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THE LEAST EIGENVALUE OF GRAPHS WHOSE COMPLEMENTS ARE UNICYCLIC

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Abstract

A graph in a certain graph class is called minimizing if the least eigenvalue of its adjacency matrix attains the minimum among all graphs in that class. Bell *et al.* have identified a subclass within the connected graphs of order n and size m in which minimizing graphs belong (the complements of such graphs are either disconnected or contain a clique of size $\frac{n}{2}$). In this paper we discuss the minimizing graphs of a special class of graphs of order n whose complements are connected and contains exactly one cycle (namely the class $\mathscr{U}_n^c$ of graphs whose complements are unicyclic), and characterize the unique minimizing graph in $\mathscr{U}_n^c$ when $n \geq 20$.

Keywords: unicyclic graph, complement, adjacency matrix, least eigenvalue.

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1. Introduction

Let $G = (V, E)$ be a simple graph with vertex set $V = V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E = E(G)$. The *adjacency matrix* of G is a matrix $A(G) = [a_{ij}]$

of order n, where $a_{ij} = 1$ if v_i is adjacent to v_j, and $a_{ij} = 0$ otherwise. Since $A(G)$ is real and symmetric, its eigenvalues are real and can be arranged as: $\lambda_1(G) \leq \lambda_2(G) \leq \cdots \leq \lambda_n(G)$. The eigenvalues of $A(G)$ are referred to as the *eigenvalues* of G. The eigenvalue $\lambda_n(G)$ is the spectral radius of $A(G)$; and there are many results in literatures concerning this eigenvalue of $A(G)$ (see, e.g. [3] for some older results).

The least eigenvalue $\lambda_1(G)$ is now denoted by $\lambda_{\min}(G)$, and the corresponding eigenvectors are called the *first eigenvectors* of G. In contrast to the largest eigenvalue, the least eigenvalue has received much less attention in the literature. In the past the main work on the least eigenvalue of a graph is focused on its bounds; see e.g. [4, 7]. Recently, the problem of minimizing the least eigenvalues of graphs subject to graph parameters has received much more attention, since two papers of Bell *et al.* [1, 2] and one paper of our group [5] appeared in the same issue of the journal Linear Algebra and Its Applications. Ye and Fan [14] discuss the connectivity and the least eigenvalue of a graph. Liu *et al.* [8] discuss the least eigenvalues of unicyclic graphs with given number of pendant vertices. Petrović *et al.* [9, 10] discuss the least eigenvalues of bicyclic graphs and get further results for the graphs of order n and size $n + k$, where $0 \leq k \leq 4$ and $n \geq k + 5$. Wang *et al.* [12, 13] discuss the least eigenvalue and the number of cut vertices of a graph. Tan and Fan [11] discuss the least eigenvalue and the vertex/edge independence number, the vertex/edge cover number of a graph.

For convenience, a graph is called *minimizing* in a certain graph class if its least eigenvalue attains the minimum among all graphs in the class. Let $\mathscr{G}(n, m)$ denote the class of connected graphs of order n and size m. Bell *et al.* (see [1, Theorem 1]) have characterized the structure of the minimizing graphs in $\mathscr{G}(n, m)$ as follows.

Theorem 1. *Let G be a minimizing graph in $\mathscr{G}(n, m)$. Then G is either*

(i) *a bipartite graph, or*

(ii) *a join of two nested split graphs (not both totally disconnected).*

We observe here that the complements of the minimizing graphs in $\mathscr{G}(n, m)$ are either disconnected or contain a clique of order at least $n/2$. This motivates us to discuss the least eigenvalue of graphs whose complements are connected and contain clique of small size. In a recent work [6] we characterized the unique minimizing graph in the class of graphs of order n whose complements are trees.

In this paper, we continue this work on the complements of unicyclic graphs, and determine the unique minimizing graph in $\mathscr{U}_n^c$ for $n \geq 20$, where $\mathscr{U}_n^c$ denotes the class of the complements of connected unicyclic graphs of order n. It is easily seen that $\mathscr{U}_n^c \subsetneq \mathscr{G}\left(n, \binom{n}{2} - n\right)$. However, for the minimizing graph in $\mathscr{U}_n^c$ the conditions of Theorem 1 do not hold.

2. PRELIMINARIES

We begin with some definitions. Given a graph G of order n, we say that a vector $X \in \mathbb{R}^n$ is *defined* on G, if there is a 1-1 map φ from $V(G)$ to the entries of X; simply written $X_u = \varphi(u)$ for each $u \in V(G)$. If X is an eigenvector of $A(G)$, then it is naturally defined on $V(G)$, *i.e.* X_u is the entry of X corresponding to the vertex u. One can find that

$$X^T AX = 2\sum_{uv\in E(G)} X_u X_v, \tag{2.1}$$

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

$$\lambda X_v = \sum_{u\in N_G(v)} X_u, \quad \text{for each vertex } \ v \in V(G), \tag{2.2}$$

where $N_G(v)$ denotes the neighborhood of v in G. The equation (2.2) is called (λ, X)-*eigenequation* of G. In addition, for an arbitrary unit vector $X \in \mathbb{R}^n$,

$$\lambda_{\min}(G) \leq X^T A(G)X, \tag{2.3}$$

with equality if and only if X is a first eigenvector of G.

In this paper all unicyclic graphs are assumed to be connected. Denote by $\mathscr{U}_n$ the set of unicyclic graphs of order n, and let $\mathscr{U}_n^c = \{G^c : G \in \mathscr{U}_n\}$, where G^c denotes the complement of G. Note that $A(G^c) = \mathbf{J} - \mathbf{I} - A(G)$, where $\mathbf{J}, \mathbf{I}$ denote the all-ones matrix and the identity matrix both of suitable sizes, respectively. So for any vector $X \in \mathbb{R}^n$,

$$X^T A(G^c)X = X^T(\mathbf{J} - \mathbf{I})X - X^T A(G)X. \tag{2.4}$$

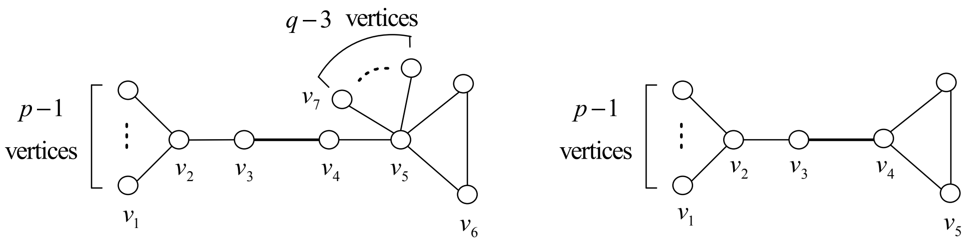

Figure 2.1. The graphs $\mathbf{U}(p, q)$ (left side) and $\mathbf{U}'(p)$ (right side).

A *star* of order n, denoted by $K_{1,n-1}$, is a tree of order n with $n-1$ pendant edges attached to a fixed vertex. The vertex of degree $n-1$ in $K_{1,n-1}$ is called the *center* of $K_{1,n}$. A cycle and a complete graph both of order n are denoted by C_n, K_n respectively. Denote by S_n^3 the graph obtained from $K_{1,n-1}$ by adding a new edge between two pendant vertices. Next, we introduce two special unicyclic graphs denoted by $\mathbf{U}(p, q)$ and $\mathbf{U}'(p)$, respectively (see Figure 2.1). $\mathbf{U}(p, q)$ is obtained from two disjoint graphs $K_{1,p}$ $(p \geq 1)$ and $S_{q+1}^3 (q \geq 3)$ by adding a new edge between one pendant vertex of $K_{1,p}$ and one pendant vertex of S_{q+1}^3. $\mathbf{U}'(p)$

is obtained from two disjoint graphs $K_{1,p}$ ($p \geq 1$) and C_3 by adding a new edge between one pendant vertex of $K_{1,p}$ and one vertex of C_3.

For a graph G containing at least one edge, it holds $\lambda_{\min}(G) \leq -1$, with equality if and only if G is a complete graph or a union of disjoint copies of complete graphs, at least one copy being nontrivial (i.e. contains more than one vertices). So, for a unicyclic graph U other than C_4, $\lambda_{\min}(U^c) < -1$. In addition, if U^c is disconnected, then U contains a complete multipartite graph as a spanning subgraph, which implies U is C_4 or S_n^3. When $n \geq 4$, $(S_n^3)^c$ consists of an isolated vertex and a connected non-complete subgraph of order $n-1$.

At the end of this section, we will discuss the least eigenvalues of $\mathbf{U}(p,q)^c$ and $\mathbf{U}'(p)^c$. Let X be a first eigenvector of the graph $\mathbf{U}(p,q)^c$ with some vertices labeled as in Figure 2.1. By eigenequations (2.2), as $\lambda_{\min}(\mathbf{U}(p,q)^c) < -1$, all the pendant vertices attached at v_2 have the same value as v_1 given by X, say X_1. Similarly, all the pendant vertices attached at v_5 have the same value as v_7, say X_7; two vertices of degree 2 on the triangle have the same value as v_6, say X_6. Write $X_{v_i} =: X_i$ for the vertices v_i's in $\mathbf{U}(p,q)^c$ for $i = 2,3,4,5$ and $\lambda_{\min}(\mathbf{U}(p,q)^c) =: \lambda_1$ for simplicity. Then by the eigenequations (2.2) on v_i for $i = 1,2,\ldots,7$, we have

$$(2.5)\quad \begin{cases} \lambda_1 X_1 &= (p-2)X_1 + X_3 + X_4 + X_5 + 2X_6 + (q-3)X_7, \\ \lambda_1 X_2 &= X_4 + X_5 + 2X_6 + (q-3)X_7, \\ \lambda_1 X_3 &= (p-1)X_1 + X_5 + 2X_6 + (q-3)X_7, \\ \lambda_1 X_4 &= (p-1)X_1 + X_2 + 2X_6 + (q-3)X_7, \\ \lambda_1 X_5 &= (p-1)X_1 + X_2 + X_3, \\ \lambda_1 X_6 &= (p-1)X_1 + X_2 + X_3 + X_4 + 2X_6 + (q-4)X_7. \end{cases}$$

Transform (2.5) into a matrix equality $(B - \lambda_1 \mathbf{I})X' = 0$, where $X' = (X_1, X_2, \ldots, X_7)^T$ and the matrix B of order 7 is easily seen. We have

$$\begin{aligned} f(\lambda;p,q) \;&:= \det(B - \lambda\mathbf{I}) = (-8 + 2p + 2q) \\ (2.6)\qquad &+(13 - 11p - 7q + 4pq)\lambda + (20 - 6q - 4qp)\lambda^2 \\ &+(-1 + 11p + 7q - 7pq)\lambda^3 + (-20 + 12p + 12q - 2pq)\lambda^4 \\ &+(-16 + 6p + 6q)\lambda^5 + (-6 + p + q)\lambda^6 - \lambda^7. \end{aligned}$$

So λ_1 is the least root of the polynomial $f(\lambda;p,q)$.

Let Y be a first eigenvector of the graph $\mathbf{U}'(p)^c$ with some vertices labeled as in Figure 2.1. By a similar discussion, all the pendant vertices attached at v_2 have the same values given by Y, say Y_1. Two vertices of degree 2 on the triangle have the same values, say Y_5. Write $Y_{v_i} =: Y_i$ for the vertices v_i's in $\mathbf{U}'(p)^c$ for $i = 2,3,4$ and $\lambda_{\min}(\mathbf{U}'(p)^c) =: \lambda_1'$ for simplicity. Then by the eigenequations (2.2) on v_i for $i = 1,2,\ldots,5$,

$$(2.7)\qquad \begin{cases} \lambda_1' Y_1 &= (p-2)Y_1 + Y_3 + Y_4 + 2Y_5, \\ \lambda_1' Y_2 &= Y_4 + 2Y_5, \\ \lambda_1' Y_3 &= (p-1)Y_1 + Y_4 + 2Y_5, \\ \lambda_1' Y_4 &= (p-1)Y_1 + Y_2, \\ \lambda_1' Y_5 &= (p-1)Y_1 + Y_2 + Y_3. \end{cases}$$

It is easily found that λ_1' is the least root of the following polynomial:

$$(2.8)\qquad \begin{aligned} g(\lambda;p) &:= (-4+2p) + (3-5p)\lambda + (6-p)\lambda^2 \\ &\quad +(1+4p)\lambda^3 + (-2+p)\lambda^4 - \lambda^5. \end{aligned}$$

Lemma 2. *If $n \geq 13$, then $\lambda_{\min}(\mathbf{U}(n-5,3)^c) < \lambda_{\min}(\mathbf{U}'(n-4)^c)$.*

Proof. Write $\lambda_{\min}(\mathbf{U}(n-5,3)^c) =: \lambda_1$, $\lambda_{\min}(\mathbf{U}'(n-4)^c) =: \lambda_1'$ for simplicity. By the above discussion, λ_1 (respectively, λ_1') is the least root of $f(\lambda; n-5, 3)$ (respectively, $g(\lambda; n-4)$). Denote

$$\bar{g}(\lambda; n-4) := (\lambda+1)^2 g(\lambda; n-4).$$

Since $\lambda_1' < -1$, λ_1' is also the least root of $\bar{g}(\lambda; n-4)$. From (2.8), $g(-3; n-4) = 171 - 19(-4+n)$, and consequently $\bar{g}(n-4, -3) \leq 0$ if $n \geq 13$. Furthermore, when $\lambda \to -\infty$, $\bar{g}(\lambda; n-4) \to +\infty$, which implies $\lambda_1' \leq -3$. Obverse that when $\lambda \leq -3$,

$$\bar{g}(\lambda; n-4) - f(\lambda; n-5, 3) = (-6+n)\lambda(1+\lambda)(-2+5\lambda+2\lambda^2) > 0.$$

In particular, $f(\lambda_1'; n-5, 3) < 0$, which implies $\lambda_{\min}(\mathbf{U}(n-5,3)^c) < \lambda_1'$. The result follows. ■

Lemma 3. *Given a positive integer $n \geq 20$, for any positive integers p, q such that $p \geq 1, q \geq 3$ and $p+q = n-2$,*

$$\lambda_{\min}(\mathbf{U}(p,q)^c) \geq \lambda_{\min}(\mathbf{U}(\lceil (n-2)/2 \rceil, \lfloor (n-2)/2 \rfloor)^c),$$

with equality if and only if $p = \lceil (n-2)/2 \rceil$ and $q = \lfloor (n-2)/2 \rfloor$.

Proof. Write $\lambda_{\min}(\mathbf{U}(p,q)^c) =: \lambda_1$ for simplicity. By (2.6), we have

$$\begin{aligned} f(\lambda; p, q) - f(\lambda; p+1, q-1) &= -\lambda(2+\lambda)(-1+2\lambda)[(p-q+1)(2+\lambda)+2], \\ f(\lambda; p, q) - f(\lambda; p-1, q+1) &= \lambda(2+\lambda)(-1+2\lambda)[(p-q-1)(2+\lambda)+2]. \end{aligned}$$

In addition, $f(-2; p, q) = -10 < 0$, which implies $\lambda_1 < -2$.

If $q \geq p+1$, then for $\lambda < -2$ we have $f(\lambda; p, q) - f(\lambda; p+1, q-1) > 0$. In particular, $f(\lambda_1; p+1, q-1) < 0$, which implies

$$\lambda_{\min}(\mathbf{U}(p+1, q-1)^c) < \lambda_1 = \lambda_{\min}(\mathbf{U}(p,q)^c).$$

If $p \geq q+3(\geq 6)$, then, by (2.6), we have $f(-3;p,q) = 241 - 19p + 23q - 21pq = 241 - 19(p-q) + (4-21p)q < 0$, which implies $\lambda_1 < -3$. Observe that $f(\lambda;p,q) - f(\lambda;p-1,q+1) > 0$ when $\lambda < -3$. In particular, $f(\lambda_1;p-1,q+1) < 0$, which implies

$$\lambda_{\min}(\mathbf{U}(p-1,q+1)^c) < \lambda_1 = \lambda_{\min}(\mathbf{U}(p,q)^c).$$

To complete the proof, we need to prove $\lambda_{\min}(\mathbf{U}(p-1,q+1)^c) < \lambda_{\min}(\mathbf{U}(p,q)^c)$ when $p = q+2$. In this case, $p = \frac{n}{2}$, $q = \frac{n}{2} - 2$, and

$$f(\lambda;p,q) - f(\lambda;p-1,q+1) = \lambda(2+\lambda)(-1+2\lambda)(4+\lambda).$$

So it is enough to prove $\lambda_1 < -4$ or

$$f\left(-4;\frac{n}{2},\frac{n}{2}-2\right) = 2376 + 582n - 36n^2 < 0.$$

If $n \geq 20$, then the above inequality holds, and hence the result follows. ■

3. Main Results

By rearranging the edges of graphs, we first give a maximization of the quadratic form $X^T A(G) X$ among all trees or all unicyclic graphs G of order n, where X is a non-negative or non-positive real vector defined on G.

Lemma 4. *Let T be a tree of order n, and let X be a non-negative or non-positive real vector defined on T whose entries are ordered so that $|X_1| \geq |X_2| \geq \cdots \geq |X_n|$, i.e. with respect to their moduli. Then*

$$\sum_{uv\in E(T)} X_u X_v \leq \sum_{i=2}^{n} X_1 X_i = \sum_{uv\in E(K_{1,n-1})} X_u X_v,$$

where X is defined on $K_{1,n-1}$ such that the center has value X_1. If, in addition, X is positive or negative, and $|X_1| > |X_2|$, then the above equality holds only if $T = K_{1,n-1}$.

Proof. We may assume X is non-negative; otherwise we consider $-X$. Let w be a vertex with value X_1 given by X. If there exists a vertex v not adjacent of w, letting v' be the neighbor of v on a path of T connecting v and w, and deleting the edge vv' and adding a new edge wv, we will arrive at a new graph (tree) T', which holds

$$\sum_{uv\in E(T)} X_u X_v \leq \sum_{uv\in E(T')} X_u X_v. \tag{3.1}$$

Repeating the process on the tree T' for the non-neighbors of w, and so on, we at last arrive at a star $K_{1,n-1}$ with w as its center, and

(3.2) $\sum_{uv \in E(T)} X_u X_v \le \sum_{uv \in E(K_{1,n-1})} X_u X_v = \sum_{i=2}^{n} X_1 X_i.$

If X is positive, $X_1 > X_2$, and w is not adjacent to all other vertices in T, then the inequality (3.1), and hence (3.2), cannot hold as an equality. The result follows. ■

Lemma 5. *Let U be a unicyclic graph of order n, and let X be a non-negative or non-positive real vector defined on U whose entries are ordered so that $|X_1| \ge |X_2| \ge \cdots \ge |X_n|$, i.e. with respect to their moduli. Then*

$$\sum_{uv \in E(U)} X_u X_v \le \sum_{i=2}^{n} X_1 X_i + X_2 X_3 = \sum_{uv \in E(S_n^3)} X_u X_v,$$

where X is defined on S_n^3 such that the vertex with degree $n-1$ has value X_1, and the other two vertices on the triangle have values X_2, X_3 respectively. If, in addition, X is positive or negative, and $|X_1| > |X_2|$, then the above equality holds only if $T = S_n^3$.

Proof. We may assume X is non-negative; otherwise we consider $-X$. Let w be a vertex with value X_1 given by X. By a similar discuss to the proof of Lemma 4, we have a graph U' of order n, in which the vertex w is adjacent to all other vertices, and

(3.3) $\sum_{uv \in E(U)} X_u X_v \le \sum_{uv \in E(U')} X_u X_v = \sum_{i=2}^{n} X_1 X_i + X_{u'} X_{v'},$

where $u'v'$ is an edge of U' not incident to w. Surely,

(3.4) $X_{u'} X_{v'} \le X_2 X_3.$

So,

(3.5) $\sum_{uv \in E(U)} X_u X_v \le \sum_{i=2}^{n} X_1 X_i + X_2 X_3 = \sum_{uv \in E(S_n^3)} X_u X_v.$

If X is positive, and $X_1 > X_2$, then the equality (3.5) holds only if (3.3) holds, which implies w is adjacent to all other vertices and consequently $U = S_n^3$. The result follows. ■

Lemma 6. *Let U be a unicyclic graph of order $n \ge 5$ such that U^c is a minimizing graph in $\mathscr{U}_n^c$, and let X be a first eigenvector of U^c. Then X contains no zero entries and has at least two positive entries and two negative entries.*

Proof. As U^c is a minimizing graph in $\mathscr{U}_n^c$, $U \ne S_n^3$. We first prove that each entry of X is nonzero. One the contrary, let $X_v = 0$ for some v. As $U \ne S_n^3$, there exists two vertices $w \in N_U(v)$ and $w' \notin N_U(v)$ such that w, w' belong to the same component of $U - v$, say U_1. Let $\hat{U}^c = U - vw + vw'$, which is also unicyclic. Since $X_v = 0$, we have $\lambda_{\min}(\hat{U}^c) = \lambda_{\min}(U^c)$ by the choice of U^c and the minimality principle based on Rayley quotient. Therefore, X is as well the first eigenvector of $\hat{U}^c$. But then, by the eigenequation at v, it follows that $X_w = X_{w'}$. So, for any vertex $u \notin N_U(v)$ in the component U_1, $X_u = X_w$. This holds for any other neighbors of v in U_1 if taking each of them in the role of w. Hence all vertices in U_1 have the same values.

If there is a nontrivial component of $U-v$, say U_2, such that v is adjacent to all vertices in U_2, then U_2 consists of exactly one edge, say pq, as U is unicyclic. By the eigenequations on p, q, we also get $X_p = X_q$. So, the vertices of each component of $U-v$ have the same values.

(i) If v is not a cut vertex of U (e.g. a pendant vertex), then $U-v$ is connected, and hence $X \geq 0$ or $X \leq 0$, a contradiction.

(ii) Now suppose v is a cut vertex of U. Let $U_1, U_2, \ldots, U_k$ $(k \geq 2)$ be the components of $U-v$, which consist of vertices with same values given by X, respectively. Note that one component of $U-v$, say U_1, contains the vertices of the (unique) cycle C of U, and all other components contain pendant vertices of U. Each vertex of $U_2 \cup \cdots \cup U_k$ has nonzero value; otherwise a pendant vertex will have zero value which yields a contradiction as in (i). If all vertices of U_1 are zero valued, then we take a vertex from U_1 lying on C in the role of v, and also obtain a contradiction as in (i). By the above discussion, all vertices but v have nonzero values.

Next if $X_r X_s > 0$, where $r \in U_i, s \in U_j$ for some distinct i, j, then let $\bar{U} = U - vw + rs$, where $w \in N_U(v)$ lies in U_i. But then $\lambda_{\min}(\bar{U}^c) < \lambda_{\min}(U^c)$, a contradiction. So $U-v$ has exactly two components U_1 and U_2, one having positive valued vertices and the other having negative valued vertices.

Finally, recalling that all vertices in U_i have the same values for $i = 1, 2$, so, by the eigenequations, all vertices in U_i have the same number of neighbors (or non-neighbors) in U_i for $i = 1, 2$. This implies $U = \mathbf{U}'(1)$ if v lies on the cycle and $U = \mathbf{U}'(2)$ otherwise. It is easily check the first eigenvector of $\mathbf{U}'(1)$ or $\mathbf{U}'(2)$ has no zero entries. So we proved the first assertion.

Now we show the second assertion. On the contrary, assume that only one vertex, say v with positive value given by X. Then any other vertex u is adjacent to v in U^c, since otherwise an eigenequation does not hold at u. So v is adjacent to all other vertices in U^c, which implies U is disconnected, a contradiction. ∎

We now arrive at the main result of this paper.

Theorem 7. *Let U be a unicyclic graph of order $n \geq 20$. Then*

$$\lambda_{\min}(U^c) \geq \lambda_{\min}(\mathbf{U}(\lceil (n-2)/2 \rceil, \lfloor (n-2)/2 \rfloor)^c),$$

with equality if and only if $U = \mathbf{U}(\lceil (n-2)/2 \rceil, \lfloor (n-2)/2 \rfloor)$.

Proof. Suppose that U^c is a minimizing graph in $\mathscr{U}_n^c$ for $n \geq 20$. The result will follow if we can show that U is the unique graph $\mathbf{U}(\lceil (n-2)/2 \rceil, \lfloor (n-2)/2 \rfloor)$.

Let X be the first eigenvector of U^c with unit length. By Lemma 6, X contains no zero entries. Denote $V_+ = \{v \in V(U^c) : X_v > 0,\}$, $V_- = \{v \in$

$V(U^c) : X_v < 0\}$, both containing at least 2 elements by Lemma 6. Denote by U_+ (respectively, U_-) the subgraph of U induced by V_+ (respectively, V_-), by E' the set of edges between V_+ and V_- in U. Since U is connected, $E' \neq \emptyset$. Obviously,

$$\begin{aligned} \sum_{vv' \in E(U)} X_v X_{v'} &= \sum_{vv' \in E(U_+)} X_v X_{v'} \\ &+ \sum_{vv' \in E(U_-)} X_v X_{v'} + \sum_{vv' \in E'} X_v X_{v'}. \end{aligned} \tag{3.6}$$

First assume $|V_-| \geq 3$. The cycle of U may contain the edges of E', or is contained in one of U_+, U_-. Without loss of generality, we assume that the cycle of U is not contained in U_+; otherwise we consider the vector $-X$ instead. Let U^* be a graph obtained from U by possibly adding some edges within V^+ and V^-, such that the subgraph of U^* induced by V^+, denoted by U^*_+, is a tree, and the subgraph of U^* induced by V^-, denoted by U^*_-, is a unicyclic graph.

In the tree U^*_+, choose a vertex, say $\mathbf{u}$, with maximum modulus among all vertices of U^*_+. By Lemma 4, we will have a star, say $K_{1,p}$ centered at $\mathbf{u}$, where $p+1 = |V^+| \geq 2$, which holds

$$\sum_{vv' \in E(U_+)} X_v X_{v'} \leq \sum_{vv' \in E(U^*_+)} X_v X_{v'} \leq \sum_{vv' \in E(K_{1,p})} X_v X_{v'}. \tag{3.7}$$

In the unicyclic graph U^*_-, choosing a vertex, say $\mathbf{w}$, with maximum modulus. By Lemma 5, we have a unicyclic graph S^3_{q+1}, where $q+1 = |V_-| \geq 3$ and the vertex $\mathbf{w}$ joins all other vertices of S^3_{q+1}, which holds

$$\sum_{vv' \in E(U_-)} X_v X_{v'} \leq \sum_{vv' \in E(U^*_-)} X_v X_{v'} \leq \sum_{vv' \in E(S^3_{q+1})} X_v X_{v'}. \tag{3.8}$$

Let $\mathbf{u}', \mathbf{w}'$ be the vertices of U_+, U_- with minimum modulus among all vertices of U_+, U_-, respectively. Then

$$\sum_{vv' \in E'} X_v X_{v'} \leq X_{\mathbf{u}'} X_{\mathbf{w}'}, \tag{3.9}$$

Now by (3.6–3.9), we have

$$\begin{aligned} \sum_{vv' \in E(U)} X_v X_{v'} &\leq \sum_{vv' \in E(K_{1,p})} X_v X_{v'} \\ &+ \sum_{vv' \in E(S^3_{q+1})} X_v X_{v'} + X_{\mathbf{u}'} X_{\mathbf{w}'} \end{aligned} \tag{3.10}$$

Since $p \geq 1$, the vertex $\mathbf{u}'$ can be chosen within the pendent vertices of $K_{1,p}$ by Lemma 4. If $q \geq 3$, $\mathbf{w}'$ can be chosen within the pendent vertices of S^3_{q+1} by Lemma 5, then from (3.10) we have

$$\begin{aligned} \tfrac{1}{2} X^T A(U) X &= \sum_{vv' \in E(U)} X_v X_{v'} \leq \sum_{vv' \in E(\mathbf{U}(p,q))} X_v X_{v'} \\ &= \tfrac{1}{2} X^T A(\mathbf{U}(p,q)) X, \end{aligned} \tag{3.11}$$

and consequently

$$\begin{aligned} \lambda_{\min}(U^c) &= X^T A(U^c) X = X^T (\mathbf{J} - \mathbf{I}) X - X^T A(U) X \\ &\geq X^T (\mathbf{J} - \mathbf{I}) X - X^T A(\mathbf{U}(p,q)) X \\ &= X^T A(\mathbf{U}(p,q)^c) X \\ &\geq \lambda_{\min}(\mathbf{U}(p,q)^c). \end{aligned} \tag{3.12}$$

If $q = 2$, that is, $S^3_{q+1} = C_3$, by a similar discussion, we have $\lambda_{\min}(U^c) \geq \lambda_{\min}(\mathbf{U}'(n-4)^c)$. By Lemma 2, $\lambda_{\min}(\mathbf{U}'(n-4)^c) > \lambda_{\min}(\mathbf{U}(n-5,3)^c)$.

Next we consider the case when $|V_-| = 2$. In this case the cycle of U cannot lies in U_-. We form a graph $U^{\#}$ from U possibly by adding some edges within V^+ and V^-, such that the subgraph of $U^{\#}$ induced by V^+ is a unicyclic graph, and the subgraph of $U^{\#}$ induced by V^- is exactly K_2. Also similar to the discussion for (3.7–3.12), we have $\lambda_{\min}(U^c) \geq \lambda_{\min}(\mathbf{U}(1, n-3))$. By Lemma 3 and the above discussion,

$$\begin{aligned}\lambda_{\min}(U^c) &\geq \lambda_{\min}(\mathbf{U}(p,q)^c) \\ &\geq \lambda_{\min}(\mathbf{U}(\lceil (n-2)/2 \rceil, \lfloor (n-2)/2 \rfloor)^c).\end{aligned} \tag{3.13}$$

By the choice of U, all equalities in (3.13) hold. So $p = \lceil (n-2)/2 \rceil, q = \lfloor (n-2)/2 \rfloor$ by Lemma 3, and consequently only the case of $|V_-| \geq 3$ occurs. Also, all equalities in (3.11) and (3.12) hold, which implies that X is a first eigenvector of $\mathbf{U}(p,q)^c$. Let $\mathbf{U}(p,q)$ have some vertices labeled as in Figure 2.1, where $v_2 = \mathbf{u}, v_3 = \mathbf{u}', v_5 = \mathbf{w}, v_4 = \mathbf{w}'$.

Assertion 1: *The vertices $v_2 = \mathbf{u}$ and $v_3 = \mathbf{u}'$ are respectively the unique ones in U_+ with maximum and minimum modulus, $v_5 = \mathbf{w}$ and $v_4 = \mathbf{w}'$ are respectively the unique ones in U_- with maximum and minimum modulus.* By Lemma 6, as X is a first eigenvector of the minimizer $\mathbf{U}(p,q)^c$, $X_{v_i} =: X_i > 0$ for $i = 1,2,3$ and $X_{v_i} =: X_i < 0$ for $i = 4,5,6,7$. By (2.5), $\lambda_1(X_4 - X_7) = -X_3 - X_4 < 0$, $\lambda_1(X_6 - X_7) = -2X_6$, $\lambda_1(X_5 - X_6) = -X_4 - (q-3)X_7$, which implies that $X_5 < X_6 < X_7 < X_4 < 0$. Also by (2.5), $\lambda_1(X_1 - X_2) > 0$, $\lambda_1(X_3 - X_1) = X_1 - X_3 - X_4 > X_1 - X_3$, which implies $X_3 < X_1 < X_2$.

Assertion 2: *$U_+ = U_+^* = K_{1,p}$, $U_- = U_-^* = S^3_{q+1}$, $E_1 = \{\mathbf{u}'\mathbf{w}'\}$, i.e. $U = \mathbf{U}(\lceil (n-2)/2 \rceil, \lfloor (n-2)/2 \rfloor)$.* By the Assertion 1 and the equality in (3.11), retracing the discussion for (3.8–3.9) and applying Lemmas 4 and 5, we get $U_+ = U_+^* = K_{1,p}$, $U_- = U_-^* = S^3_{q+1}$. From the discussion for (3.9–3.11), also by Assertion 1, E_1 consists of exactly one edge, i.e. $\mathbf{u}'\mathbf{w}'$. ■

It was proved in [5] that S^3_n is the unique minimizing graph in $\mathscr{U}_n$ when $n \geq 6$. However, when $n \geq 20$, by Theorem 7, the graph $\mathbf{U}(\lceil (n-2)/2 \rceil, \lfloor (n-2)/2 \rfloor)^c$ is the unique minimizing graph in $\mathscr{U}_n^c$. So there exists some difference on the least eigenvalue of unicyclic graphs and its complements.

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