Minimizing the least eigenvalues of unicyclic graphs with application to spectral spread

Yi-Zheng Fan a,b,∗, Yi Wang a,b, Yu-Bin Gao c

a Key Laboratory of Intelligent Computing and Signal Processing, Ministry of Education of China, Anhui University, Hefei 230039, PR China
b School of Mathematics and Computation Sciences, Anhui University, Hefei 230039, PR China
c Department of Mathematics, North University of China, Taiyuan 030051, PR China

Received 15 October 2007; accepted 13 March 2008

Submitted by S. Kirkland

Abstract

The spread of a graph is defined to be the difference between the largest eigenvalue and the least eigenvalue of the adjacency matrix of the graph. Let \( \mathcal{U}_n^k \) denote the set of connected unicyclic graphs of order \( n \) and girth \( k \), and let \( \mathcal{U}_n \) denote the set of connected unicyclic graphs of order \( n \). In this paper, we determine the unique graph with minimum least eigenvalue (respectively, the unique graph with maximum spread) among all graphs in \( \mathcal{U}_n^k \). We, finally, characterize the unique graph with minimum least eigenvalue (respectively, the unique graph with maximum spread) among all graphs in \( \mathcal{U}_n \).

© 2008 Elsevier Inc. All rights reserved.

AMS classification: 05C50; 15A18

Keywords: Unicyclic graph; Adjacency matrix; Least eigenvalue; Spread

Supported by National Natural Science Foundation of China (10601001, 60772121, 10571163), Anhui Provincial Natural Science Foundation (050460102, 070412065), NSF of Department of Education of Anhui Province (2005kj005zd), Foundation of Innovation Team on Basic Mathematics of Anhui University.

∗ Corresponding author. Address: School of Mathematics and Computation Sciences, Anhui University, Hefei 230039, PR China.

E-mail addresses: fanyz@ahu.edu.cn (Y.-Z. Fan), wangy@ahu.edu.cn (Y. Wang), ybgao@nuc.edu.cn (Y.-B. Gao).

0024-3795/$ - see front matter © 2008 Elsevier Inc. All rights reserved.
doi:10.1016/j.laa.2008.03.012
1. Introduction

For an $n \times n$ complex matrix $M$, the spread $s(M)$ of $M$ is defined as the diameter of its spectrum, i.e. $s(M) = \max_{i,j} |\lambda_i - \lambda_j|$, where the maximum is taken over all pairs of eigenvalues of $M$. There are a lot of results on the spread of matrices; see, e.g. [6,8,9,11].

Recently, the spread of graphs, as the spread of a special class of matrices, has received much attention. Let $G = (V, E)$ be a simple graph of order $n$ with vertex set $V = V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E = E(G)$. The adjacency matrix of the graph $G$ is defined to be a matrix $A = A(G) = [a_{ij}]$ of order $n$, where $a_{ij} = 1$ if $v_i$ is adjacent to $v_j$, and $a_{ij} = 0$ otherwise. Since $A$ is symmetric and real, the eigenvalues of $A$, i.e. the zeros of the characteristic polynomial $P(G, \lambda) = \det(\lambda I - A)$ of $A$, can be arranged as follows:

\[ \lambda_n(G) \geq \lambda_{n-1}(G) \geq \cdots \geq \lambda_1(G). \]

We simply call the eigenvalues and eigenvectors of $A(G)$ as those of $G$, respectively. For convenience, denote $\lambda_n(G)$ by $\lambda_{\text{max}}(G)$ and $\lambda_1(G)$ by $\lambda_{\text{min}}(G)$. If, in addition, $G$ is connected, then $A(G)$ is irreducible, the spectral radius of $A(G)$ is exactly the largest eigenvalue $\lambda_{\text{max}}(G)$; and by Perron–Frobenius Theorem, this eigenvalue is simple and there exists a unique (up to multiples) corresponding positive eigenvector, usually referred to the Perron vector of $A(G)$. The spread of the graph $G$ is defined as

\[ s(G) = \lambda_{\text{max}}(G) - \lambda_{\text{min}}(G). \]

In [10], Petrović determines all minimal graphs whose spread does not exceed 4. In [4], Gregory et al. present some lower and upper bounds for the spread of a graph. They show that path is the unique graph with minimum spread among all connected graphs of given order. However, the graph(s) with maximum spread is still unknown, and some conjectures are given as follows.

**Conjecture 1.1** [4]. The maximum spread of all graphs of order $n$ is attained only by the graph $K_{\lfloor 2n/3 \rfloor} \lor K_{n-\lfloor 2n/3 \rfloor}^c$, where $K_p$ denotes the complete graph of order $p$, $K_p^c$ is the complement of $K_p$, $G \lor H$ denotes the graph obtained from the disjoint union $G \cup H$ by adding new edges from each vertex of $G$ to each vertex of $H$.

**Conjecture 1.2** [4]. Among all graphs with $n$ vertices and $e \leq \left\lfloor \frac{n^2}{4} \right\rfloor$ edges, if $G$ is one with maximum spread, then $G$ must be bipartite.

Solving Conjecture 1.1 or characterizing the graph(s) with maximum spread among all graphs of fixed order is difficult. However, the problem is still interesting if we restrict the discussion to some special classes of graphs. In fact we may discuss Conjecture 1.2 for connected graphs with given number of edges. For trees, it is obvious that the star and the path have the maximum spread and the minimum spread among all trees with given order, respectively. For unicyclic graphs, Li et al. [7] determine the unique graph with maximum spread among all unicyclic graphs with given size of maximum matchings, and the unique graph with maximum spread among all unicyclic graphs of order $n$ when $n \geq 18$.

Recall that the girth of a graph is the minimum length of all cycles in the graph. Denote by $U_n^{k}$ the set of connected unicyclic graphs of order $n$ and girth $k$, and by $U_n$ the set of connected unicyclic graphs of order $n$. Denote by $P_k$, $C_k$, $S_k$ the path, cycle and star on $k$ vertices, respectively. Denote by $S_n^k (n \geq k \geq 3)$ the graph obtained from a cycle $C_k$ by attaching $(n - k)$ pendant edges to only one vertex of the cycle.
Lemma 1.3. (1) [5, Theorem 2; 1, Theorem 3.3] For each graph $G \in \mathcal{U}_n^k$, $\lambda_{\max}(G) \leq \lambda_{\max}(S_n^k)$ with equality if and only if $G = S_n^k$.

(2) [5, Theorem 5; 2; 1, Theorem 2.6] For each graph $G \in \mathcal{U}_n$, $\lambda_{\max}(G) \leq \lambda_{\max}(S_n^k)$ with equality if and only if $G = S_n^3$.

We prove that the graph with minimum least eigenvalue in $\mathcal{U}_n^k$ is the unique graph $S_n^k$, exactly the graph with maximum largest eigenvalue in $\mathcal{U}_n^k$ by Lemma 1.3(1). Hence $S_n^k$ is the unique graph with maximum spread among all graphs in $\mathcal{U}_n^k$. We also prove that if $G$ is one with minimum least eigenvalue in $\mathcal{U}_n$, then $G$ is $S_n^3$ if $n \geq 12$ and is $S_n^4$ if $4 \leq n \leq 11$. As a consequence, $S_n^3$ for $n \geq 6$ or $S_n^4$ for $4 \leq n \leq 5$ has the maximum spread among all graphs in $\mathcal{U}_n$. Obviously, $S_n^3$ has $n \leq \left\lfloor \frac{2n}{3} \right\rfloor$ edges (for $n \geq 4$), but $S_n^3$ is not a bipartite graph. So, Conjecture 1.2 does not hold for unicyclic graphs with order not less than 6.

The organization of this paper is as follows. In Section 2, we discuss the least eigenvalues of graphs in $\mathcal{U}_n^k$, and show that $S_n^k$ is the unique graph with minimum least eigenvalue and hence the maximum spread among all graphs in $\mathcal{U}_n^k$. In Section 3, we discuss the least eigenvalues of graphs in $\mathcal{U}_n$, and then determine the unique graph with maximum spread among all graphs in $\mathcal{U}_n$.

2. Minimizing least eigenvalue and maximizing spread among graphs in $\mathcal{U}_n^k$

Let $x = (x_1, x_2, \ldots, x_n)^T$ be a column vector in $\mathbb{R}^n$, and let $G$ be a graph on vertices $v_1, v_2, \ldots, v_n$. Then $x$ can be considered as a function defined on the vertex set of $G$, that is, for any vertex $v_i$, we map it to $x_i = x(v_i)$. We often say $x_i$ is a value of the vertex $v_i$ given by $x$. One can find that

$$x^T A(G)x = 2 \sum_{v_i, v_j \in E(G)} x(v_i) x(v_j)$$  \hspace{1cm} (2.1)

and $\lambda$ is an eigenvalue of $G$ corresponding to the eigenvector $x$ if and only if $x \neq 0$ and

$$\lambda x(v_i) = \sum_{v_j \in N_G(v_i)} x(v_j) \quad \text{for each} \ i = 1, 2, \ldots, n,$$  \hspace{1cm} (2.2)

where $N_G(v_i) = \{w : v_i w \in E(G)\}$, the neighborhood of $v_i$ in the graph $G$. Eq. (2.2) is called a $(\lambda, x)$-eigenequation of $G$.

Let $G_1, G_2$ be two disjoint connected graphs, and let $v_1 \in G_1, v_2 \in G_2$. We then obtain a new graph $G$ from $(G_1 - v_1) \cup (G_2 - v_2)$ by adding a new vertex $w$ together with edges joining $w$ and each vertex of $N_{G_1}(v_1) \cup N_{G_2}(v_2)$. Intuitively, $G$ is obtained from $G_1, G_2$ by identifying $v_1$ with $v_2$ and forming a new vertex $w$. In the following we still take $v_1$ or $v_2$ as a vertex of $G$ rather than using $w$. If $G_1$ (or $G_2$) is trivial (i.e. a graph with only one vertex), then $G = G_2$ (or $G = G_1$). If $G_1$ and $G_2$ have both at least two vertices, then $w$ is a cut vertex of $G$. Next we give a result on the variation of the least eigenvalue of a graph under the above graph operation (see Fig. 2.1).

Lemma 2.1. Let $G_1$ and $G_2$ be two disjoint nontrivial connected graphs, and let $\{v_1, v_2\} \subseteq V(G_1), u \in V(G_2)$. Let $G$ (respectively, $\bar{G}$) be obtained from $G_1, G_2$ by identifying the vertex
If there exists an eigenvector \( x \) of \( G \) corresponding to its least eigenvalue such that \( |x(v_1)| \geq |x(v_2)| \), then

\[
\lambda_{\min}(\tilde{G}) \leq \lambda_{\min}(G) \tag{2.3}
\]

with equality if and only if \( x \) is an eigenvector of \( \tilde{G} \) corresponding to its least eigenvalue, \( x(v_1) = x(v_2) \) and \( \sum_{w \in NG_2(u)} x(w) = 0 \).

**Proof.** Assume that \( x \) is a unit vector and \( x(v_1) \geq 0 \). Denote \( \alpha := \sum_{w \in NG_2(u)} x(w) \). Let \( E_1 = \{v_1 \in E(\tilde{G}) : w \in NG_2(u)\} \), \( E_2 = \{v_2 \in E(G) : w \in NG_2(u)\} \). We divide the discussion into cases, and simply write \( x(v_i) \) as \( x_i \).

**Case 1.** \( x(v_2) \geq 0 \). If \( \alpha \leq 0 \), we have

\[
\frac{1}{2} \lambda_{\min}(\tilde{G}) \leq \frac{1}{2} x^T A(\tilde{G})x = \sum_{v_i, v_j \in E(\tilde{G})} x_i x_j
\]

\[
= \sum_{v_i, v_j \in E(\tilde{G}) \setminus E_1} x_i x_j + \sum_{v_i, v_j \in E_1} x_i x_j
\]

\[
= \sum_{v_i, v_j \in E(\tilde{G}) \setminus E_1} x_i x_j + x_1 \cdot \alpha
\]

\[
\leq \sum_{v_i, v_j \in E(\tilde{G}) \setminus E_1} x_i x_j + x_2 \cdot \alpha
\]

\[
= \sum_{v_i, v_j \in E(\tilde{G}) \setminus E_1} x_i x_j + \sum_{v_i, v_j \in E_2} x_i x_j
\]

\[
= \sum_{v_i, v_j \in E(G) \setminus E_1} x_i x_j + \frac{1}{2} x^T A(G)x
\]

\[
= \frac{1}{2} \lambda_{\min}(G).
\]

If the equality holds, then \( x \) is also an eigenvector of \( \tilde{G} \) corresponding to the least eigenvalue \( \lambda_{\min}(\tilde{G}) = \lambda_{\min}(G) := \beta \). By comparing the \((\beta, x)\)-eigenequations of \( \tilde{G} \) and \( G \) on an arbitrary
vertex of $N_{G_2}(u)$ and on the vertex $v_1$, we have $x(v_1) = x(v_2)$ and $\alpha = 0$, respectively. The sufficiency is easily verified by the above inequalities.

If $\alpha > 0$, let $\bar{x}$ be obtained from $x$ only by replacing $x(w)$ by $-x(w)$ for each vertex $w \in V(G_2) \setminus \{u\}$ and preserving the values of other vertices. We have

$$\frac{1}{2} \lambda_{\min}(\tilde{G}) \leq \frac{1}{2} \bar{x}^T A(\tilde{G}) \bar{x} = \sum_{v_i v_j \in E(\tilde{G})} \bar{x}_i \bar{x}_j$$

$$= \sum_{v_i v_j \in E(\tilde{G}) \setminus (E_1 \cup E(G_2 - u))} \bar{x}_i \bar{x}_j + \sum_{v_i v_j \in E_1} \bar{x}_i \bar{x}_j + \sum_{v_i v_j \in E(G_2 - u)} \bar{x}_i \bar{x}_j.$$ 

Clearly

$$\sum_{v_i v_j \in E_1} \bar{x}_i \bar{x}_j = x_1 \cdot (-\alpha) \leq x_2 \cdot \alpha = \sum_{v_i v_j \in E_2} x_i x_j,$$

$$\sum_{v_i v_j \in E(G_2 - u)} \bar{x}_i \bar{x}_j = \sum_{v_i v_j \in E(G_2 - u)} x_i x_j.$$

Hence

$$\frac{1}{2} \lambda_{\min}(\tilde{G}) \leq \sum_{v_i v_j \in E(G)} x_i x_j = \frac{1}{2} x^T A(G) x = \frac{1}{2} \lambda_{\min}(G).$$

If the equality holds, then $\bar{x}$ is also an eigenvector of $\tilde{G}$ corresponding to the least eigenvalue $\lambda_{\min}(\tilde{G}) = \lambda_{\min}(G) := \beta$. By comparing the $(\beta, \bar{x})$-eigenequation of $\tilde{G}$ and the $(\beta, x)$-eigenequation of $G$ on the vertex $v_1$, we have $\alpha = 0$, a contradiction. Hence the above inequality holds strictly.

**Case 2.** $x(v_2) < 0$. For the case of $\alpha \leq 0$ (respectively, $\alpha > 0$), the discussion is very similar to Case 1 for $\alpha \leq 0$ (respectively, $\alpha > 0$). In both cases, inequality (2.3) cannot hold as an equality. The result follows.

**Corollary 2.2.** Let $G_0$, $G_1$ and $G_2$ be pairwisely disjoint nontrivial connected graphs, and let $\{v_1, v_2\} \subseteq V(G_0)$, $u_1 \in V(G_1)$, $u_2 \in V(G_2)$. Let $G$ be obtained by identifying the vertex $v_1$ with the vertex $u_1$ and identifying the vertex $v_2$ with the vertex $u_2$. Let $\tilde{G}$ be obtained by identifying the vertex $v_1$ first with $u_1$ and then with $u_2$. If there exists an eigenvector $x$ of $G$ corresponding to its least eigenvalue such that $|x(v_1)| \geq |x(v_2)|$, then

$$\lambda_{\min}(\tilde{G}) \leq \lambda_{\min}(G)$$

with equality if only if $x$ is an eigenvector of $\tilde{G}$ corresponding to its least eigenvalue, $x(v_1) = x(v_2)$ and $\sum_{w \in N_{G_2}(u_2)} x(w) = 0$.

**Proof.** Let $H$ be the graph obtained from $G_0$, $G_1$ by identifying the vertex $v_1$ and $u_1$. The result follows from Lemma 2.1 by viewing $H$, $G_2$ as $G_1$, $G_2$ of Lemma 2.1, respectively (see Fig. 2.2).

**Corollary 2.3.** Let $x$ be an eigenvector of $S^k_n$ ($n > k$) corresponding to its least eigenvalue, and let $w$ be the vertex on the cycle of $S^k_n$ incident to pendent edge(s). Then $w$ is the unique
vertex such that \( x(w) \) has maximum modulus among all vertices on the cycle of \( S^n_k \), and hence \( x(w) \neq 0 \).

**Proof.** Assume, to the contrary, there exists another vertex \( u \) on the cycle such that \( x(u) \) has maximum modulus and hence \( |x(u)| \geq |x(w)| \). Let \( S \) be the set of pendent vertices of \( S^n_k \). Let \( G \) be a graph obtained from \( S^n_k \) by deleting all pendent edges incident to \( w \) and attaching them to \( u \). By Lemma 2.1, \( \lambda_{\min}(G) \leq \lambda_{\min}(S^n_k) \). Obviously, \( G \cong S^n_k \), therefore, \( \lambda_{\min}(G) = \lambda_{\min}(S^n_k) \).

Hence, also by Lemma 2.1, 
\[
\lambda_{\min}(G) = \lambda_{\min}(S^n_k).
\]

By Eq. (2.2), each vertex of \( S \) has same value given by \( x \) as \( \lambda_{\min}(S^n_k) = 0 \), which implies \( x(v) = 0 \) for each \( v \in S \) and hence \( x(w) = x(u) = 0 \). So each vertex on the cycle has value 0, and then \( x = 0 \), a contradiction. Therefore, \( w \) is the unique vertex such that \( x(w) \) has maximum modulus among all vertices on the cycle of \( S^n_k \), and hence \( x(w) \neq 0 \).

**Corollary 2.4.** Let \( H \) be a star on at least three vertices whose central vertex is \( s \), and let \( t \) be any of its pendent vertices. Let \( G \) be a nontrivial connected rooted graph with a root \( r \). Denote by \( G_s \) (respectively, \( G_t \)) a graph obtained from \( G \) by identifying its root \( r \) with the vertex \( s \) (respectively, the vertex \( t \)) of \( H \). Then

\[
\lambda_{\min}(G_s) \leq \lambda_{\min}(G_t);
\]

furthermore, if \( G \) is obtained from a rooted cycle by attaching some pendent edges at its root \( r \), then the above inequality holds strictly.

**Proof.** Let \( H_1, H_2 \) be respectively the induced subgraphs of \( H \) by the vertices \( s, t \) and by the vertices of \( V(H) \setminus \{t\} \). Let \( x \) be an eigenvector of \( G_t \) (shown in Fig. 2.3a) corresponding to its least eigenvalue. If \( |x(t)| \geq |x(s)| \), then by viewing \( H_1 \) (respectively, \( G \) and \( H_2 \)) as the graph \( G_0 \) (respectively, \( G_1 \) and \( G_2 \)) of Corollary 2.2, \( \lambda_{\min}(G_s) = \lambda_{\min}(G_t) \leq \lambda_{\min}(G_i) \), where \( G_s \) is one isomorphic to \( G_s \) shown in Fig. 2.3b. If the equality holds, then \( x(t) = x(s) \) and \( \sum_{w \in N_{H_2}(s)} x(w) = 0 \) by Corollary 2.2. By Eq. (2.2), each vertex of \( N_{H_2}(s) \) has the same value given by \( x \) as \( \lambda_{\min}(G_i) \neq 0 \). Hence, \( x(w) = 0 \) for each \( w \in N_{H_2}(s) \), which implies \( x(t) = x(s) = 0 \) by Eq. (2.2).

If \( |x(t)| < |x(s)| \), by viewing \( H_1 \) (respectively, \( G \) and \( H_2 \)) as the graph \( G_0 \) (respectively, \( G_2 \) and \( G_1 \)) of Corollary 2.2, we also get the inequality \( \lambda_{\min}(G_s) \leq \lambda_{\min}(G_i) \), where \( G_s \) is shown in Fig. 2.3c. In this case the inequality holds strictly as \( x(t) \neq x(s) \).

![Fig. 2.2. The graphs G and \( \tilde{G} \) in Corollary 2.2.](image-url)
If $G$ is obtained from a rooted cycle by attaching some pendent edges at the root $r$, and inequality (2.4) holds as an equality, from above discussion we find that only does the case of $|x(t)| \geq |x(s)|$ occur, in which case $\widetilde{G}_s$ is of type $S_n^k$ for some $n$ and $k$, and $x$ is an eigenvector $\widetilde{G}_s$ corresponding to its least eigenvalue with $x(t) = 0$, a contradiction to Corollary 2.3. □

Corollary 2.5. Let $G$ be a graph of order $n$ which is obtained from a cycle $C_k$ by attaching $l$ pendent edges and $m$ pendent edges respectively to two distinct vertices of the cycle, where $l \geq 1$, $m \geq 1$ and $k + l + m = n$. Then

$$\lambda_{\min}(S_n^k) < \lambda_{\min}(G).$$

Proof. Let $u$, $w$ be two distinct vertices on the cycle of $G$ incident to $l$, $m$ pendent edges, respectively. Let $x$ be an eigenvector of $G$ corresponding to its least eigenvalue. We may assume that $|x(w)| \geq |x(u)|$. Then by Corollary 2.2, $\lambda_{\min}(\widetilde{G}) \leq \lambda_{\min}(G)$, where $\widetilde{G}$ is obtained from the cycle $C_k$ by attaching $l + m$ pendent edges to the vertex $w$. Clearly, $\widetilde{G} \cong S_n^k$, and then $\lambda_{\min}(S_n^k) \leq \lambda_{\min}(G)$. If the equality holds, by Corollary 2.2, $x(u) = x(w)$, and $\sum_{v \in S} x(v) = 0$, where $S$ is the set of pendent vertices adjacent to $u$ in the graph $G$. By Eq. (2.2), each vertex of $S$ has the same value given by $x$, and hence has value 0, which implies $x(w) = x(u) = 0$ also by Eq. (2.2). By Corollary 2.2, $x$ is also an eigenvector of $\widetilde{G} \cong S_n^k$ corresponding to its least eigenvalue with $x(w) = 0$, a contradiction to Corollary 2.3. □

Corollary 2.6. Let $G$ be a nontrivial connected graph containing a vertex $u$, and let $G(k, l)$ ($k \geq 1$) be a graph obtained from $G$ by attaching two hanging paths $P_k$ and $P_l$ at the vertex $u$ (i.e. by identifying $u$ first with one pendant vertex of $P_k$ and then with one pendant vertex of $P_l$). Then for $l \geq 2$,

$$\lambda_{\min}(G(k, l)) \leq \lambda_{\min}(G(k + l − 1, 1)).$$

Proof. Let $u$, $w$ be two pendent vertices of the hanging path $P_{k+l-1}$ of $G(k + l − 1, 1)$ shown in Fig. 2.4a, where $u$ is the common vertex of $G$ and $P_{k+l-1}$. Let $v$ be the $k$th vertex of the path $P_{k+l-1}$ (counted from $u$), and let $P_k$ (respectively, $P_l$) be the sub-path of $P_{k+l-1}$ connecting $u$ and $v$ (respectively, $v$ and $w$). Let $x$ be an eigenvector of $G(k + l − 1, 1)$ corresponding to
its least eigenvalue. If $|x(u)| \geq |x(v)|$, by viewing $P_k$ (respectively, $G$ and $P_l$) as the graph $G_0$ (respectively, $G_1$ and $G_2$) of Corollary 2.2, then

$$\lambda_{\text{min}}(G(k, l)) \leq \lambda_{\text{min}}(G(k + l - 1, 1)),$$

where $G(k, l)$ is shown in Fig. 2.4b.

If $|x(u)| < |x(v)|$, then by viewing $P_k$ (respectively, $G$ and $P_l$) as the graph $G_0$ (respectively, $G_2$ and $G_1$) of Corollary 2.2, the above inequality also holds, in which case $G(k, l)$ is shown in Fig. 2.4c. □

**Theorem 2.7.** Let $C\{T_{ni}\} \in \mathcal{V}_{k}^{n}$, which is obtained from a cycle $C_k$ on vertices $c_1, c_2, \ldots, c_k$ by identifying $c_i$ with the root of a rooted tree $T_{ni}$ of order $n_i$ for each $i = 1, 2, \ldots, k$, where $n_i \geq 1$ and $\sum_{i=1}^{k} n_i = n$. Let $C\{S_{ni}\}$ (respectively, $C\{P_{ni}\}$) be obtained from $C\{T_{ni}\}$ by replacing each $T_{ni}$ by a rooted star $S_{ni}$ with the center as its root (respectively, a rooted path $P_{ni}$ with one pendent vertex as its root). Then

$$\lambda_{\text{min}}(C\{S_{ni}\}) \leq \lambda_{\text{min}}(C\{T_{ni}\}) \leq \lambda_{\text{min}}(C\{P_{ni}\}).$$

**Proof.** Assume that $T_{ni} \neq S_{ni}$ (including roots) for some $n_i$. Let $v$ be a vertex in $T_{ni}$ such that $d(v) > 2$ and $d(v, c_i)$ is largest among all vertices of $T_{ni}$, where $d(v, c_i)$ denotes the distance of $v$ to $c_i$. Then there are at least two hanging paths attached at $v$. For any hanging path $P_t$ ($t \geq 3$) at $v$, if $P_t$ is replaced by identifying the second vertex of $P_t$ (counted from $v$) with $v$, denoted the resulting graph as $G$, then by Corollary 2.6, $\lambda_{\text{min}}(G) \leq \lambda_{\text{min}}(C\{T_{ni}\})$. If $t \geq 4$, then we continue the above procedure for the hanging path $P_{t-1}$ of $G$ attached at $v$. Repeatedly using Corollary 2.6, then $P_t$ is at last replaced by a star $S_t$ with its center identified with $v$, and the least eigenvalue of resulting graph is not larger than that of $C\{T_{ni}\}$.

Repeating the same procedure for other hanging paths at $v$, we then get a star with $v$ being its center whose order is equal to the sum of above paths. Let $w$ be a vertex in $T_{ni}$, adjacent to $v$, and belonging to the unique path between $c_i$ and $v$. By Corollary 2.4, the least eigenvalue is not increased when all pendant edges at $v$ are relocated such that they become the pendant edges at
w. Note that $d(w, c_i) = d(v, c_i) - 1$. Repeating the same procedure for any other vertex as $v$, we arrive at $C\{S_{n_i}\}$, as desired.

Assume that $T_{n_i} \neq P_{n_i}$ (including roots) for some $n_i$. Let $v$ be a vertex defined in the first paragraph. By Corollary 2.6, when any two hanging paths at $v$ are replaced by a single path with length equal to the sum of the two paths, then the least eigenvalues is not decreased. Repeating this procedure (for any other vertex as $v$), we arrive at $C\{P_{n_i}\}$, as desired. □

**Theorem 2.8.** Let $G \in \mathcal{U}^k_n$. Then

$$\lambda_{\min}(G) \geq \lambda_{\min}(S^k_n)$$

with equality if and only if $G = S^k_n$.

**Proof.** Let $G = C\{T_{n_i}\}$ defined as in Theorem 2.7. Assume that $G \neq S^k_n$. If there exists exactly one $n_i$, say $n_1$, such that $n_1 > 1$, i.e. $G$ is obtained from a cycle $C_k$ by identifying one vertex with some vertex of a tree $T_{n_1}$ of order $n_1$, then according the procedure in the first and second paragraphs of the proof of Theorem 2.7

$$\lambda_{\min}(G) \geq \lambda_{\min}(\tilde{G}) \geq \lambda_{\min}(S^k_n),$$

where $\tilde{G}$ is obtained from $S^k_m$ by attaching $(n - m)$ pendent edges to one of its pendent vertices for some integer $m$ with $k + 1 \leq m \leq n - 1$. By Corollary 2.4, $\lambda_{\min}(\tilde{G}) > \lambda_{\min}(S^k_n)$, and the result follows in this case.

If there exist more than one $n_i$’s such that $n_i > 1$, by Theorem 2.7, $\lambda_{\min}(G) \geq \lambda_{\min}(C\{S_{n_i}\})$. So it is enough to deal with $C\{S_{n_i}\}$. Repeatedly using Corollary 2.2, we have

$$\lambda_{\min}(G) \geq \lambda_{\min}(\widehat{G}) \geq \lambda_{\min}(S^k_n),$$

where $\widehat{G}$ is obtained from $S^k_m$ by attaching $n - m$ pendent edges to some vertex on the cycle with degree 2 for some integer $m$ with $k + 1 \leq m \leq n - 1$. By Corollary 2.5, $\lambda_{\min}(\widehat{G}) > \lambda_{\min}(S^k_n)$. The result also follows. □

By Lemma 1.3(1) and Theorem 2.8, we get the following result.

**Theorem 2.9.** Let $G \in \mathcal{U}^k_n$. Then

$$s(G) \leq s(S^k_n)$$

with equality if and only if $G = S^k_n$.

3. Minimizing least eigenvalue and maximizing spread among graphs in $\mathcal{U}_n$

In this section, we first determine the graph(s) whose least eigenvalue attains the minimum among all graphs in $\mathcal{U}_n$, and then characterize the graph(s) with maximum spread among all graphs in $\mathcal{U}_n$.

**Lemma 3.1.** For $3 \leq k \leq n - 1$, $\lambda_{\max}(S^k_{n+1}) < \lambda_{\max}(S^k_n)$.

**Proof.** For the case of $3 \leq k \leq n - 1$, let $w$ be the unique vertex on the cycle of $S^k_n$ incident to pendent edge(s). Let $x$ be a unit Perron vector of $A(S^k_n)$. We claim that $x(w) > x(v)$ for any other
vertex $v$ on the cycle of $S_n^k$. If not, let $u$ be a vertex on the cycle with $x(u) \geq x(w)$. Let $G$ be obtained from $S_n^k$ by deleting all pendent edges incident to $w$ and attaching them to $u$. Then by Eq. (2.1)
\[
\lambda_{\max}(G) \geq x^T A(G)x \geq x^T A(S_n^k)x = \lambda_{\max}(S_n^k).
\]
Note that $G \cong S_n^k$ and hence $\lambda_{\max}(G) = \lambda_{\max}(S_n^k):= \alpha$. So, $x$ is also a Perron vector of $A(G)$.

However, by the $(\alpha, x)$-eigenvalues of $S_n^k$ and $G$ on the vertex $w$ (or $u$), we get a contradiction as $x$ has all entries positive. If $k = n$, then $S_n^k = C_n$ and $A(C_n)$ has the all ones vector as a Perron vector.

In this case we choose any vertex of $S_n^k$ as the vertex $w$.

For $3 \leq k \leq n - 1$, let $w$ be the vertex of $S_n^{k+1}$ chosen as above. Let $u$ be a vertex on the cycle of $S_n^{k+1}$ with distance 2 to $w$, and let $\tilde{u}$ be the vertex on the cycle of $S_n^{k+1}$ lying between $u$ and $w$. Let $G$ be obtained from $S_n^{k+1}$ by deleting the edge $u\tilde{u}$ of and adding a new edge $uw$. Then $G \cong S_n^k$, and if $x$ is unit Perron vector of $A(S_n^{k+1})$, then
\[
\lambda_{\max}(S_n^k) = \lambda_{\max}(G) \geq x^T A(G)x \geq x^T A(S_n^{k+1})x = \lambda_{\max}(S_n^{k+1}).
\]

The above inequality cannot hold as an equality, otherwise $x$ is a Perron vector of $A(G)$ and this will cause a contradiction by considering the eigenequations of $G$ and $S_n^{k+1}$ on the vertex $w$.

**Lemma 3.2.** For $2 \leq k \leq \frac{n-1}{2}$
\[
\lambda_{\min}(S_n^{2k+1}) > \lambda_{\min}(S_n^{2k})
\]
and if $G$ is a graph whose least eigenvalue attains the minimum among all graphs in $\mathcal{U}_n$, then $G$ is either $S_n^3$ or $S_n^4$.

**Proof.** Let $C_{2k+1}$ be the cycle of $S_n^{2k+1}$ with vertices labeled as $c_1, c_2, \ldots, c_{2k+1}$ (in anticlockwise way), where $c_1$ is adjacent to pendent vertices if $n > 2k + 1$. Note that there exists an automorphism $\varphi$ of $S_n^{2k+1}$ which maps $c_i$ to $c_{2k+3-i}$ for $i = 2, 3, \ldots, k + 1$ and preserves other vertices. Let $x$ be a unit eigenvector of $S_n^{2k+1}$ corresponding to the least eigenvalue. If $n > 2k + 1$, we may assume $x(c_1) > 0$ by Corollary 2.3. If $n = 2k + 1$, we may choose a vertex as $c_1$ such that $x(c_1) > 0$. Define a vector $x_{\varphi}$ such that $x_{\varphi}(v) = x(\varphi(v))$ for each vertex $v$ of $S_n^{2k+1}$. Then $x_{\varphi}$, and hence $x + x_{\varphi}$ (as $x(c_1) \neq 0$), is also an eigenvector of $S_n^{2k+1}$ corresponding to the least eigenvalue.

By above discussion, there exists a unit eigenvector $x$ of $S_n^{2k+1}$ corresponding to the least eigenvalue such that
\[
x(c_i) = x(c_{2k+3-i}) \quad \text{for} \quad i = 2, 3, \ldots, k + 1.
\]

Let $x(c_{k+1}) = x(c_{k+2}) := \alpha$. If $\alpha = 0$, then by Eq. (2.2), $x(c_k) = x(c_{k-1}) = \cdots = x(c_1) = 0$, a contradiction. If $\alpha > 0$, then $x(c_{k+3}) < 0$ by Eq. (2.2) as $\lambda_{\min}(S_n^{2k+1}) < 0$. Similarly, if $\alpha < 0$ then $x(c_{k+3}) > 0$. So in both cases, we have
\[
x(c_{k+1})x(c_{k+2}) > x(c_{k+1})x(c_{k+3}).
\]
Now replacing the edge $c_{k+1}c_{k+2}$ of $S_n^{2k+1}$ by $c_{k+1}c_{k+3}$, we get a new graph $H \in \mathcal{U}_n^{2k}$, and
\[
\lambda_{\min}(H) \leq x^T A(H)x < x^T A(S_n^{2k+1})x = \lambda_{\min}(S_n^{2k+1}).
\]
By Theorem 2.8
\[
\lambda_{\min}(S_n^{2k}) \leq \lambda_{\min}(H) < \lambda_{\min}(S_n^{2k+1}).
\]
The first result follows.
Next we prove the second result. Suppose that $G$ is a graph whose least eigenvalue attains the minimum among all graphs in $\mathcal{U}_n$. Then $G = S^k_n$ for some integer $k$ by Theorem 2.8. If $k$ is even, then $k = 4$; otherwise, by Lemma 3.1, $\lambda_{\text{max}}(S^k_n) < \lambda_{\text{max}}(S^3_n)$, and by the fact that $S^k_n, S^4_n$ are both bipartite

$$\lambda_{\min}(S^k_n) = -\lambda_{\max}(S^k_n) > -\lambda_{\max}(S^4_n) = \lambda_{\min}(S^4_n),$$

which yields a contradiction. If $k$ is odd, then $k = 3$; otherwise, $k = 2l + 1$ for some $l \geq 2$, and by the result we have proved

$$\lambda_{\min}(S^{2l+1}_n) > \lambda_{\min}(S^{2l}_n) \geq \lambda_{\min}(S^4_n),$$

which also yields a contradiction. The result follows. □

Lemma 3.3 [3]. Let $G$ be a graph containing a vertex $u$, and let $\mathcal{C}(u)$ be the set of all cycles of $G$ containing $u$. Then

$$P(G, \lambda) = \lambda P(G - u, \lambda) - \sum_{v \in N_G(u)} P(G - u - v, \lambda) - 2 \sum_{Z \in \mathcal{C}(u)} P(G - V(Z), \lambda).$$

Lemma 3.4 [3]. Let $G$ be a graph of order $n$, and let $V' \subseteq V(G)$ consisting of $k$ vertices. Then

$$\lambda_i(G) \leq \lambda_i(G - V') \leq \lambda_i+k(G) \quad \text{for } 1 \leq i \leq n - k.$$

Lemma 3.5 [12]. If $4 \leq n \leq 11$, then $\lambda_{\min}(S^4_n) < \lambda_{\min}(S^3_n)$; and if $n \geq 12$, then $\lambda_{\min}(S^3_n) < \lambda_{\min}(S^4_n)$.

Proof. By Lemma 3.3, we get

$$P(S^3_n, \lambda) = \lambda^{n-4}[\lambda^4 - n\lambda^2 - 2\lambda + (n - 3)], \quad P(S^4_n, \lambda) = \lambda^{n-4}[\lambda^4 - n\lambda^2 + 2(n - 4)].$$

Obviously, $\lambda_{\min}(S^4_n) = -\sqrt{\frac{n+\sqrt{(n-4)^2+16}}{2}}$. Let $f(\lambda) = \lambda^4 - n\lambda^2 - 2\lambda + (n - 3)$. Then $f(\lambda)$ have the same nonzero roots as $P(S^3_n, \lambda)$, and $f(\lambda_{\min}(S^4_n)) = 5 - n + \sqrt{2(n + \sqrt{(n-4)^2+16})}$. With help of the software MATHEMATICA, we get $f(\lambda_{\min}(S^4_n)) > 0$ if $4 \leq n \leq 11$, $f(\lambda_{\min}(S^4_n)) < 0$ if $n \geq 12$. By Lemma 3.4

$$\lambda_{\min}(S^4_n) \leq \lambda_{\min}(S^4_n - u) = \lambda_{\min}(S^3_{n-1}) = \lambda_{\min}(S^3_n - w) \leq \lambda_2(S^3_n),$$

where $u$ is a vertex on the cycle of $S^4_n$ with distance 2 to the vertex with maximum degree if $n > 4$ and $u$ is chosen arbitrarily if $n = 4$, and $w$ is a vertex of $S^3_n$ with degree 2. Then the results follow. □

Note that in [12] the authors give a similar proof of Lemma 3.5. Here we rewrite the proof for completeness. By Lemmas 3.2 and 3.5, we have the following theorem.

Theorem 3.6. Let $G \in \mathcal{U}_n$. Then

(1) if $4 \leq n \leq 11$, $\lambda_{\min}(G) \geq \lambda_{\min}(S^4_n)$, with equality if and only if $G = S^4_n$;
(2) if $n \geq 12$, $\lambda_{\min}(G) \geq \lambda_{\min}(S^3_n)$, with equality if and only if $G = S^3_n$. 

Theorem 3.7. Let $G \in \mathcal{U}_n$. Then

1) if $n = 4, 5$, $s(G) \leq s(S^4_n)$, with equality if and only if $G = S^4_n$;
2) if $n \geq 6$, $s(G) \leq s(S^3_n)$, with equality if and only if $G = S^3_n$.

Proof. Suppose $G$ is one with maximum spread among all graphs in $\mathcal{U}_n$. Then by Theorem 2.9, $G = S^k_n$ for some integer $k$. By Lemmas 3.1 and 3.2, $G$ is $S^3_n$ or $S^4_n$. If $n \geq 12$, the result holds by Lemma 1.3(2) and Theorem 3.6. If $n \leq 11$, we verify the result by the software MATHEMATICA; see Fig. 3.1. □

References