Forbidden subgraphs for graphs of bounded spectral radius, with applications to equiangular lines

Zilin Jiang∗†, Alexandr Polyanskii∗‡

Abstract

The spectral radius of a graph is the largest eigenvalue of its adjacency matrix. Let \( F(\lambda) \) be the family of connected graphs of spectral radius \( \leq \lambda \). We show that \( F(\lambda) \) can be defined by a finite set of forbidden subgraphs for every \( \lambda < \lambda^* := \sqrt{2 + \sqrt{5}} \approx 2.058 \), whereas \( F(\lambda) \) cannot for every \( \lambda \geq \lambda^* \). The study of forbidden subgraphs characterization for \( F(\lambda) \) is motivated by the problem of estimating the maximum cardinality of equiangular lines in the \( n \)-dimensional Euclidean space \( \mathbb{R}^n \) — a family of lines through the origin such that the angle between any pair of them is the same. Denote by \( N_\alpha(n) \) the maximum number of equiangular lines in \( \mathbb{R}^n \) with angle \( \arccos \alpha \). We establish an approach to determine the constant \( c_\alpha \) in \( N_\alpha(n) = c_\alpha n + O_\alpha(1) \) for every \( \alpha > \frac{1}{1 + 2\sqrt{2}} \).

Besides we prove that for every graph \( G \) of average degree \( d \geq 2 \), there exists a vertex \( v_0 \) of \( G \) such that \( \lambda_1(H) \geq 2 \cos\left(\frac{\pi}{k+2}\right)\sqrt{d - 1} \), where \( H \) is the subgraph consisting of all vertices within distance \( k \) of \( v_0 \). Combining this with the proof strategy used to pin down the constant \( c_\alpha \), we show that \( N_\alpha(n) \leq 1.49n + O_\alpha(1) \) for every \( \alpha \neq \frac{1}{3}, \frac{1}{5}, \frac{1}{1 + 2\sqrt{2}} \), which improves a recent result of Balla, Dräxler, Keevash and Sudakov.

1 Introduction

The spectral radius of a graph \( G \), denoted by \( \lambda_1(G) \), is the largest eigenvalue of its adjacency matrix. Let \( F(\lambda) \) be the family of connected graphs of spectral radius \( \leq \lambda \). It is well known that \( \lambda_1 \) is monotone in the sense that \( \lambda_1(G_1) \leq \lambda_1(G_2) \) if \( G_1 \) is a subgraph of \( G_2 \), moreover \( \lambda_1(G_1) < \lambda_1(G_2) \) if \( G_1 \) is a proper subgraph of a connected graph \( G_2 \). This implies that \( F(\lambda) \) is closed under taking subgraphs. It is natural to ask if \( F(\lambda) \) can be defined by a finite set of forbidden subgraphs. We determine the threshold \( \lambda^* \) below which the answer is yes.

∗Department of Mathematics, the Technion – Israel Institute of Technology, Technion City, Haifa 32000.
†Email: jiangzilin@technion.ac.il. Supported in part by ISF grant nos 1162/15, 936/16.
‡Moscow Institute of Physics and Technology and Institute for Information Transmission Problems RAS. Email: alexander.polyanskii@yandex.ru. Supported in part by ISF grant no. 409/16, and by the Russian Foundation for Basic Research through grant nos 15-01-99563 A, 15-01-03530 A.
Theorem 1. For every $\lambda < \lambda^* := \sqrt{2 + \sqrt{5}}$, there exist finitely many graphs $G_1, G_2, \ldots, G_n$ such that $F(\lambda)$ consists exactly of the connected graphs which do not contain any of $G_1, G_2, \ldots, G_n$ as a subgraph. However, the same conclusion does not hold for every $\lambda \geq \lambda^*$.

The motivation to understand the forbidden subgraphs characterization for $F(\lambda)$ comes from the problem of estimating the maximum cardinality $N(n)$ of equiangular lines in the $n$-dimensional Euclidean space $\mathbb{R}^n$ — a family of lines through the origin such that the angle between any pair of them is the same. It is considered to be one of the founding problems of algebraic graph theory to determine $N(n)$. The “absolute bound” $N(n) \leq \binom{n+1}{2}$ was established by Gerzon (see [LS73 Theorem 3.5]). A remarkable construction of de Caen [dC00] shows that $N(n)$ equals $\frac{2}{9}(n+1)^2$ for $n$ of the form $n = 6 \cdot 4^k - 1$ (see [GY16] for a generalization and [JW15] for an alternative constructions). In these constructions, the common angle tends to $\pi/2$ as dimension grows.

The question of determining the maximum number $N_\alpha(n)$ of equiangular lines in $\mathbb{R}^n$ with common angle $\arccos \alpha$ was first raised by Lemmens and Seidel [LS73] in 1973, who showed that $N_{1/3}(n) = 2n - 2$ for $n \geq 15$ and also conjectured that $N_{1/5}(n)$ equals $\lfloor 3(n-1)/2 \rfloor$ for sufficiently large $n$. This was later confirmed by Neumaier [Neu89] (see also [GKMS16]). Besides, the “relative bound” $N_\alpha(n) \leq \frac{1}{\lambda^2} n$ is only valid in small dimensions $n < 1/\alpha^2$ (see [vLS66] Lemma 6.1 and [LS73 Theorem 3.6]).

A general bound due to Neumann [LS73] Theorem 3.4 states that $N_\alpha(n) \leq 2n$ unless $1/\alpha$ is an odd integer. For many years, a linear upper bound for $N_\alpha(n)$ was not known when $1/\alpha$ is an odd integer bigger than $5$. An important progress was recently made by Bukh [Buk16], who proved that $N_\alpha(n) \leq c_\alpha n$ for some $c_\alpha = 2^{O(1/\alpha^2)}$. Subsequently, Balla, Dräxler, Keevash and Sudakov [BDKS17] drastically improved the upper bound to $N_\alpha(n) \leq 1.93n$ for sufficiently large $n$ relative to $\alpha$ whenever $\alpha \neq \frac{1}{3}$. A universal upper bound $N_\alpha(n) \leq (2/3\alpha^2 + 4/7)n + 2$ for all $n \in \mathbb{N}$ when $1/\alpha$ is an odd integer was later found by Glazyrin and Yu [GY16].

We combine Theorem 1 and the framework developed in [BDKS17] to establish a result of the form $N_\alpha(n) = c_\alpha n + O(1)$ for all $\alpha > \alpha_* := \frac{1}{1+2\sqrt{5}}$.

Theorem 2. Suppose $\alpha > \alpha_* := \frac{1}{1+2\sqrt{2+\sqrt{5}}}$. The maximum number $N_\alpha(n)$ of equiangular lines in $\mathbb{R}^n$ with angle $\arccos \alpha$ equals $\frac{k}{k-1} : n + O(1)$, where $k_\alpha$ is the smallest $k$ such that $\frac{2}{k} \alpha$ is the spectral radius of a graph on $k$ vertices. If $k_\alpha = \infty$, then $N_\alpha(n) = n + O(1)$.

Remark 1. Throughout, as all the big-O notations depend on $\alpha$, we suppress the subscript in $O_\alpha(\cdot)$.

Applying the above theorem to the connected graphs with $\leq 3$ vertices,

![Graph with 3 vertices](https://example.com/graph.png)

whose spectral radii are $1, \sqrt{2}$ and $2$ respectively, we obtain the old results $N_{1/3}(n) = 2n + O(1)$, $N_{1/5}(n) = \frac{3}{2}n + O(1)$ and surprisingly a new result $N_{1/(1+2\sqrt{5})}(n) = \frac{3}{2}n + O(1)$. This refutes the
second part of Conjecture 6.1 in [BDKS17]. The first part of the conjecture, which was also raised by Bukh [Buk16, Conjecture 8], says the following.

**Conjecture A.** The maximum number of equiangular lines in \( \mathbb{R}^n \) with angle \( \arccos \alpha \) equals \( \frac{1}{\frac{n}{\alpha}+1} \cdot n + O(1) \) if \( 1/\alpha \) is an odd natural number.

One can check that \( k_\alpha = (1/\alpha + 1)/2 \) if \( 1/\alpha \) is an odd natural number. Theorem [2] motivates the following stronger conjecture.

**Conjecture B.** The maximum number \( N_\alpha(n) \) of equiangular lines in \( \mathbb{R}^n \) with angle \( \arccos \alpha \) equals \( \frac{k_\alpha}{k_\alpha-1} \cdot n + O(1) \), where \( k_\alpha \) is defined as in Theorem [2]. If \( k_\alpha = \infty \), then \( N_\alpha(n) = n + O(1) \).

One of the unknown cases that are not addressed by Theorem 2 is \( \alpha = 1/7 \). Conjecture A asserts that \( N_{1/7}(n) = \frac{4}{3}n + O(1) \). For such cases, we develop the following spectral result.

**Lemma 3.** Let \( G \) be a graph with average degree \( d \geq 2 \). There exists a vertex \( v_0 \) of \( G \) such that \( \lambda_1(H) \geq 2 \cos(\frac{\pi}{k+1})\sqrt{d-1} \), where \( H \) is the subgraph consisting of all vertices within distance \( k \) of \( v_0 \).

Combining Lemma 3 with the proof strategy for Theorem 2 we derive an upper bound of \( N_\alpha(n) \).

The rest of the paper is organized as follows. In Section 2 we prove Theorem 1. In Section 3.1 we review the framework developed by Balla et al.. In Section 3.2 we apply Theorem 1 to estimate \( N_\alpha(n) \) for \( \alpha > \alpha_* \), and in Section 3.3 we extrapolate our method to obtain an upper bound on \( N_\alpha(n) \) for \( \alpha \leq \alpha_* \). In the concluding section we discuss evidences supporting Conjecture A and a possible extension of our method.

## 2 Forbidden subgraphs of \( \mathcal{F}(\lambda) \)

Suppose there is a finite forbidden subgraphs characterization, say \( G_1, G_2, \ldots, G_n \) for \( \mathcal{F}(\lambda) \). By the monotonicity of spectral radius, we know that no graph has spectral radius in \( (\lambda, \min \{ \lambda_i(G_i) : i \in [n] \}) \). Let \( \Lambda_1 \) consist of the spectral radius of all graphs or all orders, and denote by \( \lim \Lambda_1 \) the set of limit points of \( \Lambda_1 \) and \( \lim_+ \Lambda_1 := \{ \lambda \in \mathbb{R} : (\lambda, \lambda + \varepsilon) \cap \Lambda_1 \neq \emptyset \text{ for all } \varepsilon > 0 \} \) the set of right-sided limit points of \( \Lambda_1 \). The contrapositive of the above observation says that \( \mathcal{F}(\lambda) \) does not have a finite forbidden subgraphs characterization for all \( \lambda \in \lim_+ \Lambda_1 \).

Hoffman was interested in a related set \( R \) consisting of the spectral radius of all symmetric matrices of all orders with non-negative integer entries, and he proved the following theorem on \( \lim R \).

**Theorem 4** (Hoffman [Hof72]). For \( n = 1, 2, \ldots, \) let \( \beta_n \) be the positive root of

\[
x^{n+1} = 1 + x + \cdots + x^{n-1}.
\]

Let \( \alpha_n = \beta_n^{1/2} + \beta_n^{-1/2} \). Then \( 2 = \alpha_1 < \alpha_2 < \cdots \) are all limit points of \( R \) smaller than \( \lim_n \alpha_n = \lambda^* \).
In fact, Hoffman proved the above theorem by first showing [Hof72, Proposition 2.1] that $\Lambda_1 = R$. He also computed the limit of spectral radii of several families of graphs. We compile some of his computation and other relevant results in the following lemma, the proof of which is presented in Appendix A. We use the notation $\alpha_n \nearrow \alpha$ if $\alpha_1 < \alpha_2 < \ldots$ and $\lim_n \alpha_n = \alpha$, and $\alpha_n \searrow \alpha$ if $\alpha_1 > \alpha_2 > \ldots$ and $\lim_n \alpha_n = \alpha$.

**Lemma 5.** Let $\alpha_n$ be defined as in Theorem 4. Denote by $C_n$ the cycle with $n$ vertices, $P_n$ the path with $n$ vertices and $S_n$ the star with $n$ leaves. Define $A_n, B_{m,n}, D_n, E_{m,n}, F_n$ as below. (a) $\lambda_1(A_n) \nearrow 3/\sqrt{2}$, (b) $\lambda_1(B_{m,n}) \searrow \alpha_n$ for fixed $n$, (c) $\lambda_1(C_n) = 2$, (d) $\lambda_1(D_n) \searrow \lambda^*$, (e) $\lambda_1(E_{m,n}) \nearrow \alpha_m$ for fixed $m$, (f) $\lambda_1(F_n) \nearrow \lambda^*$, (p) $\lambda_1(P_n) = 2 \cos(\frac{2}{m+1}) > 2$, (s) $\lambda_1(S_n) = \sqrt{n}$.

The work of finding all the limit points of $\Lambda_1$ was completed by Shearer.

**Theorem 6** (Shearer [She89]). For any $\lambda \geq \lambda^*$, there exists a sequence of distinct graphs $G_1, G_2, \ldots$ such that $\lim \lambda_1(G_i) = \lambda$.

Note that Theorem 6 implies that $\lim \Lambda_1 \supset [\lambda^*, \infty)$. Thus by the observation at the beginning of the section, the second half of Theorem 1 is proved.

**Proof of the first half of Theorem 1.** We break the proof into two cases.

**Case 1:** $\lambda < 2$. Note that $S_4 \notin F(\lambda)$ and $P_n \notin F(\lambda)$ for some $n$. Clearly, a connected graph $G$ that contains neither $S_4$ nor $P_n$ has at most $4^n$ vertices. Therefore

$$\{S_4, P_n\} \cup \{\text{connected graph } G \notin F(\lambda) \text{ with } \leq 4^n \text{ vertices} \}$$

is a finite forbidden subgraphs characterization for $F(\lambda)$.

**Case 2:** $2 \leq \lambda < \lambda^*$. Choose $m \geq 2$ such that $\alpha_{m-1} \leq \lambda < \alpha_m$, where $\alpha_m$ is as defined in Theorem 4. Then choose $n$ such that $A_n, E_{m,n}, F_n \notin F(\lambda)$. Note that $S_5 \notin F(\lambda)$, $B_{1,m}, B_{2,m}, \ldots, B_{m,m} \notin F(\lambda)$ and $D_2, D_3, \ldots, D_{m+n} \notin F(\lambda)$. We claim that if a connected graph $G$ contains none of

$$\mathcal{G}_0 := \{S_5, A_n, B_{1,n}, B_{2,n}, \ldots, B_{m,n}, D_2, D_3, \ldots, D_{m+n}, E_{m,n}, F_n\},$$

then $G$ is a path, a cycle, $E_{i,j}$ for some $i < m$, or its number of vertices is bounded by a constant, say $b$, which will be determined by the argument below. In fact, because $G$ does not contain

\footnote{It was asserted that $\lambda_1(A_n) \nearrow 4/\sqrt{3}$ in [Hof72]. This is a mistake but it will not affect the main result of [Hof72] as long as the limit is $> \lambda^*$.}
is a finite forbidden subgraphs characterization for $G$ does not contain $D_2, D_3, \ldots$, and so $G$ must be a tree or a cycle. We may assume that $G$ is a tree but not a path. As $G$ does not contain $S_5$, $G$ is a tree of maximum degree $\leq 4$. If the maximum degree is indeed 4, then $G$ would contain $A_n$ when $G$ has sufficiently many vertices. Hereafter, we may assume that the maximum degree of $G$ is 3 exactly. Because $G$ does not contain $F_n$, when $G$ has sufficiently many vertices, every vertex of degree 3 will be adjacent to a leave, in other words, $G$ is a caterpillar tree of maximum degree 3. Moreover, since $G$ does not contain $B_{1,m}, B_{2,m}, \ldots, B_{m,n}, E_{m,n}$, $G$ has only one vertex of degree 3, hence $G$ must be one of $E_{i,j}$ for $i < m$. Notice that the spectral radii of paths and cycles are at most $2 \leq \lambda$ and the spectral radius $\lambda_1(E_{i,j}) < \alpha_i \leq \alpha_{m-1} \leq \lambda$ for all $i < m$. Therefore the claim implies that

$$G_0 \cup \{\text{connected graph } G \notin \mathcal{F}(\lambda) \text{ with } \leq b \text{ vertices}\}$$

is a finite forbidden subgraphs characterization for $\mathcal{F}(\lambda)$. 

\[ \square \]

### 3 Equiangular lines

#### 3.1 The framework to estimate $N_\alpha(n)$

We shall set the ground by briefly reviewing the framework to estimate $N_\alpha(n)$ developed in [BDKS17]. We advise the readers who are interested in the details of the framework to read at least Section 2.1 of [BDKS17].

**Definition 1.** Let $L$ be a subset of the interval $[-1, 1]$. A finite non-empty set $C$ of unit vectors in $\mathbb{R}^n$ is called a spherical $L$-code if $\langle v_1, v_2 \rangle \in L$ for any pair of distinct vectors $v_1, v_2$ in $C$. The Gram matrix $M_C$ are given by $(M_C)_{i,j} = \langle v_i, v_j \rangle$, and the underlying graph $G_C$ is defined as follows: let $C$ be its vertex set and for any distinct $v_i, v_j \in C$, we put the edge $(v_i, v_j)$ if and only if $\langle v_i, v_j \rangle < 0$.

By choosing a unit vector in the direction of each line in a set of equiangular lines with angle $\arccos \alpha$ in $\mathbb{R}^n$, we obtain a spherical $\{ \pm \alpha \}$-code $C = \{v_1, \ldots, v_m\}$ in $\mathbb{R}^n$. One can show that the clique number of $G_C$ is $\leq 1 + \alpha^{-1}$. By Ramsey’s theorem, if $|C|$ is large enough, then $G_C$ contains an independent set of size, say $t$. Assume that $I = \{v_1, \ldots, v_t\} \subset C$ is an independent set in $G_C$. By properly switching $v_i$ to $-v_i$ for some $i > t$, we may assume that the degree of $v_i$ to $I$ is at most $t/2$ for all $i > t$. One can then show that the number of vertices that are not independent from $I$ in $G_C$ is bounded by $b = O_{\alpha,t}(1)$. Without loss of generality, assume that each vertex in $\{v_{b+1}, \ldots, v_m\}$ is independent from $I$. Denote by $v'_i$ the normalized projection of $v_i$ onto the orthogonal complement of span($I$). It can be shown that $C' := \{v'_b, \ldots, v'_m\}$ is a spherical $L(\alpha, t)$-code, where

$$L(\alpha, t) := \left\{ -\sigma \cdot \left(1 - \frac{1}{1 + \alpha^{-1}}\right), \frac{1}{1 + \alpha^{-1}} \right\} \text{ and } \sigma := \frac{2\alpha}{1 - \alpha}.$$ 

We wrap up the above discussion in the following lemma, which is essentially [BDKS17] Lemma 2.8. The slight difference in the statement originates from our need to estimate $N_\alpha(n)$ up to a constant error relative to $\alpha$. However, the same proof goes through without alteration.
Lemma 7 (Lemma 2.8 of Balla et al. [BDKS17]). Let $\alpha \in (0, 1)$ and $t \in \mathbb{N}$ be fixed. For any spherical $\{\pm\alpha\}$-code $C$ in $\mathbb{R}^n$, there exists a spherical $L(\alpha, t)$-code $C'$ in $\mathbb{R}^n$ such that $|C| \leq |C'| + O_{\alpha, t}(1)$.

As $t$ goes to $\infty$, $L(\alpha, t)$ approaches $\{-\sigma, 0\}$. One of the connections between spherical $\{\pm\alpha\}$-codes and spherical $\{-\sigma, 0\}$-codes is the following. We shall denote by $I_n$ the identity matrix of order $n$ and $J_n$ the all-ones matrix of order $n$, and we suppress the subscripts when the order of the matrices are clear from the context.

Lemma 8. Let $\alpha \in (0, 1)$ and $\sigma = 2\alpha/(1-\alpha)$. For any spherical $\{-\sigma, 0\}$-code $C_0$ in $\mathbb{R}^k$, there exists a spherical $\{\pm\alpha\}$-code $C$ in $\mathbb{R}^n$ such that $|C| \geq \lfloor n^2 \alpha^2 \rfloor |C_0|$. In particular, the maximum number $N_\alpha(n)$ of equiangular lines in $\mathbb{R}^n$ with angle $\arccos \alpha$ is $\geq \lfloor n^2 \alpha^2 \rfloor k_\alpha$, where $k_\alpha$ is defined as in Theorem 2.

In the case $k_\alpha = \infty$, we have $N_\alpha(n) \geq n$.

Proof. Given a spherical $\{-\sigma, 0\}$-code $C_0$ in $\mathbb{R}^k$. Let $m = \lfloor n^2 \alpha^2 \rfloor$ and $M_0$ be the Gram matrix of $C_0$. Consider the matrix $M := (1-\alpha)M_0 \otimes I_m + \alpha J$ of order $m |C_0|$. One can check that $M$ is semipositive definite and rank($M$) $\leq m \cdot \text{rank}(C_0) + 1 \leq mk + 1 \leq n$. Moreover, the diagonal entries are ones and the off-diagonal entries are either $-\alpha$ or $\alpha$. Therefore $M$ can be realized as the Gram matrix of a spherical $\{\pm\alpha\}$-code in $\mathbb{R}^n$ of size $m |C_0|$.

When $k_\alpha < \infty$, it suffices to construct a spherical $\{-\sigma, 0\}$-code $C_0$ in $\mathbb{R}^{ka-1}$ of size $k_\alpha$. Because $1/\sigma = \frac{1-\alpha}{2\alpha}$ is the spectral radius of a graph $G$ on $k_\alpha$ vertices, $I - \sigma A$ is positive semidefinite, where $A$ is the adjacency matrix of $G$. Moreover, rank($I - \sigma A$) $\leq k_\alpha - 1$. Clearly, $I - \sigma A$ can be realized as the Gram matrix of a spherical $\{-\sigma, 0\}$-code in $\mathbb{R}^{ka-1}$ of size $k_\alpha$.

When $k_\alpha = \infty$, one can check that $(1 - \alpha)I_n + \alpha J_n$ can be realized as the Gram matrix of a spherical $\{\pm\alpha\}$-code in $\mathbb{R}^n$ of size $n$.

3.2 Application of Theorem 1

We recall two classical results — a fact about the spectral radius of a connected graph and a necessary condition on eigenvalues of the sum of two matrices.

Theorem 9 (Corollary of Perron–Frobenius theorem [Pro12, Per07]). For every connected graph $G$, $\lambda_1(G)$ has multiplicity 1, with an eigenvector whose components are all positive.

Theorem 10 (Weyl’s inequality [Wey12]). Given two $n \times n$ Hermitian matrices $A$ and $B$. Denote the eigenvalues of $A$ as $\lambda_1(A) \geq \lambda_2(A) \geq \cdots \geq \lambda_n(A)$, and similarly denote the eigenvalues of $B$ and $A + B$. Whenever $0 \leq i, j, i + j < n$, $\lambda_{i+j+1}(A + B) \leq \lambda_{i+1}(A) + \lambda_{j+1}(B)$.

The motivation of the proof for Theorem 2 comes from the following observation. Suppose $C'$ is a spherical $L(\alpha, t)$-code in $\mathbb{R}^n$. Let $M_{C'}$ be its Gram matrix, $G'$ its underlying graph with adjacency matrix $A'$. The matrices $M_{C'}$ and $A'$ are related by

$$
\left(1 + \frac{1}{t + \alpha^{-1} + 1}\right) M_{C'} = I - \sigma A' + \frac{1}{t + \alpha^{-1} - 1} J.
$$
Since $M_{C'}$ is positive semidefinite and one has the freedom to choose $t$ large, it seems plausible that $I - \sigma A'$ is positive semidefinite as well. In this case, one can easily finish the proof. Unfortunately, the positive eigenvalue of $J$ is $|C'|$ that is not bounded. This allows $I - \sigma A'$ to have a negative eigenvalue, in other words, the spectral radius of $G'$ is $> \lambda = 1/\sigma$. Theorem 1 roughly says that the reason for $\lambda_1(G') > \lambda$ is local, that is, $G'$ contains a forbidden subgraph of bounded size. Therefore, a priori we can choose $t$ large to get a contradiction from $I - \sigma A'$ not being positive semidefinite.

Proof of Theorem 2. In view of Lemma 8, it suffices to show that $N_\alpha(n) \leq k_\alpha \cdot n + O(1)$. Let $I$ be the Gram matrix of $C'$ where $G'$ contains $G$ components, say $G_1, \ldots, G_m$ respectively. We claim that $G_i$ does not contain any graph in $\mathcal{I}$ for all $i \in [m].$ Suppose on the contrary that $G_i$ contains a graph $G \in \mathcal{I}$. Without loss, assume that $i = 1$. Let $G'_1$ with vertex set $C'_1$ be the minimal induced subgraph of $G_1$ that contains $G$ as a subgraph. Apparently $v(G'_1) = v(G)$. By the monotonicity of $\lambda_1$ and the choice of $t$ in (1), we obtain

$$1 - \sigma \lambda_1(G'_1) + \frac{v(G'_1)}{t + \alpha - 1} < 0$$

where $v(G)$ denotes the number of vertices in $G$.

By Lemma 7, there exists a spherical $L(\alpha, t)$-code $C'$ in $\mathbb{R}^n$ such that $|C| \leq |C'| + O(1)$. Let $M_{C'}$ be the Gram matrix of $C'$, and $G_{C'}$ the underlying graph. We decompose $G_{C'}$ into $m$ connected components, say $G_1, \ldots, G_m$, with vertex sets $C_1, \ldots, C_m$ respectively. We claim that $G_i$ does not contain any graph in $\mathcal{I}$ for all $i \in [m]$. Suppose on the contrary that $G_i$ contains a graph $G \in \mathcal{I}$. Without loss, assume that $i = 1$. Let $G'_1$ with vertex set $C'_1$ be the minimal induced subgraph of $G_1$ that contains $G$ as a subgraph. Apparently $v(G'_1) = v(G)$. By the monotonicity of $\lambda_1$ and the choice of $t$ in (1), we obtain

$$1 - \sigma \lambda_1(G'_1) + \frac{v(G'_1)}{t + \alpha - 1} < 0.$$  

(2)

Let $M_{C'_1}$ be the Gram matrix of $C'_1$ and let $A'_1$ be the adjacency matrix of $G'_1$. These two matrices are related by the equation

$$
\left(1 + \frac{1}{t + \alpha - 1}\right) M_{C'_1} = I - \sigma A'_1 + \frac{1}{t + \alpha - 1} J.
$$

Using the fact that $\lambda_1(J) = v(G'_1)$ and (2), we know from Weyl’s inequality that the least eigenvalue of $M_{C'_1}$ is negative. This contradicts with the fact that a Gram matrix is positive semidefinite.

Because $\mathcal{I}$ is a forbidden subgraphs characterization for $\mathcal{F}(\lambda)$, by the claim $G_i \in \mathcal{F}(\lambda)$, that is $\lambda_1(G_i) \leq \lambda$, for all $i \in [m]$. In other words, $I - \sigma A_i$ is positive semidefinite, where $A_i$ is the adjacency matrix of $G_i$. By Theorem 9, $\text{rank}(I - \sigma A_i) \geq |C_i| - 1$ and equality holds if and only if
\[ \lambda_1(A_i) = 1/\sigma = \lambda. \] Finally, we use the relation

\[ \left(1 + \frac{1}{t + \alpha^{-1} - 1}\right) M_{C'} = \begin{pmatrix} I - \sigma A_1 & \cdots & \cdots & \cdots \\ \cdots & I - \sigma A_2 & \cdots & \cdots \\ \cdots & \cdots & \ddots & \cdots \\ \cdots & \cdots & \cdots & I - \sigma A_m \end{pmatrix} + \frac{1}{t + \alpha^{-1} - 1} J \]

to estimate the rank of \( M_{C'} \)

\[ n \geq \text{rank}(M_{C'}) \geq \left( \sum_{i=1}^{m} \text{rank}(I - \sigma A_i) \right) - 1. \] (3)

If \( k_\alpha \) is finite, we know that if \( \lambda_1(A_i) = \lambda = \frac{1}{2\alpha}, \) then \( |C_i| \leq k_\alpha \) and so \( \text{rank}(I - \sigma A_i) \geq (1 - 1/k_\alpha) |C_i| \). Therefore we always have \( \text{rank}(I - \sigma A_i) \geq (1 - 1/k_\alpha) |C_i|. \) By (3), we obtain

\[ n \geq \left( 1 - \frac{1}{k_\alpha} \right) \left( \sum_{i=1}^{m} |C_i| \right) - 1 = \left( 1 - \frac{1}{k_\alpha} \right) |C'| - 1 \geq \left( 1 - \frac{1}{k_\alpha} \right) |C| - O(1), \]

which is equivalent to the desired inequality after multiplying \( \frac{k_\alpha}{k_\alpha - 1} \). Otherwise since \( k_\alpha = \infty, \) we get \( \text{rank}(I - \sigma A_i) \geq |C_i| \) and \( n \geq (\sum_{i=1}^{m} |C_i|) - 1 = |C'| - 1 \geq |C| - O(1). \)

3.3 An improved upper bound on \( N_\alpha(n) \)

In this section, we prove \( N_\alpha(n) \leq 1.49n + O(1). \) We recall the following spectral techniques. Again, Lemma 11 is stated differently from [BDKS17, Lemma 2.13], and the same proof works line by line.

Lemma 11 (Lemma 2.10 of Bella et al. [BDKS17]). Let \( C \) be a spherical \( L(\alpha, t) \)-code in \( \mathbb{R}^n \) and let \( G_C \) be the underlying graph of \( C \) of average degree \( d \). Then \( |C| \leq (1 + d\sigma^2) \cdot \text{rank}(I - \sigma A), \) where \( \sigma = \frac{2\alpha}{1 - \alpha} \) and \( A \) is the adjacency matrix of \( G_C \).

Lemma 12 (Lemma 2.13 of Balla et al. [BDKS17]). Let \( G \) be a graph with minimum degree \( \delta \geq 2. \) Let \( v_0 \) be a vertex of \( G \) and let \( H \) be the subgraph consisting of all vertices within distance \( k \) of \( v_0. \) Then \( \lambda_1(H) \geq \frac{2k}{k+1} \sqrt{\delta - 1}. \)

Lemma 3 can be seen as an averaged version of Lemma 12. By Lemma 5(p), the coefficient in Lemma 3 \( 2 \cos(\frac{\pi}{k+2}) = \lambda_1(P_{k+1}), \) where \( P_{k+1} \) is the path with \( k+1 \) vertices. Notice that \( \lambda_1(P_{k+1}) > \frac{2k}{k+1}, \) the average degree of \( P_{k+1}, \) which is the coefficient in Lemma 12.

Remark 2. Lemma 3 is asymptotically tight when \( d \) is a prime plus one due to the existence of regular graphs of high girth. The Ramanujan graphs constructed independently by Margulis [Mar82] and Lubotzky, Phillips and Sarnak [LPS88] are \( d \)-regular graphs on \( n \) vertices of girth \( \Omega_d(\log n). \) Locally, a subgraph of these Ramanujan graphs of bounded size looks like a \( d \)-regular tree, whose spectral radius is bounded from above by the spectral radius \( 2\sqrt{d-1} \) of the infinite \( d \)-regular tree.
Proof of Lemma 3. Since removing leaf vertices from a graph of average degree $d \geq 2$ cannot decrease its average degree, without loss of generality, we may assume that the minimum degree of $G$ is $\geq 2$. A walk $(v_1, v_2, v_3, \ldots)$ on $G$ is non-backtracking if $v_i \neq v_{i+2}$ for all $i$. For all $i \geq 0$, define $W_i$ to be the set of all non-backtracking walks $(v_1, v_2, v_3, \ldots, v_i)$ on $G$ of length $i + 1$. Define the forest $T$ as follows: the vertex set is $\bigcup_{i=0}^{k} W_i$ and two vertices $(u_1, u_2, \ldots, u_k)$ and $(v_1, v_2, \ldots, v_j)$ are adjacent if and only if $|i - j| = 1$ and $u_k = v_k$ for $k = -1, 0, \ldots, \min(i, j)$. For every $e = (v_1, v_0) \in W_0$, denote by $T_e$ the connected component of $T$ containing $e$. We also denote by $G_{t_0}$ the subgraph of $G$ consisting of all vertices within distance $k$ of $v_0$.

We claim that $\lambda_1(T_e) \leq \lambda_1(G_{t_0})$ for every $e = (v_1, v_0) \in W_0$. Let $s_i$ and $t_i$ be the number of closed walks of length $i$ starting respectively at $e$ in $T_e$ and $v_0$ in $G_{t_0}$. It is well known that $\lambda_1(T_e) = \limsup \sqrt{s_i}$ and $\lambda_1(G_{t_0}) = \limsup \sqrt{t_i}$. We naturally map a closed walk $e = e_0, e_1, \ldots, e_i = e$ in $T_e$ to a closed walk $v_0, v_1, \ldots, v_i = v_0$ in $G_{t_0}$, where $v_j$ is the terminal vertex of the non-backtracking walk $e_j$ for $j = 0, 1, \ldots, i$. One can show that this map is injective, and so $s_i \leq t_i$ for all $i$, from which the claim follows.

Set $\lambda = \lambda_1(P_{k+1}) = 2 \cos(\pi/k+2)$. Because $\lambda_1(T) = \max \{\lambda_1(T_e) : e \in W_0\}$, it suffices to prove $\lambda_1(T) \geq \sqrt{d} - 1$. Consider the non-backtracking random walk on $T$, where the start vertex $w_0 = (v_1, v_0)$ is chosen uniformly at random from $W_0$ and, for $i \in [k]$, at $i$th step the next vertex $w_i = (v_1, v_0, \ldots, v_i)$ is chosen uniformly from the available choices in $W_i$. The transition matrix of this walk is

$$P_{(u_1, u_0, \ldots, u_k), (u_1, u_0, \ldots, u_k+1)} = \frac{1}{d(u_i) - 1},$$

where $d(v)$ denotes the degree of $v$ in $G$. Clearly $|W_0| = d|V(G)|$. Since $W_i$ is a finite set and $w_i = (v_1, v_0, \ldots, v_i)$ is a random element of $W_i$ with distribution

$$p(w_i) := \frac{1}{d|V(G)|} \prod_{j=0}^{i-1} \frac{1}{d(v_j) - 1},$$

for any $c : W_i \to \mathbb{R}$, the basic identity of importance sampling allows us to represent $\sum_{w \in W_i} c(w)$ as follows:

$$\sum_{w \in W_i} c(w) = \sum_{w \in W_i} p(w) \frac{c(w)}{p(w)} = E[c(w_i)/p(w_i)].$$

(4)

Let $(x_0, x_1, \ldots, x_k) \in \mathbb{R}^{k+1}$ be an eigenvector of $P_{k+1}$ such that $x_0, x_1, \ldots, x_k > 0$. Define the vector $f : V(T) \to \mathbb{R}$ by $f(w) = x_i \sqrt{p(w)}$ for $w \in W_i$, and define the matrix $A$ to be the adjacency matrix of the forest $T$. For $w = (u_1, u_0, \ldots, u_i)$, denote by $w^- = (u_1, u_0, \ldots, u_{i-1})$. By the importance sampling identity (4), we observe that

$$\langle f, f \rangle = \sum_{i=0}^{k} \sum_{w \in W_i} f(w)^2 = \sum_{i=0}^{k} E(x_i^2) = \sum_{i=0}^{k} x_i^2,$$

$$\frac{1}{2} \langle f, Af \rangle = \sum_{i=1}^{k} \sum_{w \in W_i} f(w^-) f(w) = \sum_{i=1}^{k} E\left[ x_{i-1} x_i \sqrt{p(w^-)/p(w)} \right] = \sum_{i=1}^{k} x_{i-1} x_i E\left[ \sqrt{d(v_{i-1}) - 1} \right].$$

9
As is easily verified by induction, $(v_{i-1}, v_i)$ is uniformly distributed on $W_0$ for all $i = 0, 1, \ldots, k$, thus $\Pr (v_j = v) = \frac{d(v)}{d(V(G))} = \pi(v)$ for all $v \in V(G)$ and $j = 0, 1, \ldots, k$. Since each $v_j$ has distribution $\pi$ and the fact that $x \mapsto x\sqrt{x-1}$ is convex on $[2, \infty]$, Jensen’s inequality gives

$$\frac{1}{2} \langle f, Af \rangle = \sum_{i=1}^{k} x_{i-1} x_i \sum_{v \in V(G)} \frac{d(v)}{d(V(G))} \sqrt{d(v) - 1} \geq \sqrt{d-1} \sum_{i=1}^{k} x_{i-1} x_i.$$  

Finally we invoke the Rayleigh principle $2 \sum_{i=1}^{k} x_{i-1} x_i = \lambda \sum_{i=0}^{k} x_i^2$ and $\lambda(T) \geq \langle f, Af \rangle / \langle f, f \rangle$. \hfill \Box

**Remark 3.** See the expository note by Levin and Peres [LPT11] for other applications of the importance sampling identity.

**Theorem 13.** Let $N_\alpha(n)$ be the maximum number of equiangular lines in $\mathbb{R}^n$ and let $\sigma := \frac{2\alpha}{1-\alpha}$. If $\sigma \leq 1/2$, then $N_\alpha(n) \leq \left(1 + \frac{1}{4} + \varepsilon \right)n + O_{\alpha, \varepsilon}(1)$ for every $\varepsilon > 0$. In particular, for every $\varepsilon > 0$, $N_{1/7}(n) \leq (4/3 + 1/36 + \varepsilon)n + O_{\varepsilon}(1)$.

**Proof.** Let $\lambda := 1/\sigma$. The stratagem is to find a finite partial forbidden subgraphs characterization $G_0$, consisting graphs of spectral radius $\lambda$, in the following sense: if a connected graph $G$ does not contain any of $G_0$, then either $G \in \mathcal{F}(\lambda)$ or $G$ has average degree $\leq d$ for some constant $d$. We claim that if such $G_0$ exists, then

$$N_\alpha(n) \leq \left(1 + \max \left\{ \frac{1}{k_\alpha - 1}, d\sigma^2 \right\} \right)n + O_{\alpha, d}(1). \quad (5)$$

The proof of the claim follows the outline of the proof for Theorem 2.

Suppose $C$ is a spherical $\{\pm \alpha\}$-code in $\mathbb{R}^n$. We choose $t$ large enough so that $\mathbb{I}$ holds for all $G \in \mathcal{G}_0$. By Lemma 11, there exists a spherical $L(\alpha, t)$-code $C'$ in $\mathbb{R}^n$ such that $|C| \leq |C'| + O(1)$. Define $M_{C'}, G_{C'}, G_1, \ldots, G_m, C_1, \ldots, C_m, A_1, \ldots, A_m$ as in the proof of Theorem 2. The same claim that $G_i$ does not contain any graph in $\mathcal{G}_0$ holds for all $i \in [n]$. By our choice of $\mathcal{G}_0$, we know that either $\lambda_1(G_i) \leq \lambda$ or the average degree of $G_i$ is $\leq d$. In the former case, we can show that $|C_i| \leq \left(1 + \frac{1}{k_\alpha - 1}\right) \cdot \text{rank}(I - \sigma A_i)$. Whereas, in the latter case, we can apply Lemma 11 and get $|C_i| \leq \left(1 + d\sigma^2\right) \cdot \text{rank}(I - \sigma A_i)$. Summing up these estimations for $|C_i|$ yields (5).

We choose $k$ large enough so that $\sqrt{2\sqrt{1 + 4\varepsilon}} < \lambda' := 2\cos\left(\frac{\pi}{k+2}\right) < 2$, and we choose $D \in \mathbb{N}$ such that $S_D \notin \mathcal{F}(\lambda)$.

Suppose $G$ has average degree $\leq (\lambda/\lambda')^2 + 1$ and it has maximum degree $< D$. Because $\sigma \leq 1/2$, hence $d > (2/\lambda')^2 + 1 > 2$, Lemma 9 implies that there exists a vertex $v_0$ of $G$ such that $\lambda_1(H) \geq \lambda'\sqrt{d-1} > \lambda$, where $H$ is the subgraph consisting of all vertices within distance $k$ of $v_0$. This means that $G$ contains a subgraph $H \notin \mathcal{F}(\lambda)$ on $\leq D^k$ vertices. Thus we can apply the claim above to $d = (\lambda/\lambda')^2 + 1$ and

$$\mathcal{G}_0 := \{S_D\} \cup \left\{\text{connected graph } G \notin \mathcal{F}(\lambda) \text{ with } \leq D^k \text{ vertices} \right\}.$$  

Since $d\sigma^2 = (1/\lambda')^2 + \sigma^2 < 1/4 + \sigma^2 + \varepsilon$, the upper bound (5) becomes

$$N_\alpha(n) \leq \left(1 + \max \left\{ \frac{1}{k_\alpha - 1}, \frac{1}{4} + \sigma^2 + \varepsilon \right\} \right)n + O_{\alpha, \varepsilon}(1).$$
Because the complete graph on \( k_\alpha \) vertices has the largest spectral radius \( k_\alpha - 1 \) among all graphs on \( k_\alpha \) vertices, we know that \( \lambda \leq k_\alpha - 1 \), hence \( \sigma \geq 1/(k_\alpha - 1) \). This implies that \( 1 + 4 + \sigma^2 \geq 7 \sigma \) subsumes \( 1/(k_\alpha - 1) \).

**Corollary 14.** The maximum number of equiangular lines in \( \mathbb{R}^n \) with angle \( \arccos \alpha \) is \( \leq 1.49n + O(1) \) if \( \alpha \notin \{1/3, 1/5, 1/(1 + 2\sqrt{2}) \} \).

**Proof.** Set \( \sigma_* := 1/\lambda^* \approx 0.486 \). On the one hand, Theorem 2 implies that \( N_\alpha(n) \leq \frac{3}{4}n + O(1) \) if \( \sigma \in (\sigma_*, \infty) \cap \{1, 1/2, 1/\sqrt{2} \} \). On the other hand, because \( \sigma_2^* < 0.24 \), Theorem 13 implies that if \( \sigma \leq \sigma_* \) then \( N_\alpha(n) \leq \left(1 + \frac{1}{4} + \sigma^2 + (0.24 - \sigma_2^*)\right)n + O(1) \leq 1.49n + O(1) \).

4 Concluding remarks

Besides Theorem 2 and Lemma 8 we discuss two other evidences supporting Conjecture 13. The key parameter \( k_\alpha \) in the conjecture is the smallest \( k \) such that \( \lambda := \frac{1 - \alpha}{2\alpha} \) is the spectral radius of a graph on \( k \) vertices. Clearly, if \( k_\alpha < \infty \), then

1. \( \lambda \) is an algebraic integer — it is a root of some monic polynomial with coefficients in \( \mathbb{Z} \),
2. \( \lambda \) is totally real — its conjugate elements are in \( \mathbb{R} \),
3. \( \lambda \) is the largest among its conjugate elements by Perron–Frobenius theorem.

On the converse, Bass, Estes and Guralnick [BEG94 Corollary 0.7] proved that any totally real algebraic integer is the eigenvalue of the adjacency matrix of some regular graph. It would be interesting to study a complete set of necessary conditions for the spectral radius of a graph.

Notice that \( \deg \lambda \geq \deg \alpha \), where \( \deg \alpha \) denotes the algebraic degree of \( \alpha \). Conjecture 13 predicts that \( N_\alpha(n) \leq \frac{\deg \alpha}{\deg \alpha - 1} \cdot n + O(1) \). This is indeed a cheap bound on \( N_\alpha(n) \).

**Proposition 15.** If \( \lambda = \frac{1 - \alpha}{2\alpha} \) is a totally real algebraic integer, then \( N_\alpha(n) \leq \frac{\deg \alpha}{\deg \alpha - 1} \cdot n + O(1) \). Otherwise \( n \leq N_\alpha(n) \leq n + 1 \).

**Proof.** Let \( C \) be a spherical \( \{\pm \alpha\}\)-code in \( \mathbb{R}^n \). Let \( M_C \) be its Gram matrix, \( G_C \) its underlying graph, and \( A \) the adjacency matrix of \( G \). We know that \( M_C = (1 - \alpha)(I - \sigma A) + \alpha J \), where \( \sigma = 1/\lambda \). If \( \lambda \) is not a totally real algebraic integer, then \( \lambda \) is not an eigenvalue of \( A \), hence \( \mathop{\mathrm{rank}}(I - \sigma A) = |C| \) and so \( n \geq \mathop{\mathrm{rank}}(M_C) \geq |C| - 1 \). Together with Lemma 8 we have \( n \leq N_\alpha(n) \leq n + 1 \). If \( \lambda \) is an algebraic number, then \( \mathop{\mathrm{rank}}(I - \sigma A) \geq (1 - \frac{1}{\deg \lambda})|C| \) and so \( n \geq \mathop{\mathrm{rank}}(M_C) \geq (1 - \frac{1}{\deg \lambda})|C| - 1 \).

The special case \( \lambda = \lambda^* \) of Proposition 15 supplements Theorem 2. Observe that one of the conjugate elements of \( \lambda^* \) is \( \sqrt{2 - \sqrt{5}} \) which is not real. This means \( N_{1/(1 + 2\sqrt{2})}(n) = n + O(1) \).

Lemma 8 and Proposition 15 would imply that Conjecture 13 in the equality case \( k_\alpha = \deg \alpha \). Note that \( k_\alpha = \deg \alpha \) if and only if \( \lambda = \frac{1 - \alpha}{2\alpha} \) is the spectral radius of a graph with irreducible characteristic polynomial. A result of Mowshowitz [Mow71] (see [GM81, Theorem 3.8] for a generalization) states that a graph with irreducible characteristic polynomial has trivial automorphism group. Such graphs are known as asymmetric graphs. Erdős and Rényi [ER63] showed that asymmetric graphs have at
least 6 vertices and there are 8 asymmetric graphs on 6 vertices. Interestingly, these 8 graphs all indeed have irreducible characteristic polynomial. Moreover, their spectral radii are larger than \( \lambda^* \), for which Theorem 2 fails to address.

Hereafter we assume that \( \lambda \) is a totally real algebraic integer. Suppose \( \lambda \) is not the largest among its conjugate elements. Conjecture 3 thus asserts that \( N_\alpha(n) = n + O(1) \). This is indeed the case.

**Proposition 16.** Suppose \( \lambda = \frac{1-\alpha}{2\alpha} \) is a totally real algebraic integer. If \( \lambda \) is not the largest among its conjugate elements, \( n \leq N_\alpha(n) \leq n + 2 \).

**Proof.** We denote by \( \lambda_{-i}() \) and \( \lambda_i() \) respectively the \( i \)th smallest eigenvalue and the \( i \)th largest eigenvalue of a matrix. Let \( \lambda' > \lambda \) be a conjugate element of \( \lambda \). Let \( C \) be a spherical \( \{\pm\} \)-code in \( \mathbb{R}^n \). Let \( M_C \) be its Gram matrix, \( G_C \) its underlying graph, and \( A \) the adjacency matrix of \( G \). We know that \( M_C = (1-\alpha)(I-\sigma A) + \alpha J \). Assume for the sake of contradiction that \( \text{rank}(I-\sigma A) \leq |C| - 2 \), that is, \( \lambda \) is an eigenvalue of \( A \) with multiplicity \( \geq 2 \), then \( 1-\sigma \lambda' < 0 \) is an eigenvalue of \( I-\sigma A \) with multiplicity \( \geq 2 \), hence \( \lambda_{-2}(I-\sigma A) < 0 \). By Weyl’s inequality, \( 0 \leq \lambda_{-1}(M_C) \leq (1-\alpha)\lambda_{-2}(I-\sigma A) + \alpha \lambda_2(J) < 0 \). This is a contradiction. Therefore \( \text{rank}(I-\sigma A) \geq |C| - 1 \) and so \( n \geq \text{rank}(M_C) \geq |C| - 2 \). Together with Lemma 8 we have \( n \leq N_\alpha(n) \leq n + 2 \).

Lastly, we remark on a possible extension of our method. Our proof strategy would yield Conjecture 3 provided that \( \mathcal{F}(\lambda) \) has a finite partial forbidden subgraphs characterization \( \mathcal{G}_0 \subset \mathcal{F}(\lambda)^c \) in the following sense: if a graph \( G \) does not contain any graph in \( \mathcal{G}_0 \), then either \( G \in \mathcal{F}(\lambda) \) or \( \lambda \) is an eigenvalue of \( G \) with multiplicity \( \leq v(G)/k_\alpha \). In this direction, Woo and Neumaier [WN07] investigated the structure of graphs whose spectral radius is in \( (2, 3/\sqrt{2}] \). In particular, such a graph is either an open quipu\(^2\), a closed quipu\(^3\) or a dagger\(^4\). One can prove that the multiplicity of any nonzero eigenvalue is at most 2.

**Acknowledgements**

Thanks to Boris Bukh for introducing equiangular lines to the first author, and to Jun Su and Sebastian Cioab˘a for some useful correspondence.

**References**

[BDKS17] Igor Balla, Felix Dräxler, Peter Keevash, and Benny Sudakov. Equiangular lines and spherical codes in euclidean space. *Inventiones mathematicae*, Jul 2017. [arXiv:1606.06620 [math.CO]]

\(^2\)An open quipu is a tree of maximum degree 3 such that all vertices of degree 3 lie on a path.

\(^3\)A closed quipu is a connected graph of maximum degree 3 such that all vertices of degree 3 lie on a unique cycle.

\(^4\)A dagger is \( A_n \) defined in Lemma 5.
[BEG94] Hyman Bass, Dennis R. Estes, and Robert M. Guralnick. Eigenvalues of symmetric matrices and graphs. *J. Algebra*, 168(2):536–567, 1994.

[Buk16] Boris Bukh. Bounds on equiangular lines and on related spherical codes. *SIAM J. Discrete Math.*, 30(1):549–554, 2016. arXiv:1508.00136[math.CO]

[dC00] D. de Caen. Large equiangular sets of lines in Euclidean space. *Electron. J. Combin.*, 7:Research Paper 55, 3, 2000.

[ER63] P. Erdős and A. Rényi. Asymmetric graphs. *Acta Math. Acad. Sci. Hungar*, 14:295–315, 1963.

[Fro12] Ferdinand Georg Frobenius. Über matrizen aus nicht negativen elementen. 1912.

[GKMS16] Gary Greaves, Jacobus H. Koolen, Akihiro Munemasa, and Ferenc Szöllösi. Equiangular lines in Euclidean spaces. *J. Combin. Theory Ser. A*, 138:208–235, 2016. arXiv:1403.2155[math.CO]

[GM81] C. D. Godsil and B. D. McKay. Spectral conditions for the reconstructibility of a graph. *J. Combin. Theory Ser. B*, 30(3):285–289, 1981.

[GY16] Alexey Glazyrin and Wei-Hsuan Yu. Upper bounds for s-distance sets and equiangular lines. 2016. arXiv:1611.09479[math.MG]

[Hof72] Alan J. Hoffman. On limit points of spectral radii of non-negative symmetric integral matrices. pages 165–172. Lecture Notes in Math., Vol. 303, 1972.

[JW15] Jonathan Jedwab and Amy Wiebe. Large sets of complex and real equiangular lines. *J. Combin. Theory Ser. A*, 134:98–102, 2015. arXiv:1501.05395[math.CO]

[LP17] David A. Levin and Yuval Peres. Counting Walks and Graph Homomorphisms via Markov Chains and Importance Sampling. *Amer. Math. Monthly*, 124(7):637–641, 2017.

[LPS88] A. Lubotzky, R. Phillips, and P. Sarnak. Ramanujan graphs. *Combinatorica*, 8(3):261–277, 1988.

[LS73] P. W. H. Lemmens and J. J. Seidel. Equiangular lines. *J. Algebra*, 24:494–512, 1973.

[Mar82] G. A. Margulis. Explicit constructions of graphs without short cycles and low density codes. *Combinatorica*, 2(1):71–78, 1982.

[Mow71] Abbe Mowshowitz. Graphs, groups and matrices. pages 509–522, 1971.

[Neu89] A. Neumaier. Graph representations, two-distance sets, and equiangular lines. *Linear Algebra Appl.*, 114/115:141–156, 1989.
A Proof of Lemma 5

We need the characteristic polynomials for paths and cycles. The readers are invited to prove them by reduction and induction.

**Lemma 17.** Denote $p_n$ and $q_n$ the characteristic polynomials of $P_n$ and $C_n$ respectively. Then

\[ p_0(x) = 1, \quad p_1(x) = x, \quad p_n = xp_{n-1}(x) - p_{n-2}(x), \quad q_{n+1}(x) = p_{n+1}(x) - p_{n-1}(x) - 2, \quad \text{for all } n \geq 2. \]

Moreover, the recursions give

\[ p_n(x) = \frac{\theta^n}{1 - \theta^2} + \frac{\theta^{-n}}{1 - \theta^2}, \quad q_n(x) = \theta^n + \theta^{-n} - 2, \quad (6) \]

where $\theta = \theta(x) := \frac{x + \sqrt{x^2 - 4}}{2}$.

**Proof of Lemma 5(c).** Clearly, for every regular graph, its spectral radius equals its degree. \(\square\)

**Proof of Lemma 5(p).** The characteristic polynomial $p_n$ of $P_n$ satisfies $p_n(2 \cos \omega) = \sin((n+1)\omega)/\sin \omega$. Thus the eigenvalues of $P_n$ are $2 \cos \frac{k\pi}{n+1}$, where $k \in [n]$.

**Proof of Lemma 5(s).** It follows from the characteristic polynomial of $S_n$, which is $x^{n-1}(x^2 - n)$.

For the proof of other facts in Lemma 5 we shall use the following lemmas due to Hoffman.

**Lemma 18** (Lemma 3.4 of Hoffman [Hof72]). Let $A_{n-1}$ be a principal submatrix of order $n - 1$ of a symmetric matrix $A_0$ of order $n$ with non-negative entries. Define $A_{i+1}$ recursively by

\[ A_{i+1} = \begin{pmatrix} A_i & e_i^T \\ e_i & 0 \end{pmatrix}, \quad \text{where } e_i = \begin{pmatrix} 0 & \cdots & 0 & 1 \end{pmatrix}. \]
Assume further that $\lim_{i \to \infty} \lambda_1(A_i) > 2$. Then $\lim_{i \to \infty} \lambda_1(A_i)$ is the largest positive root of

$$
\left(\frac{x + \sqrt{x^2 - 4}}{2}\right) p_0(x) = p_{-1}(x),
$$

(7)

where $p_i$ is the characteristic polynomial of $A_i$ for $i = -1, 0$.

**Definition 2.** Let $G$ be a connected graph, and let $v$ be a vertex of $G$. Denote $(G, v, n)$ the graph obtained from $G$ by appending a path of $n$ vertices to $G$ at $v$. Let $G_1, G_2$ be disjoint connected graphs, and let $v_1, v_2$ be vertices of $G_1, G_2$ respectively. Define $(G_1, v_1, n, v_2, G_2)$ to be the graph obtained from $G_1$ and $G_2$ by joining them by a path of $n$ vertices connecting $v_1$ and $v_2$.

**Remark 4.** When we apply Lemma 18 to the adjacency matrix of a graph, we get the following interpretation. Let $G$ be a connected graph, and let $v$ be a vertex of $G$. Assume further that $\lambda_1(G, v, n) \geq 2$ for some $n$, then $\lim_{i \to \infty} \lambda_1(A_n)$ is the largest positive root of (7), where $p_{-1}, p_0$ are the characteristic polynomials of $G \setminus \{v\}$ and $G$ respectively.

**Lemma 19** (Proposition 4.2 of Hoffman [Hof72]). Let $G_1, G_2$ be disjoint connected graphs, $v_1, v_2$ vertices of degree $\geq 2$ of $G_1, G_2$ respectively. Then

$$\lim \lambda_1(G_1, v_1, n, v_2, G_2) = \max \{\lim \lambda_1(G_1, v_1, n), \lim \lambda_1(G_2, v_2, n)\}.$$

**Definition 3.** Let $e$ be an edge of a graph $G$. If there exists a path in $G$, $x_1, x_2, \ldots, x_k$ where $x_k$ and $x_k$ are the end vertices of $e$, and the degrees of $x_1, x_2, \ldots, x_k$ are respectively $1, 2, 2, \ldots, 2$, then $e$ is said to be on an end path of $G$.

**Lemma 20** (Proposition 4.1 of Hoffman [Hof72]). Let $G$ be a connected graph with $\lambda_1(G) > 2$, $e = (x, y)$ an edge of $G$ not on an end path of $G$, $G$ not a cycle. Let $G_e^+$ be the graph obtained from $G$ by deleting edge $e$, and adding a vertex $z$ adjacent to $x$ and $y$ only. Then $\lambda_1(G_e^+) < \lambda_1(G)$.

By the monotonicity of the spectral radius and Lemma 20, the monotonicity of the spectral radii of each family of graphs in Lemma 5 follows immediately. We are left to compute the limits.

**Proof of Lemma 5(a).** Note that $A_n = (S_3, v, n)$, where $v$ is the vertex of degree 3 in $S_3$. Note that $\lambda_1(A_1) = 2$. By Remark 4, $\lim \lambda_1(A_n)$ is the largest positive root of

$$
\left(\frac{x + \sqrt{x^2 - 4}}{2}\right) x^2(x^2 - 3) = x^3,
$$

which turns out to be $3/\sqrt{2}$. \hfill \Box
Proof of Lemma 5(f). Note that $F_n = (P_5, v, n)$, where $v$ is the third vertex of $P_5$. Observe that $\lambda_1(F_2) = 2$. By Remark 4, $\lim \lambda_1(F_n)$ is the largest positive root of
\[
\left( \frac{x + \sqrt{x^2 - 4}}{2} \right) (x^5 - 4x^3 + 3x) = (x^2 - 1)^2,
\]
which turns to be the positive root $\lambda^*$ of $x^4 - 4x^2 - 1$.

Proof of Lemma 5(e). For the $m = 1$ case, it is well known that $\lambda_1(E_{1,n})$ is at least the average degree $2 + 4/n$ and so $\lim \lambda_1(E_{1,n}) \geq 2$. On the other hand, assume for the sake of contradiction that $\lim \lambda_1(E_{1,n}) > 2$. By Remark 4, $\lim \lambda_1(E_{1,n})$ is the largest positive root of
\[
\left( \frac{x + \sqrt{x^2 - 4}}{2} \right) x (x^2 - 2) = x^2,
\]
which turned out to be 2 contradicting the assumption $\lim \lambda_1(E_{1,n}) > 2$.

For the $m \geq 2$ case, because $\lambda_1(E_{m,8}) \geq \lambda_1(E_{2,8}) = 2$ and $E_{m,n} = (P_{m+2}, v, n)$, where $v$ is the second vertex of $P_{m+2}$, Remark 4 and Lemma 17 gives that $\lim_{n \to \infty} E_{m,n}$ is the largest positive root of
\[
\theta p_{m+2}(x) = xp_m(x),
\]
where $\theta$ and $p_i$ are defined as in Lemma 17. From this and \( \theta \), using $x = \theta + 1/\theta$, $z = \theta^2$, we seek the largest root of
\[
z^{m+1} = 1 + z + \cdots + z^{m-1}.
\]
In view of Theorem 4, this proves that $z = \beta_m$ and $\lim_{n \to \infty} \lambda_1(E_{m,n}) = \alpha_m$.

Proof of Lemma 5(b). Let $v_1$ be the vertex in $S_2$ of degree 2 and $v_2$ be second vertex in $P_{n+2}$. By Lemma 19,
\[
\lim_{m \to \infty} \lambda_1(B_{m,n}) = \max \left\{ \lim_{m \to \infty} \lambda_1(S_2, v_1, m), \lim_{m \to \infty} \lambda_1(P_{n+2}, v_2, m) \right\}
= \max \left\{ \lim_{m \to \infty} \lambda_1(E_{1,m}), \lim_{m \to \infty} \lambda_1(E_{n,m}) \right\} = \alpha_n.
\]

Proof of Lemma 5(d). Let $M_n$ be the adjacency matrix of $D_n$ and let $r_n$ be its characteristic polynomial. By expanding the determinant of $xI - M_n$ along the row of the leaf of $D_n$, one obtains
\[
r_n(x) = xq_{n+1}(x) - p_n(x),
\]
where $p_n$ and $q_{n+1}$ are defined as in Lemma 17. Using $x = \theta + 1/\theta$ and $z = \theta^2$, we seek the largest root of $(z^2 - z - 1)(1 - z^{-(n+1)}) = 2z^{-n/2}(z^{1/2} + z^{-1/2})$. As $z > 1$, we get $z^2 - z - 1 > 0$, hence $z > \phi$, where $\phi = \frac{1 + \sqrt{5}}{2}$ is the golden ratio. As $n \to \infty$, the largest root tends to $\phi$, and so $\lambda_1(D_n) \sim \phi^{1/2} + \phi^{-1/2} = \lambda^*$. \qed

16