1}\right) E_{v_0,v_0}$$

is positive definite, where v_0 is the vertex in $V(F_R, 0) \setminus V(F)$.

Proof. We claim that $\lambda_1(G_S, \ell-1) > -\lambda$. Assume for the sake of contradiction that $\lambda_1(G_S, \ell-1) = -\lambda$. Let $\boldsymbol{x}\colon V(G_S, \ell - 1) \to \mathbb{R}$ be an eigenvector of $(G_S, \ell - 1)$ associated with $-\lambda$. Let $v_0 \dots v_\ell$ be the path of length ℓ that is added to G to obtain (G_S, ℓ). We extend $\boldsymbol{x}$ to $\tilde{\boldsymbol{x}}\colon V(G_S, \ell) \to \mathbb{R}$ by setting $\tilde{x}_{v_\ell} = 0$. Since $\tilde{\boldsymbol{x}}^\intercal A_{(G_S,\ell)}\tilde{\boldsymbol{x}} = -\lambda\tilde{\boldsymbol{x}}^\intercal\tilde{\boldsymbol{x}}$, and $\lambda_1(G_S, \ell) = -\lambda$, the nonzero vector $\tilde{\boldsymbol{x}}$ is an

Figure 6: The claw graph C and the diamond graph D.

eigenvector of (G_S, ℓ). Using $-\lambda x_{v_i} = \sum_{u \sim v_i} x_u$ for $i \in \{\ell, \dots, 1\}$, one can then prove by induction that $x_{v_i} = 0$ for $i \in \{\ell, \dots, 0\}$. Therefore the vector $\boldsymbol{x}$ restricted to $V(G)$ is an eigenvector of G associated with $-\lambda$, which contradicts with the assumption that $\lambda(G) > -\lambda$.

Coming back to the proof of the lemma, we partition the matrix $A_{(F_R,\ell,G_S)} + \lambda I$ into the following blocks:

$$\begin{pmatrix} A_{(F_R,0)} + \lambda I & B \\ B^\intercal & C \end{pmatrix}.$$

Since $C = A_{(G_S,\ell-1)} + \lambda I$, and $\lambda_1(G_S, \ell - 1) > -\lambda$ from the claim, the block C is positive definite. Therefore, the above block matrix is positive definite if and only if the Schur complement $A_{(F_R,0)} + \lambda I - BC^{-1}B^\intercal$ of C is positive definite. Since the only nonzero row of B is its v_0-th row, say B_{v_0}, the matrix $BC^{-1}B^\intercal$ simplifies to $\left(B_{v_0} C^{-1} B_{v_0}^\intercal\right) E_{v_0,v_0}$.

It suffices to verify that $B_{v_0} C^{-1} B_{v_0}^\intercal = \lambda/2 + \sqrt{\lambda^2/4 - 1}$. Notice that the block matrix

$$\begin{pmatrix} \lambda/2 + \sqrt{\lambda^2/4 - 1} & B_{v_0} \\ B_{v_0}^\intercal & C \end{pmatrix}$$

is precisely the matrix in Corollary 27, and so it is singular. Since the block C is non-singular, its Schur complement $\lambda/2 + \sqrt{\lambda^2/4 - 1} - B_{v_0} C^{-1} B_{v_0}^\intercal$ must be zero. □

Proof of Lemma 24. Simply notice that the matrix criterion in Lemma 28 is independent from ℓ. □

4 Characterization of the rooted graphs

Consider an augmented path extension of a rooted graph F_R in $\mathcal{G}(\lambda^*) \setminus \mathcal{G}(2)$. Clearly, $(F_R, 0)$ is connected, and furthermore Lemma 6 implies that $\lambda_1(F_R, 0,) > -\lambda^*$.

To characterize such rooted graphs F_R, we need the following sufficient condition for line graphs, which is an immediate consequence of [14, Theorem 4]. The claw graph and the diamond graph are defined in Figure 6.

Theorem 29 (Theorem 4 of van Rooij and Wilf [14])**.** *Every graph that contains neither the claw graph nor the diamond graph as a subgraph is a line graph.* □

The following computation, together with Lemma 6, roughly speaking, enables us to forbid certain subgraphs in the rooted graph F_R.

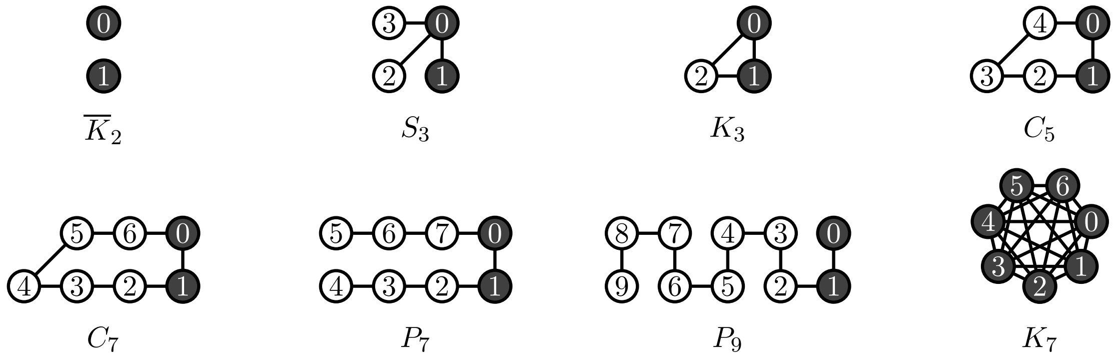

Figure 7: The rooted graphs in Proposition 30.

Proposition 30. *For every rooted graph F_R in Figure 7, the smallest eigenvalue of $(F_R, 0, \therefore)$ is less than $-\lambda^*$.*

Proof. We shall prove that $\lambda_1(F_R, 0, \therefore) < -101/50 = -2.02$. Our computation is straightforward. We label the rooted graphs in Figure 7 by `K2C, S3, K3, C5, C7, P7, P9, K7`. For each rooted graph F_R, we output the determinant of $A_{(F_R,0,\therefore)} + (101/50)I$, which turns out to be negative. Our code is available as the ancillary file `forb_rooted_graphs.rb` in the arXiv version of the paper.

Lemma 31. *For every rooted graph F_R, if $(F_R, 0)$ is connected and $\lambda_1(F_R, 0, \therefore) > -\lambda^*$, then there exists a connected bipartite single-rooted graph H_r such that*

(a) F_R is the line graph of H_r,

(b) every vertex of H is at most 8 from r as long as r is not a leaf of H,

(c) and the maximum degree of H is at most 7.

Proof. Suppose that F_R is a rooted graph such that $(F_R, 0)$ is connected and $\lambda_1(F_R, 0, \therefore) > -\lambda^*$. Let $\overline{K}_2$, S_3, K_3, C_5, C_7, P_7, P_9 and K_7 be the eight rooted graphs defined in Figure 7.

We first prove that the claw graph C is not a subgraph of $(F_R, 1)$. Assume for the sake of contradiction that C is a subgraph of $(F_R, 1)$. Then C is also a subgraph of $(F_R, 2)$. Let v_2 be the vertex in $V(F_R, 2) \setminus V(F_R, 1)$, and let $v_2 u_1 \dots u_\ell$ be a shortest path (possibly of length 0) from v_2 to a vertex u_ℓ at distance 1 from C in $(F_R, 2)$. Label the vertices of C as in Figure 6, and let $S \subseteq \{0, 1, 2, 3\}$ be the nonempty subset of vertices of C that are adjacent to u_ℓ in $(F_R, 2)$. Notice that the augmented path extension $(F_R, 2, \therefore)$ contains

$$\begin{aligned}
(\overline{K}_2, \ell+1, \therefore) &\text{ when } S = \{0\}\,; \\
(\overline{K}_2, \ell+2, \therefore) &\text{ when } |S| = 1 \text{ and } 0 \notin S; \\
(S_3, \ell, \therefore) &\text{ when } |S \cap \{1,2,3\}| = 1 \text{ and } 0 \in S; \\
(\overline{K}_2, \ell, \therefore) &\text{ when } |S \cap \{1,2,3\}| \geq 2,
\end{aligned}$$

as a subgraph, which yields a contradiction in view of Lemma 6 and Proposition 30.

We next prove that the diamond graph D is not a subgraph of $(F_R, 1)$. Assume for the sake of contradiction that D is a subgraph of $(F_R, 1)$. Let v_1 be the vertex in $V(F_R, 1) \setminus V(F_R, 0)$, and let $v_1 u_1 \dots u_\ell$ be a shortest path (possibly of length 0) from v_1 to a vertex u_ℓ at distance 1 from D. Label the vertices of D as in Figure 6, and let $S \subseteq \{0, 1, 2, 3\}$ be the nonempty subset of vertices of D that are adjacent to u_ℓ in $(F_R, 1)$. Notice that the augmented path extension $(F_R, 1, \therefore)$ contains

$$\begin{aligned}
(\overline{K}_2, \ell+1, \therefore) &\text{ when } S = \{0\} \text{ or } S = \{2\}\,; \\
(K_3, \ell+1, \therefore) &\text{ when } S = \{1\} \text{ or } S = \{3\}\,; \\
(\overline{K}_2, \ell, \therefore) &\text{ when } S \supseteq \{1, 3\}\,; \\
(K_3, \ell, \therefore) &\text{ when } |S| \geq 2 \text{ and } S \not\supseteq \{1, 3\}\,,
\end{aligned}$$

as a subgraph, which yields a contradiction in view of Lemma 6 and Proposition 30.

At this point, Theorem 29 implies that there exists a graph H' such that $(F_R, 1)$ is the line graph of H'. Let v_0 be the vertex in $V(F_R, 0) \setminus V(F)$, and let v_1 be the vertex in $V(F_R, 1) \setminus V(F_R, 0)$. We identify the two vertices v_0 and v_1 of $(F_R, 1)$ with two edges e_0 and e_1 of H'. Since $v_0 v_1$ is an edge of $(F_R, 1)$, the edges e_0 and e_1 shares a common vertex in H'. Let r, u_0, u_1 be the vertices of H' such that $e_0 = r u_0$ and $e_1 = u_0 u_1$. Since v_1 is a leaf of $(F_R, 1)$ and $v_0 v_1$ is a pedant edge of $(F_R, 1)$, we deduce that u_1 is a leaf of H', and u_0 is a leaf of $H' - u_1$. Let $H = H' - \{u_0, u_1\}$. Clearly F_R is the line graph of H_r. Since $(F_R, 1)$ is connected, so are H' and H.

To finish the proof of (a), we need to further show that H is bipartite. Assume for the sake of contradiction that H contains an odd cycle C_k of length k as a subgraph that is not necessarily induced. Take a shortest path P of length ℓ between r and C_k. Notice that the edges in P and C_k induce the following graph as a subgraph of $(F_R, 0, \therefore)$:

$$\begin{aligned}
(K_3, \ell, \therefore) &\text{ when } k = 3; \\
(C_5, \ell, \therefore) &\text{ when } k = 5; \\
(C_7, \ell, \therefore) &\text{ when } k = 7; \\
(P_7, \ell, \therefore) &\text{ when } k \geq 9,
\end{aligned}$$

which yields a contradiction in view of Lemma 6 and Proposition 30.

We are left to prove (b) and (c). Assume for the sake of contradiction that r is not a leaf of H, and there exists a vertex u_9 at distance 9 from r in H. Take a shortest path $P := r u_1 \dots u_9$ between r and u_9. Since r is not a leaf of H, we can choose a neighbor of r, say u_0, in H that is not on P. Notice that these edges $r u_0, r u_1, u_1 u_2, \dots, u_8 u_9$ in H induce $(P_9, 0, \therefore)$ as a subgraph of $(F_R, 0, \therefore)$, which yields a contradiction in view of Proposition 30. Lastly, assume for the sake of contradiction that there exists a vertex u with degree at least 8 in H. Take a shortest path P of length ℓ between r and u in H. We can choose neighbors of u, say $u_1, \dots, u_7$, in H that is not on

P. Notice that the edges of P together with the edges $uu_1, \ldots, uu_7$ induce $(K_7, \ell, \therefore)$ as a subgraph of $(F_R, 0, \therefore)$, which yields a contradiction in view of Lemma 6 and Proposition 30. $\square$

We need one more ingredient on augmented path extensions that are not in $\mathcal{G}(2)$.

Lemma 32. *For every rooted graph F_R and every $\ell \in \mathbb{N}$, if the smallest eigenvalue of $(F_R, \ell, \therefore)$ is less than -2, then the same holds for $(F_R, \ell+1, \therefore)$.*

Proof. Let $v_0 \ldots v_\ell$ be the path of length ℓ added to the disjoint union of F and the rooted graph $\therefore$ to obtain $(F_R, \ell, \therefore)$, and let $v_{-1}v_0 \ldots v_\ell$ be the corresponding path of length $\ell + 1$ to obtain $(F_R, \ell+1, \therefore)$. Suppose that $\lambda_1(F_R, \ell, \therefore) < -2$. We can pick a nonzero vector $\boldsymbol{x} \colon V(F_R, \ell, \therefore) \to \mathbb{R}$ such that $\boldsymbol{x}^\intercal A_{(F_R,\ell,\therefore)}\boldsymbol{x} < -2\boldsymbol{x}^\intercal\boldsymbol{x}$. Define the vector $\tilde{\boldsymbol{x}} \colon V(F_R, \ell+1, \therefore) \to \mathbb{R}$ by

$$\tilde{x}_v = \begin{cases} -x_v & \text{if } v \in V(F); \\ -x_{v_0} & \text{if } v = v_{-1}; \\ x_v & \text{otherwise.} \end{cases}$$

Clearly, $\tilde{\boldsymbol{x}}^\intercal A_{(F_R,\ell+1,\therefore)}\tilde{\boldsymbol{x}} = \boldsymbol{x}^\intercal A_{(F_R,\ell,\therefore)}\boldsymbol{x} - 2x_{v_0}^2$ and $\tilde{\boldsymbol{x}}^\intercal\tilde{\boldsymbol{x}} = \boldsymbol{x}^\intercal\boldsymbol{x} + x_{v_0}^2$. In particular, $\tilde{\boldsymbol{x}}$ is a nonzero vector that satisfies $\tilde{\boldsymbol{x}}^\intercal A_{(F_R,\ell+1,\therefore)}\tilde{\boldsymbol{x}} < -2\tilde{\boldsymbol{x}}^\intercal\tilde{\boldsymbol{x}}$, which implies that $\lambda_1(F_R, \ell+1, \therefore) < -2$ according to the Rayleigh principle. $\square$

We are in the position to establish the qualitative version of the second part of our classification theorem.

Proof of Theorem 5. Let the family $\mathcal{H}$ consist of the connected bipartite single-rooted graphs H_r such that r is not a leaf of H, and $\lambda_1(L(H_r), 0, \therefore) > -\lambda^*$. To satisfy (a), let the family $\mathcal{F}$ consist of the line graphs of the single-rooted graphs in $\mathcal{H}$. The family $\mathcal{H}$ includes the trivial single-rooted graph K_1, of which the line graph is the null graph K_0, whose augmented path extension $(K_0, \ell, \therefore)$ is simply E_ℓ.

Lemma 31 implies that every rooted graph H_r in $\mathcal{H}$ has radius at most 8 and maximum degree at most 7, and so both $\mathcal{H}$ and $\mathcal{F}$ are finite.

For (b), consider a connected augmented path extension $(F_R, \ell, \therefore)$ with smallest eigenvalue in $(-\lambda^*, -2)$. Without loss of generality, we may assume that either $F_R = K_0$ or $|R| \geq 2$. The former case is trivial because F_R is the line graph of the single-rooted graph $K_1 \in \mathcal{H}$. For the latter case where $|R| \geq 2$, since $(F_R, 0)$ is connected and $\lambda_1(F_R, 0, \therefore) > -\lambda^*$ via Lemma 6, Lemma 31 provides $H_r \in \mathcal{H}$ such that F_R is the line graph of H_r.

For (c), consider a rooted graph F_R in $\mathcal{F}$. By definition, $\lambda_1(F_R, 0, \therefore) > -\lambda^*$, and so the smallest eigenvalue of $(F_R, \ell, \therefore)$ is more than $-\lambda^*$ via Lemma 6 for every $\ell \in \mathbb{N}$. Note that the augmented path extension $(F_R, 6, \therefore)$ contains E_6 as a subgraph, whose smallest eigenvalue is less than -2. Let $\ell_0 \in \mathbb{N}$ be the smallest $\ell \in \mathbb{N}$ such that $\lambda_1(F_R, \ell, \therefore) < -2$. In particular, $\ell_0 \leq 6$. In view of Lemma 32, we know that $\lambda_1(F_R, \ell, \therefore) < -2$ if and only if $\ell \geq \ell_0$. $\square$

5 Enumeration of the rooted graphs

The proof of Theorem 5 on Page 15 has already characterized the members of $\mathcal{H}$. In this section, we enumerate all members of $\mathcal{H}$, and describe them concisely by their maximal members.

Definition 33. Given two single-rooted graphs H_r and H'_s, we say that H_r is a *general subgraph* of H'_s if there exists an injective graph homomorphism from H to H' that maps r to s.

The enumeration of $\mathcal{H}$ is achieved by a computer search. To supplement Theorem 5(c), we also output for each $H_r \in \mathcal{H}$ the smallest value of $\ell_0 \in \{0, \dots, 6\}$ for which $\lambda_1(L(H_r), \ell_0,) \in (-\lambda^*, -2)$.

Theorem 34. *Let the family $\mathcal{H}$ consist the connected bipartite single-rooted graphs H_r such that r is not a leaf of H, and $\lambda_1(L(H_r), 0,) > -\lambda^*$. Let $\mathcal{H}^*$ be the subfamily of $\mathcal{H}$ that consists members that are maximal under general subgraphs.*

(a) For every general subgraph H_r of a member in $\mathcal{H}^*$, if H is connected, and r is not a leaf of H, then H_r is in $\mathcal{H}$.

(b) There are a total of 794 members of $\mathcal{H}$ with the following statistics.[2]

size	*0*	*2*	*3*	*4*	*5*	*6*	*7*	*8*	*9*	*10*	*11*	*12*	*13*	*14*
#	*1*	*1*	*2*	*6*	*14*	*42*	*107*	*190*	*194*	*136*	*68*	*27*	*4*	*2*

(c) There are a total of 48 members of $\mathcal{H}^*$, which are listed in Figure 8.

Proof. For (a), consider a general subgraph H_r of $H'_s \in \mathcal{H}$. Since $(L(H_r), 0,)$ is a subgraph of $(L(H'_s), 0,)$, we know that $\lambda_1(L(H_r), 0,) > -\lambda^*$.

To enumerate the members in $\mathcal{H}$, notice that for every member $H_r \in \mathcal{H}$, except the trivial single-rooted graph K_1, there exists a sequence of members $H_r^{(2)}, \dots, H_r^{(n)} = H_r$ of $\mathcal{H}$ such that, $H_r^{(2)}$ is , and $H^{(i+1)}$ is obtained from $H^{(i)}$ by adding an edge, which is incident to at least one vertex of $H^{(i)}$, for every $i \in \{2, \dots, n-1\}$. This allows us to search for more non-trivial members of $\mathcal{H}$ by adding a new edge to the existing ones.

We store members of $\mathcal{H}$ in the hash `dict` based on their size, and store those that are maximal under general subgraphs in the array `maximal`. At the start, `dict[0]` consists of the trivial singled-rooted graph K_1, `dict[2]` consists of , and `m` increases from `2`.

Whenever `dict[m]` is nonempty, we iterate through members of `dict[m]`. For each H_r in `dict[n]`, we carry out the following steps.

(i) We add a new edge to H_r in every possible way to obtain new connected bipartite single-rooted graphs H'_r.

[2] The *size* of a graph is the number of its edges.

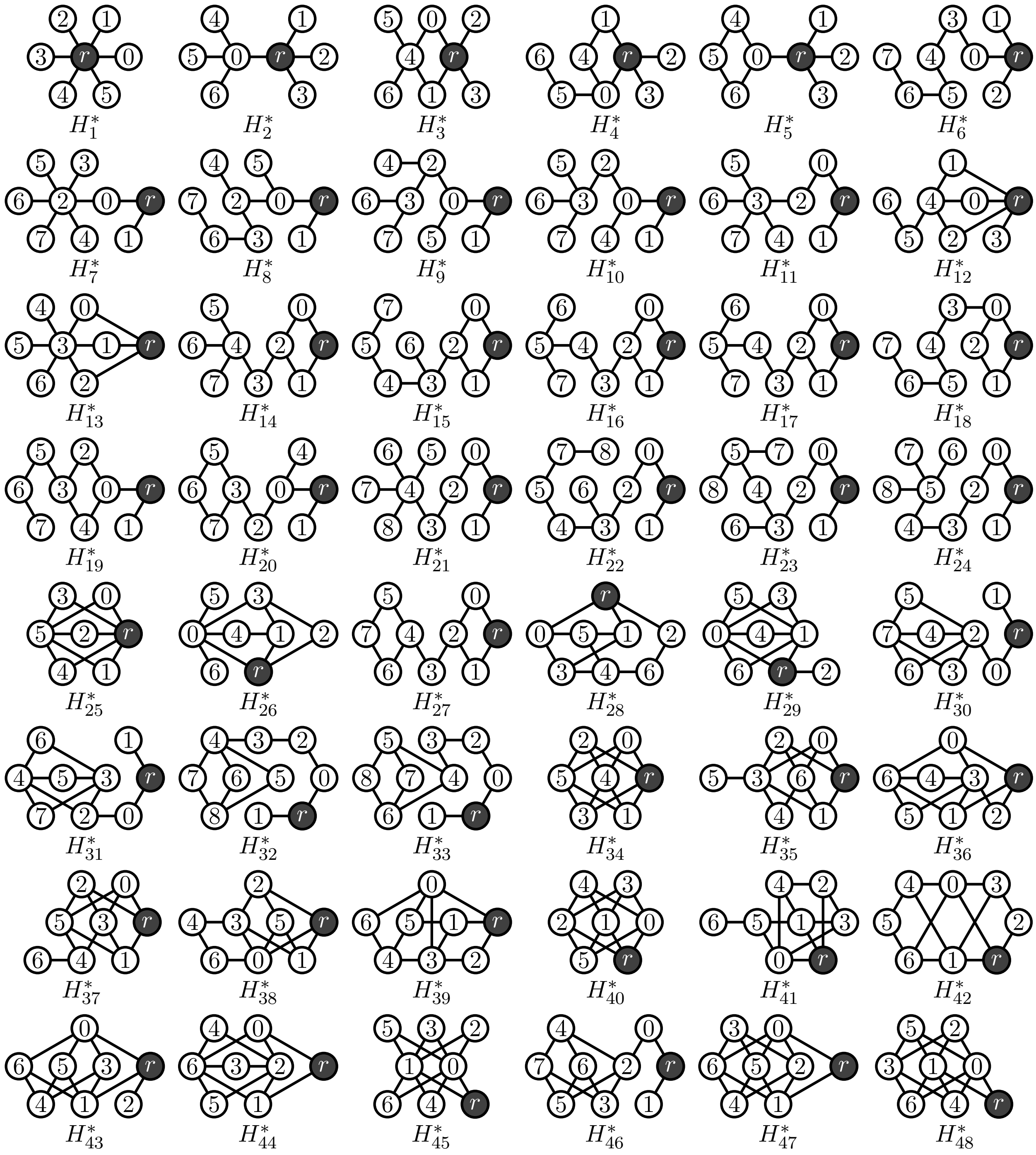

Figure 8: Single-rooted graphs of $\mathcal{H}$ that are maximal under general subgraphs.

(ii) We admit those H'_r with $\lambda_1(L(H'_r), 0,) > -\lambda^*$ to `dict[m+1]` (cf. Sections 5.1 and 5.2).

(iii) We append H_r to `maximal` when no H'_r was admitted to `dict[m+1]`.

For each H_r in `dict`, we output H_r as a string of the form `u[1]u[2]...u[2e-1]u[2e]` which lists the edges `u[1]u[2],...,u[2e-1]u[2e]` of H_r, and we designate `r` to represent the root of H_r in the string. We also output the smallest value of $\ell_0 \in \{0, \dots, 6\}$ such that $\lambda_1(L(H_r), \ell_0,) < -2$ (cf. Section 5.3). Finally, we output the maximal single-rooted graphs stored in `maximal`.

Our code and its output are available as the ancillary files `enum_rooted_graphs.rb` and `enum_rooted_graphs.txt` in the arXiv version of the paper.

For the rest of this section, we share further details of our implementation.

5.1 Positive definiteness of $A_{G'} + \lambda^* I$

Before we admit a single-rooted graph H'_r to `dict[m+1]`, we need to check whether $A_{G'} + \lambda^* I$ is positive definite, where $G' = (L(H'_r), 0,)$. Since H'_r is obtained from H_r in `dict[m]` by adding a new edge, the graph $G := (L(H_r), 0,)$ can be obtained from G' be removing a vertex. Since $A_G + \lambda^* I$ is already positive definite, according to Sylvester's criterion, it suffices to check whether the determinant of $A_{G'} + \lambda^* I$ is positive. To avoid the irrational number λ^*, we use two rational approximations λ^*_- and λ^*_+:

$$2.0198008850 \approx 18259/9040 =: \lambda^*_- < \lambda^* < \lambda^*_+ := 91499/45301 \approx 2.0198008874,$$

One of the following two cases might happen.

Case 1: $\det(A_{G'} + \lambda^*_- I) > 0$. Since $A_G + \lambda^*_- I$ is positive definite, so is $A_{G'} + \lambda^*_- I$ according to Sylvester's criterion. In this case, we can assert that $A_{G'} + \lambda^* I$ is positive definite.

Case 2: $\det(A_{G'} + \lambda^*_+ I) < 0$. Since the matrix $A_{G'} + \lambda^*_+ I$ is not positive definite, we can assert that $A_{G'} + \lambda^* I$ is not positive definite either.

Otherwise, we raise an exception, which never occurs for all graphs encountered throughout the computer search.

5.2 Hash function of single-rooted graphs

When we admit a single-rooted graph H'_s to `dict[m+1]`, we need to check whether it is isomorphic to an existing member of `dict[m+1]`. To efficiently detect isomorphic duplicates, we maintain a hash table `@hash` of existing members of `dict[m+1]` using the following hash function.

For a bipartite single-rooted graph H_r, its hash value is a triple `[dr, dA, dB]`, where `dr` is the degree of r in H, `dA` is the degree sequence of the vertices in the part that contains r, and `dB` is the degree sequence of the vertices in the part that does not contain r. Clearly, when two bipartite single-rooted graphs are isomorphic, their hash values are equal.

This allows us to test isomorphism between H'_s and any existing member of `dict[m+1]` by examining only the members of `@hash[hv]`, where `hv` is the hash value of H'_s.

5.3 Positive semidefiniteness of $A_G + 2I$

When we calculate the smallest ℓ_0, according to Sylvester's criterion, checking whether $A_G + 2I$ is positive semidefinite involves checking whether all principal minors of $A_G + 2I$ are nonnegative. To make this subroutine more efficient, we need the following fact.

Theorem 35 (Theorem 2.5 of Bussemaker and Neumair [2]). *There is no graph whose smallest eigenvalue is in* $(\lambda_1(E_6), -2)$, *where* $\lambda_1(E_6) \approx -2.006594$. □

Corollary 36. *For every graph* G, *the matrix* $A_G + 2I$ *is positive semidefinite if and only if the matrix* $A_G + (305/152)I$ *is positive definite.*

Proof. Since $\lambda_1(E_6) < -305/152 < -2$, the smallest eigenvalue of G is at least -2 if and only if it is more than $-305/152$. □

In our implementation, we assert that $A_G + 2I$ is positive semidefinite if and only if all the *leading* principal minors of $A_G + (305/152)I$ are positive.

6 Enumeration of the maverick graphs

We need the following technical result on the generation of maverick graphs.

Definition 37 (Witness). Given a graph G, a quadruple (u_0, u_1, u_2, u_c) of distinct vertices is a *witness for an augmented path extension* if u_0u_1, u_1u_2 and u_0u_c are the only edges of G that are not in $G - \{u_1, u_2, u_c\}$.

Remark. As the name suggests, a graph G has a witness for an augmented path extension if and only if G is an augmented path extension of a rooted graph.

Lemma 38. *For every maverick graph* M *on* n *vertices, there exists a sequence* $K_2 = G_2, \ldots, G_n = M$ *of connected graphs satisfying the following three properties.*

(i) For every $i \in \{3, \ldots, n\}$, $\lambda_1(G_i) > -\lambda^*$, *and there exists* $v_i \in V(G_i)$ *such that* $G_{i-1} = G_i - v_i$.

(ii) If $n \geq 10$, *then* $\lambda_1(G_{10}) < -2$.

(iii) If $n \geq 11$ *and* G_{10} *has a unique witness for an augmented path extension, then* G_{11} *is not an augmented path extension.*

The proof requires the following fact about graphs with smallest eigenvalue less than -2 that are minimal under subgraphs.

Theorem 39 (Kumar, Rao and Singhi [12]). *Every minimal forbidden subgraph for the family $\mathcal{G}(2)$ of graphs with smallest eigenvalue at least -2 has at most 10 vertices.* $\square$

Proof of Lemma 38. Suppose M is a maverick graph on n vertices. Since M is connected, M is not a null graph, and $\lambda_1(M) > -\lambda^*$, the case where $n \leq 9$ is trivial. Hereafter, we may assume that $n \geq 10$. Theorem 39 provides a connected subgraph G_{10} of M on 10 vertices such that $\lambda_1(G_{10}) < -2$. We can then easily build the other connected graphs in the sequence using G_{10}.

In the case where $n \geq 11$ and G_{10} has a unique witness, say (u_0, u_1, u_2, u_c), of an augmented path extension, since M is not an augmented path extension, there exists a vertex $v_{11} \in V(M) \setminus V(G_{10})$ that is adjacent to at least of one of u_1, u_2 and u_c in M. We can specifically choose $G_{11} = M[V(G_{10}) \cup \{v_{11}\}]$. Assume for the sake of contradiction that G_{11} to have a witness (u_0', u_1', u_2', u_c'). It must be the case that $u_0' = u_0$, $u_1' = u_c$, $u_2' = v_{11}$, $u_c' \notin \{u_0, u_1, u_2, u_c\}$, and u_0u_1, u_1u_2, u_0u_c, u_cv_{11} and u_0u_c' are the only edges of G that are not in $G - \{u_1, u_2, u_c, u_c'\}$. Thus G_{10} has another witness (u_0, u_1, u_2, u_c'), which contradicts the uniqueness of the witness (u_0, u_1, u_2, u_c) for G_{10}. $\square$

The enumeration of all maverick graphs is achieved by a computer search.

Proof of Theorem 8. To enumerate the maverick graphs, we store the graphs that can possibly occur in a sequence described by Lemma 38 in the hash `dict` based on their order. At the start, `dict[2]` consists of a single graph K_2 and `n` increases from `2`.

Whenever `dict[n]` is nonempty, we iterate through members of `dict[n]`. For each G in `dict[n]`, we carry out the following five steps.

(i) We connect a new vertex to a nonempty vertex subset S of G in every possible way to obtain new graphs $G' = (G_S, 0)$. See Section 6.1 for a more efficient implementation.

(ii) We store those G' with $\lambda_1(G') > -\lambda^*$ in a temporary array `candidates`.

(iii) In view of Lemma 38(ii), when `n = 9`, we remove G' from `candidates` when $\lambda_1(G') < -2$.

(iv) In view of Lemma 38(iii), when `n = 10`, we remove G' from `candidates` when G has a unique witness for an augmented path extension, and G' is an augmented path extension (cf. Section 6.2).

(v) We merge `candidates` into `dict[n+1]` (cf. Section 6.3).

We append the maverick graphs among the members in `dict[n]` to the array `mavericks`. To select the maverick graphs, we reject members of `dict[n]` with smallest eigenvalue at least -2 when `n = 2,...,9`, and we always reject augmented path extensions in `dict[n]`.

Our program terminates at `n = 20` because `dict[20]` is empty. Our code and its output are available as the ancillary files `enum_maverick_graphs.rb` and `enum_maverick_graphs.txt` in the arXiv version of the paper.

Remark. On a MacBook Pro equipped with an Apple M1 Pro chip and 16 GB of memory, the program initially completed its task in under 25 minutes. With the assistance of ChatGPT 4.0, we rewrote the code in Julia, a dynamically typed programming language designed for high performance, enabling it to finish in under 8 minutes on the same machine. The code is available as `enum_maverick_graphs.jl` in the arXiv version of the paper.

We reuse the techniques discussed in Sections 5.1 and 5.3 to check positive definiteness and positive semidefiniteness of matrices. We share additional details of our implementation below.

6.1 Adding a new vertex

To accelerate the generation of graphs, we capitalize on the computation done for G in `dict[n]` based on the following observation. Suppose that G is a graph such that $\lambda_1(G) > -\lambda^*$. Let $\mathcal{S} = \{S \subseteq V(G) \colon \lambda_1(G_S, 0) > -\lambda^*\}$. For every $S \in \mathcal{S}$, and every $U \subseteq V(G')$, where $G' = (G_S, 0)$, note that $\lambda_1(G'_U, 0) > -\lambda^*$ implies that $\lambda_1(G_{U \cap V(G)}, 0) > -\lambda^*$, which is equivalent to $U \cap V(G) \in \mathcal{S}$. In other words, when we connect a new vertex to a nonempty subset U of $G' = (G_S, 0)$ with $S \in \mathcal{S}$, we only need to iterate through U with $U \cap V(G) \in \mathcal{S}$.

To keep track of the set $\mathcal{S}$ defined for G, we add an attribute `@possible_subets`, a list of distinct nonempty vertex subsets of G, to each graph G. For the graph K_2 in `dict[2]`, its `@possible_subsets` consists of all the nonempty vertex subsets of K_2. For each G in `dict[n]`, instead of connecting a new vertex, say v', to a nonempty vertex subset S of G in every possible way, we connect v' to S for every S in `@possible_subsets` of G. To obtain `@possible_subsets` of the graphs obtained from G, we initially set `new_possible_subsets` to be the list with a single vertex subset $\{v'\}$. For each S in `@possible_subsets` of G, check whether $\lambda_1(G_S, 0) > -\lambda^*$, and if so, we append both S and $S \cup \{v'\}$ to `new_possible_subsets`, and we append $(G_S, 0)$ to `candidates`. Finally, we set `@possible_subsets` of each graph G' in `candidates` as `new_possible_subsets`.

6.2 Finding witnesses

Given a graph G, to find its witnesses for an augmented path extension, we iterate through all edges u_1u_2 of G with $d(u_1) = 2$ and $d(u_2) = 1$, check whether the vertex u_0, that is, the other neighbor of u_1, is adjacent to a leaf u_c, and we output all quadruples (u_0, u_1, u_2, u_c).

6.3 Hash function of graphs and generalized degrees

When we add a graph G in `candidates` to `dict[n+1]`, we need to check whether it is isomorphic to an existing member of `dict[n+1]`. To that end, we maintain a hash table `@hash` of existing

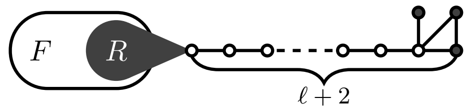

Figure 9: The twisted path extension $(F_R, \ell,)$.

members of `dict[n+1]` using the following hash function.

For a vertex v of a graph G, the *generalized degree* of v in G is the pair `[dv, dw]`, where `dv` is the degree of v in G, and `dw` is the size of the neighborhood of v (that is, the subgraph of G induced by all vertices adjacent to v). The hash value of a graph G is then the sorted sequence of generalized degrees. Clearly, when two graphs are isomorphic, their hash values are equal, and moreover, the generalized degree of a vertex is preserved under isomorphism.

This allows us to test isomorphism between G and any existing member of `dict[n+1]` by examining only the members of `@hash[hv]`, where `hv` is the hash value of G. In addition, when we attempt to build an isomorphism between G and a member G' of `@hash[hv]`, we only map a vertex of G to a vertex of G' that has the same generalized degree.

7 Twisted maverick graphs

A visual examination of the maverick graphs reveals that a notable portion of them look alike.

Definition 40 (Twisted path extension and twisted maverick graph)**.** Given a rooted graph F_R and $\ell \in \mathbb{N}$, the *twisted path extension* of the rooted graph F_R is the path augmentation $(F_R, \ell,)$. See Figure 9 for a schematic drawing. Given a graph G, a quadruple (u_0, u_1, u_2, u_c) of distinct vertices is a *witness for a twisted path extension* if u_0u_1, u_0u_2, u_1u_2 and u_0u_c are the only edges of G that are not in $G - \{u_1, u_2, u_c\}$. A maverick graph is *twisted* if it is a twisted path extension of a rooted graph.

A direct computer screening of the maverick graphs produced in Section 6 reveals that roughly a quarter of them are twisted.

Theorem 41. *There are a total of 1161 twisted maverick graphs with the following statistics.*

order	*10*	*11*	*12*	*13*	*14*	*15*	*16*	*17*	*18*	*19*
#	*48*	*133*	*220*	*236*	*210*	*162*	*96*	*40*	*13*	*3*

Proof. For each maverick graph, we find its witnesses for a twisted path extension as follows: we iterate through all edges u_1u_2 of G with $d(u_1) = d(u_2) = 2$, check whether u_1 and u_2 shares a common neighbor, if so, check whether the common neighbor, say u_0, is adjacent to a leaf u_c, and output all quadruples (u_0, u_1, u_2, u_c). Once a witness is found for a maverick graph, we assert that it is twisted. As it turns out, every maverick graph that is twisted has a unique witness. Our code and its output are available as the ancillary files `enum_twisted_mavericks.rb` and `enum_twisted_mavericks.txt` in the arXiv version of the paper.

For the proof of Corollary 9, we need the following connection between twisted path extensions and augmented path extensions.

Proposition 42. *For every rooted graph F_R and $\ell \in \mathbb{N}$, if $\lambda_1(F_R, \ell, \therefore) \leq -2$, then $\lambda_1(F_R, \ell, \therefore) \leq \lambda_1(F_R, \ell, \because)$.*

Proof. Let $\lambda > 1$ to be chosen later, and let v_0 be the vertex in $V(F_R, \ell) \setminus V(F_R, \ell - 1)$. In the case where $\ell = 0$, instead let v_0 be the vertex in $V(F_R, \ell) \setminus V(F_R)$. Denote by E_{v_0,v_0} the unit matrix where the (v_0, v_0)-entry with value 1 is the only nonzero entry.

We claim that $\lambda_1(F_R, \ell, \therefore) \geq -\lambda$ if and only if

$$A_{(F_R,\ell)} + \lambda I - \left(\frac{2\lambda - 2}{\lambda^2 - 1} + \frac{1}{\lambda}\right) E_{v_0,v_0} \tag{2}$$

is positive semidefinite. Indeed, we partition the matrix $A_{(F_R,\ell,\therefore)} + \lambda I$ into blocks:

$$\begin{pmatrix} A_{(F_R,\ell)} & B \\ B^\intercal & C \end{pmatrix}$$

Since $C = A_{\circ\circ} + \lambda I$ and $\lambda > 1$, the block C is positive definite. Therefore, the Schur complement $A_{(F_R,\ell)} + \lambda I - BC^{-1}B^\intercal$ of C is positive semidefinite. Since the only nonzero row of B is its v_0-th row, say B_{v_0}, the matrix $BC^{-1}B^\intercal$ simplifies to $B_{v_0}C^{-1}B_{v_0}^\intercal E_{v_0,v_0}$. We then compute directly:

$$B_{v_0}C^{-1}B_{v_0}^\intercal = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}^\intercal \begin{pmatrix} \lambda & 1 & \\ 1 & \lambda & \\ & & \lambda \end{pmatrix}^{-1} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \frac{2\lambda - 2}{\lambda^2 - 1} + \frac{1}{\lambda}.$$

Similarly, we can prove that $\lambda_1(F_R, \ell, \because) \geq -\lambda$ if and only if

$$A_{(F_R,\ell)} + \lambda I - \left(\frac{\lambda}{\lambda^2 - 1} + \frac{1}{\lambda}\right) E_{v_0,v_0} \tag{3}$$

is positive semidefinite. Finally, take $\lambda = -\lambda_1(F_R, \ell, \therefore) \geq 2$, and observe that the matrix in (3) minus the matrix in (2) is equal to the matrix $(\lambda - 2)/(\lambda^2 - 1)E_{v_0,v_0}$, which is positive semidefinite. $\square$

Proof of Corollary 9. Suppose that G is a connected graph on at least 18 vertices such that $\lambda_1(G) \in (-\lambda^*, -2)$. In view of Theorems 8 and 41, G is either an augmented path extension or a twisted maverick graph. We break the rest of the proof into two cases.

Case 1: G is an augmented path extension. In view of Lemmas 6 and 31, there exists a connected bipartite single-rooted graph H_r and $\ell \in \mathbb{N}$ such that G is $(L(H_r), \ell, \because)$. Let (u_0, u_1, u_2, u_c) be the witness for the augmented path extension. Clearly u_c is a leaf of G, and $G - u_c$ is the path extension $(L(H_r), \ell + 2)$, which is the line graph of the bipartite graph $(H_r, \ell + 3)$. We are left to prove the

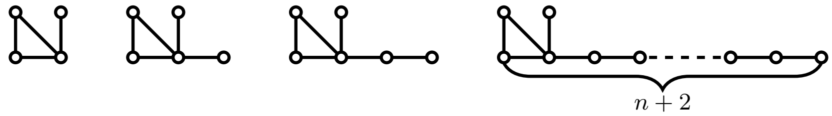

Figure 10: E'_0, E'_1, E'_2 and E'_n.

uniqueness of such a leaf. We claim that there exists a neighbor of u_0 in $G - \{u_1, u_2, u_c\}$, that is not a leaf of G. Assume for the sake of contradiction that every neighbor of u_0 in $G - \{u_1, u_2, u_c\}$ is a leaf of G. In this case, $\ell = 0$ and F_R is a null graph with more than one vertex, which contradicts with the connectedness of H_r. Let u_{-1} be such a neighbor of u_0. Then $\{u_{-1}, u_0, u_1, u_c\}$ induces a star S_3 with 3 leaves in G. Since a line graph cannot contain S_3 as a subgraph, and u_c is the only leaf of G in $\{u_{-1}, u_0, u_1, u_c\}$, we have to remove u_c from G to obtain a line graph.

Case 2: G is a twisted maverick graph $(F_R, \ell,)$. In view of Proposition 42, $\lambda_1(F_R, \ell,) > -\lambda^*$. By Lemmas 6 and 31, there exists a connected bipartite single-rooted graph H_r such that F_R is $L(H_r)$. Let (u_0, u_1, u_2, u_c) be the witness for the twisted path extension. Clearly u_c is a leaf of G, and $G - u_c$ is the graph $(L(H_r), \ell,)$, which is the line graph of the bipartite graph $(H_r, \ell + 1,)$ The proof for the uniqueness of such a leaf follows exactly that of the previous case. ☐

Remark. The order 18 in Corollary 9 is the smallest possible because of the two maverick graphs of order 17 that are not twisted — each has a unique leaf, and its removal results in a graph that contains the star S_3 as a subgraph.

8 Beyond the classification theorem of $\mathcal{G}(\lambda^*) \setminus \mathcal{G}(2)$

In this section, we explore graphs whose smallest eigenvalues are slightly below $-\lambda^*$. To see why Theorem 3 generalizes beyond $-\lambda^*$, notice that in the process of deriving Theorem 3 in Section 2, the constant λ^* plays an essential role only in Lemma 21. In [10, Appendix A], Jiang and Polyanskii already noted that $\lambda^* \approx 2.01980$ can be replaced with $101/50 = 2.02$ in Lemma 21. To obtain the best constant, we define the following graphs, and compute the limit of their smallest eigenvalues.

Proposition 43. *For every $n \in \mathbb{N}$, define the graph E'_n as the path extension $(, n)$ in Figure 10. The smallest eigenvalue of E'_n decreases to $-\lambda'$, where*

$$\lambda' := \gamma + 1/\gamma \approx 2.02124$$

and γ is the unique positive root of $x^4 + x^3 = x^2 + 2$.

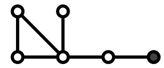

Figure 11: The rooted graph E_2'.

Proof. Using Lemma 26, we know that the matrix

$$\begin{pmatrix} r & 1 & 1 & 1 \\ 1 & x & 1 & 0 \\ 1 & 1 & x & 0 \\ 1 & 0 & 0 & x \end{pmatrix}$$

is singular when $x = \lambda'$, where $r = x/2 + \sqrt{x^2/4 - 1}$. Substituting x by $r + 1/r$, the determinant of the above matrix is equal to $r^4 - r^2 + 2r + 2/r - 2/r^2 - 3$, which factors into $(r^4 + r^3 - r^2 - 2)(r^2 - r + 1)/r^2$. Since γ is the unique positive root of $r^4 + r^3 - r^2 - 2$, and no root of $r^2 - r + 1$ is real, it must be the case that $\lambda' = \gamma + 1/\gamma$. $\square$

Besides E_2, the graph E_2' is also one of the 31 minimal forbidden subgraphs for the family $\mathcal{D}_\infty$ of generalized line graphs. As it turns out, E_2' is the bottleneck case in Lemma 21.

Proposition 44. *For every minimal forbidden subgraph F for the family $\mathcal{D}_\infty$ of generalized line graphs, if F is not isomorphic to E_2, and F_R is not the rooted graph E_2' in Figure 11, then* $\lim_{\ell\to\infty} \lambda_1(F_R, \ell) < -95/47$ *for every nonempty vertex subset R of F.*

We postpone the computer-assisted proof of Proposition 44 to Appendix A. Now we prove Theorem 10 for every $\lambda \in (\lambda^*, \lambda')$.

Proof of Theorem 10. Pick an arbitrary $\lambda \in (\lambda^*, \lambda')$. Since $\lambda' \approx 2.02124 < 2.02127 \approx 95/47$, in view of Proposition 44, we can replace the constant λ^* in Lemma 21 with λ. The rest of the proof follows exactly that of Theorem 3 on Page 8. $\square$

Remark. For $n \geq 6$, the graph E_n' is in $\mathcal{G}(\lambda') \setminus \mathcal{G}(2)$. Since it is not an augmented path extension, Theorem 10 no longer holds for $\lambda \geq \lambda'$.

To show that it is impossible to generalize Theorem 5, we need the following result on the set of smallest graph eigenvalues.

Theorem 45 (Theorem 2.19 of Jiang and Polyanskii [10])**.** *For every $\lambda > \lambda^*$, there exist graphs $G_1, G_2, \ldots$ such that* $\lim_{n\to\infty} \lambda_1(G_n) = -\lambda$. $\square$

Proof of Theorem 11. Fix $\lambda > \lambda^*$. Assume for the sake of contradiction that there exists a finite family $\mathcal{F}$ of rooted graphs and $N \in \mathbb{N}$ such that every graph G on more than N vertices, if $\lambda_1(G) \in (-\lambda, -\lambda^*)$, then G is isomorphic to an augmented path extension of a rooted graph in $\mathcal{F}$. By Lemma 25, for each rooted graph $F_R \in \mathcal{F}$, we can set $a(F_R) := \lim_{\ell\to\infty} \lambda_1(F_R, \ell,)$. We can then pick an open interval $I \subset (-\lambda, -\lambda^*)$ that avoids the finite set $\{a(F_R) \colon F_R \in \mathcal{F}\}$. Note that only finitely many graphs have their smallest eigenvalues in I, which contradicts with Theorem 45. $\square$

9 Concluding remarks

Since Theorem 10 holds for every $\lambda \in (\lambda^*, \lambda')$, we ask the following natural question.

Problem 46. *Classify all the connected graphs with smallest eigenvalue in* $(-\lambda', -\lambda^*)$. *In particular, classify such graphs on sufficiently many vertices.*

To conclude the paper, we reiterate a similar problem raised in [10] on *signed graphs*, which are graphs whose edges are each labeled by $+$ or $-$. When we talk about eigenvalues of a signed graph $G^{\pm}$ on n vertices, we refer to its *signed adjacency matrix* — the $n \times n$ matrix whose (i, j)-th entry is 1 if ij is a positive edge, -1 if ij is a negative edge, and 0 otherwise.

Problem 47. *Classify all the connected signed graphs with smallest eigenvalue in* $(-\lambda^*, -2)$. *In particular, classify such signed graphs on sufficiently many vertices.*

Understanding such signed graphs, and extending their classification beyond $-\lambda^*$ would offer insights into spherical two-distance sets. We refer the reader to [10, Section 5] for the relevant discussion.

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A Computer-assisted proofs

Proof of Propositions 22 and 44. For the exceptional case in Proposition 44 where F_R is the rooted graph in Figure 11, the path extension (F_R, ℓ) is just $E'_{\ell+3}$, whose smallest eigenvalue approaches $-\lambda'$ as $\ell \to \infty$ according to Proposition 43. We strengthen the other inequalities in Proposition 44 by replacing λ' with $95/47$.

In view of Lemma 26, for each rooted graph F_R considered in Propositions 22 and 44, to show $\lim_{\ell\to\infty} \lambda_1(F_R, \ell) < -95/47$, we only need to show that

$$A_{(F_R,0)} + (95/47)I - (95/94 - 3\sqrt{21}/94)E_{v_0,v_0}$$

is not positive semidefinite, where v_0 is the vertex in $V(F_R, 0)\setminus V(F)$. Since $95/94-3\sqrt{21}/94 > 6/7$, to show that the above matrix is not positive semidefinite, it suffices to show the matrix

$$A_{(F_R,0)} + (95/47)I - (6/7)E_{v_0,v_0} \tag{4}$$

with rational entries is not positive semidefinite.

Our implementation is straightforward. We iterate through the 7-vertex graphs labeled by `A1,...,A39` and the 8-vertex graphs labeled by `B1,...,B4` in Proposition 22, and the minimal forbidden subgraphs, labeled by `G1,...,G31`, for the family $\mathcal{D}_\infty$ in Proposition 44. For each graph F, we check whether $A_F + (95/47)I$, a principal submatrix of the matrix in (4), is positive semidefinite. Since 95/47, which is not an algebraic integer, cannot be a graph eigenvalue, we instead check whether $A_F + (95/47)I$ is positive definite. If so, we output the nonempty vertex subsets R of F, for which the determinant of the matrix in (4) is nonnegative.

In the output, either F is isomorphic to E_3 or E_2, or F_R is the exceptional rooted graph in Figure 11. Therefore the output of our program serves as the proof of the strict inequalities in Propositions 22 and 44.

Our code is available as the ancillary file `path_extension.rb` in the arXiv version of this paper. We provide the input as `path_extension.txt` for the convenience of anyone who wants to program independently. In the input, each line contains the label of the graph and the string of the form `u[1]u[2]...u[2e-1]u[2e]`, which lists the edges `u[1]u[2],...,u[2e-1]u[2e]` of the graph. The first line represents the graph E_2, the next 4 lines represent $B_1,\dots,B_4$ in Figure 4, and the rest lines represent the 31 minimal forbidden subgraphs for $\mathcal{D}_\infty$.