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First Eigenvalue of Nonsingular Mixed Unicyclic Graphs with Fixed Number of Branch Vertices

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Abstract. Mixed graphs are graphs whose edges may be directed or undirected. The first eigenvalue of a mixed graph is the least nonzero eigenvalue of its Laplacian matrix. We determine the unique mixed graphs with minimum first eigenvalue over all nonsingular mixed unicyclic graphs with fixed number of branch vertices, and the unique graph with minimum least signless Laplacian eigenvalue over all nonbipartite unicyclic graphs with fixed number of branch vertices.

1. Introduction

A mixed graph is a graph whose edges may be directed or undirected. This concept generalizes both the classical approach of orienting all edges and the unoriented approach, see, e.g., [2, 10]. Let G be a mixed graph with vertex set $V(G) = \{v_1, \ldots, v_n\}$ and edge set $E(G)$. Then G is obtainable from an undirected graph by assigning arbitrary orientations (two possible directions) to some of its edges. This undirected graph is called the underlying graph of G, denoted by $\widetilde{G}$. For $e \in E(G)$, the sign of e, denoted by $\mathrm{sgn}_G(e)$ (or $\mathrm{sgn}(e)$ simply), is defined as $\mathrm{sgn}_G(e) = -1$ if e is oriented and $\mathrm{sgn}_G(e) = 1$ otherwise. The adjacency matrix $A(G)$ of G is defined as the $n \times n$ matrix (a_{ij}) such that $a_{ij} = \mathrm{sgn}(v_i, v_j)$ if $(v_i, v_j) \in E(G)$, and $a_{ij} = 0$ otherwise. For each $v \in V(G)$, the degree of v in G, denoted by $d_G(v)$ (or $d(v)$ simply), is the number of neighbors of v in $\widetilde{G}$. The matrix $L(G) = A(G) + D(G)$ is the Laplacian matrix of G, where $D(G)$ is the degree diagonal matrix of G whose diagonal entries are vertex degrees of G.

Since $L(G)$ is symmetric and positive semi-definite, the eigenvalues of $L(G)$ are all nonnegative real numbers. The first eigenvalue of G is the least nonzero eigenvalue of $L(G)$, denoted by $\lambda(G)$.

Let $\overrightarrow{G}$ be the all-oriented graph obtained from G by assigning to each unoriented edge of G an arbitrary orientation. Note that $L(\overrightarrow{G})$ is the classical Laplacian matrix of $\widetilde{G}$.

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A mixed graph G is singular (or nonsingular) if $L(G)$ is singular (or nonsingular). A cycle is nonsingular if and only if it has odd number of unoriented edges, see [1, Lemma 1].

A signature matrix is a diagonal matrix with ± 1 along its diagonal. Let S be a signature matrix of order n. Then $S^T L(G) S$ is the Laplacian matrix of a mixed graph, denoted by ${}^S G$, which has the same underlying graph with G. Obviously, $L(G)$ and $L({}^S G)$ have the same spectrum and the singularity of each cycle in G and ${}^S G$ is unchanged.

Lemma 1.1. [1,15] *Let G be a connected mixed graph. Then the following statements are equivalent:*

(a) *G is singular;*

(b) *G does not contain a nonsingular cycle;*

(c) *there exists a signature matrix S such that $S^T L(G) S = L(\overrightarrow{G})$.*

Suppose G is connected. If G is singular, then by Lemma 1.1, $L(G)$ and $L(\overrightarrow{G})$ have the same spectrum, and hence the first eigenvalue of G is equal to the algebraic connectivity of $\widetilde{G}$ [8]. Suppose that G is nonsingular. By Lemma 1.1, G contains at least one nonsingular cycle, and thus G has a spanning nonsingular unicyclic subgraph. Therefore, it is natural to study the first eigenvalue of a nonsingular mixed unicylic graph.

Fan [5] studied the problems on minimizing and maximizing the first eigenvalue over all nonsingular mixed unicyclic graphs with fixed girth. Up to a signature matrix, Fan et al. [7] determined the unique graphs with minimum first eigenvalue over all nonsingular mixed unicyclic graphs with fixed girth. Liu et al. [13] considered the same question for mixed graphs with fixed number of pendant vertices, and determined the unique graph with the minimum first eigenvalue. More results on the eigenvalues of $L(G)$ and related topics may be found in [4, 6, 12, 15].

An ordinary graph G is a mixed graph with no edge oriented. In this case, $L(G)$ is just the signless Laplacian matrix of $G = \widetilde{G}$, and $\lambda(G)$ is the least signless Laplacian eigenvalue of G if G is a connected non-bipartite graph [3]. Let G be a connected non-bipartite graph on $n \geq 3$ vertices. Cardoso et al. [3] showed that the minimum value of $\lambda(G)$ is attained solely by the unicyclic graph obtained from a triangle by attaching a path at one of its terminal vertices.

A vertex of a graph is a branch vertex (or branching vertex) if its degree is at least three. The branch vertices are often used to analyze graph structures. A tree with at most one branch vertex is called a spider [11]. The problem of generating spanning trees with minimum number of branch vertices was introduced by Gargano et al. [9] and has been studied over the past decade, see, e.g. [14].

In this paper, we determine in Theorem 3.7 the unique mixed graphs (up to a signature matrix) with minimum first eigenvalue in the class of all nonsingular mixed unicyclic graphs with $n \geq 5$ vertices and k branch vertices for $k = 1, \dots, \lfloor \frac{n}{2} \rfloor$. We determine in Corollary 3.8 the unique graph with minimum least signless Laplacian eigenvalue in the class of all nonbipartite unicyclic graphs with $n \geq 5$ vertices and k branch vertices for $k = 1, \dots, \lfloor \frac{n}{2} \rfloor$.

2. Preliminaries

Let G be a mixed graph with $V(G) = \{v_1, \dots, v_n\}$. For $v \in V(G)$, let $N_G(v)$ be the set of neighbors of v in G. A first eigenvector of G is an eigenvector of $L(G)$ corresponding to $\lambda(G)$. A column vector $x = (x_{v_1}, \dots, x_{v_n})^\top \in \mathbb{R}^n$ can be considered as a function defined on $V(G)$ which maps vertex v_i to x_{v_i}, i.e., $x(v_i) = x_{v_i}$ for $i = 1, \dots, n$. One can find that

$$x^T L(G) x = \sum_{(u,v) \in E(G)} (x_u + \operatorname{sgn}(u,v) x_v)^2,$$

and λ is an eigenvalue of G with eigenvector x if and only if $x \neq 0$ and

$$(\lambda - d_G(v)) x_v = \sum_{u \in N_G(v)} \operatorname{sgn}(u,v) x_u,$$

which is called the eigenequation (of G) at v. Moreover, if G is nonsingular, then for a nonzero vector $x \in \mathbb{R}^n$,

$$\lambda(G) \leq \frac{x^T L(G) x}{x^T x}$$

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

Let $\mathcal{U}$ be the set of mixed unicyclic graphs with all edges oriented except an (arbitrary) edge on the (unique) cycle. By Lemma 1.1 and [1, Lemma 1], a mixed unicyclic graph with unique cycle C is nonsingular if and only if C has odd number of unoriented edges. Thus each mixed unicyclic graph in $\mathcal{U}$ is nonsingular.

Lemma 2.1. [5] *Let G be a connected mixed graph and G_0 a spanning nonsingular unicyclic subgraph of G. Then there exists a signature matrix S such that $S^T L(G) S = L({}^S G)$ and ${}^S G_0 \in \mathcal{U}$.*

By Lemma 2.1, to study the spectrum of $L(G)$ for a nonsingular unicyclic graph G, it suffices to study the spectrum of $L({}^S G)$ with ${}^S G \in \mathcal{U}$.

Lemma 2.2. [7] *Let $G \in \mathcal{U}$ and let x be a first eigenvector of G. Then there exists a signature matrix S such that ${}^S G \in \mathcal{U}$ and Sx is a nonnegative first eigenvector of ${}^S G$.*

A path which starts from w in a mixed graph is a path from w to some other vertex.

Lemma 2.3. [5,7] *Let G be a mixed graph in $\mathcal{U}$ with n vertices and let $x \in \mathbb{R}^n$ be a first eigenvector of G. Then the following statements are true:*

(i) *There exists a vertex u on the cycle of G such that $x_u \neq 0$;*

(ii) *There exists at most one vertex v on the cycle of G such that $x_v = 0$;*

(iii) *For each vertex w on the cycle with $d(w) \geq 3$, every path P which starts from w and contains no vertices of the cycle except w has the property that the entries of x at the vertices of P form an increasing (decreasing, zero, respectively) sequence along this path if $x_w > 0$ ($x_w < 0$, $x_w = 0$, respectively).*

Let I_n be the unit matrix of order n.

Lemma 2.4. *Let $G, G' \in \mathcal{U}$ with $\widetilde{G} = \widetilde{G'}$ and let x be a first eigenvector of G. Suppose that (v_1, v_g) is the unique unoriented edge of G'. Then there exists a signature matrix S such that $L(G') = L(^S G)$ and $(Sx)_{v_1} = x_{v_1}$.*

Proof. Let $V(G) = V(G') = \{v_1, \ldots, v_n\}$ and $C_g = v_1 \cdots v_g v_1$ be the unique cycle of G. If (v_1, v_g) is also the unique unoriented edge of G, then $L(G') = L(G) = L(^S G)$ for $S = I_n$. Suppose that (v_i, v_{i+1}) is the unique unoriented edge of G, where $1 \leq i \leq g - 1$. Let G_1 and G_2 be the two components of $G - (v_1, v_g) - (v_i, v_{i+1})$ with $v_1 \in V(G_1)$. Let $S = \mathrm{diag}(s_{v_1}, \ldots, s_{v_n})$ such that $s_v = 1$ if $v \in V(G_1)$ and $s_v = -1$ if $v \in V(G_2)$. Since $L(^S G) = S^T L(G) S$, we have $\mathrm{sgn}_{^S G}(u, v) = s_u s_v \,\mathrm{sgn}_G(u, v)$. Then

$$\mathrm{sgn}_{^S G}(v_1, v_g) = s_{v_1} s_{v_g} \,\mathrm{sgn}_G(v_1, v_g) = 1 = \mathrm{sgn}_{G'}(v_1, v_g),$$
$$\mathrm{sgn}_{^S G}(v_i, v_{i+1}) = s_{v_i} s_{v_{i+1}} \,\mathrm{sgn}_G(v_i, v_{i+1}) = -1 = \mathrm{sgn}_{G'}(v_i, v_{i+1}),$$

and for $(u, v) \in E(G_1) \cup E(G_2)$,

$$\mathrm{sgn}_{^S G}(u, v) = s_u s_v \,\mathrm{sgn}_G(u, v) = -1 = \mathrm{sgn}_{G'}(u, v).$$

Thus $L(G') = L(^S G)$. Since $S_{v_1 v_1} = 1$, we have $(Sx)_{v_1} = x_{v_1}$. □

For vertex-disjoint nontrivial connected mixed graphs G_1 and G_2 with $u \in V(G_1)$ and $v \in V(G_2)$, $G_1 uv G_2$ be the mixed graph obtained from G_1 and G_2 by identifying u and v.

Lemma 2.5. [13] *Let G_1 and G_2 be two vertex-disjoint mixed graphs, where $G_1 \in \mathcal{U}$ with $u, v \in V(G_1)$, and G_2 is an all-oriented nontrivial tree with $w \in V(G_2)$. Let G (G', respectively) be the mixed graph obtained from G_1 and G_2 by identifying vertex u (v, respectively) in G_1 with vertex w in G_2, see Figure 2.1. Let x be a nonnegative first eigenvector of G. If $x_u \leq x_v$, then*

$$\lambda(G) \geq \lambda(G')$$

with equality if and only if $x_u = x_v$ and $d_{G_2}(w) x_w = \sum_{z \in N_{G_2}(w)} x_z$.

Figure 2.1: The mixed graphs G and G' in Lemma 2.5.

For mixed graphs G and G' in Lemma 2.5, we say that G' is obtained from G by moving G_2 from u to v.

3. Mixed graphs minimizing the first eigenvalue

For a signature matrix S and a mixed graph G, $\widetilde{{}^S G} = \widetilde{G}$, and thus a vertex in ${}^S G$ and G have the same degree.

Let $\mathcal{UM}(n,k)$ be the set of nonsingular mixed unicyclic graphs of order n with k branch vertices, where $n \geq 4$ and $1 \leq k \leq \lfloor \frac{n}{2} \rfloor$. Let G be a mixed graph in $\mathcal{UM}(n,k)$ with minimum first eigenvalue. Let $\mathbb{UM}(n,k) = \mathcal{UM}(n,k) \cap \mathcal{U}$. By Lemmas 2.1 and 2.2, up to a signature matrix, we may assume that $G \in \mathcal{U}$ and that x is a unit nonnegative first eigenvector of G. Then $G \in \mathbb{UM}(n,k)$.

It is shown in [5] that $\lambda(G) \leq \frac{3}{n}$, and thus $\lambda(G) < 1$, which will be used in our proof.

Let $C_g = v_1 \cdots v_g v_1$ be the unique cycle of G. For $v \in V(G)$, let $d(v, C_g)$ be the length of a shortest path connecting v and some vertex on C_g. Note that $d(v, C_g) = 0$ if $v \in V(C_g)$.

A pendant path of G is a path, in which one terminal vertex is a branch vertex, the other terminal vertex is a pendant vertex, and each internal vertex (if any exists) is of degree two in G.

Lemma 3.1. *For $i = 1, \ldots, g$, let T_i be the component of $G - E(C_g)$ containing v_i. Suppose that $x_{v_i} = 0$ for some i. Then*

(i) *$T_i \cong K_1$, or*

(ii) *$T_i \cong K_2$ and all vertices on the cycle are branch vertices.*

Proof. Suppose that $T_i \ncong K_1$. We need only to show that $T_i \cong K_2$ and all vertices on the cycle are branch vertices.

Obviously, v_i is a branch vertex. By Lemma 2.3(ii), for each $v_j \in V(C_g)$ with $j \neq i$, we have $x_{v_j} > 0 = x_{v_i}$. Suppose that v_j is not a branch vertex for some $j \neq i$. Let G' be the mixed graph obtained from G by moving T_i from v_i to v_j. Obviously, $G' \in \mathbb{UM}(n,k)$. By Lemma 2.5, $\lambda(G') < \lambda(G)$, a contradiction. Thus each v_j with $j \neq i$ is a branch vertex.

Suppose that T_i is not a star with center v_i. Then there exists a vertex $w \in V(T_i) \cap N(v_i)$ such that $d(w) \geq 2$. Let T_w be the component of $G - (v_i, w)$ containing w. Let G'' be the mixed graph obtained from G by moving T_w from w to a pendant vertex v in some T_j with $j \neq i$. Obviously, $G'' \in \mathbb{UM}(n,k)$. By Lemma 2.3(iii), $x_v > x_{v_j} > 0 = x_{v_i} = x_w$ for $j \neq i$. By Lemma 2.5, $\lambda(G'') < \lambda(G)$, a contradiction. Thus T_i is a star with center v_i. Now suppose that $T_i \ncong K_2$. Then there are at least two distinct pendant vertices at v_i. Let z be one such pendant vertex. Let G^* be the mixed graph obtained from G by removing (v_i, z) and adding (v_j, z) for some $j \neq i$. Obviously, $G^* \in \mathbb{UM}(n,k)$. By Lemma 2.5, $\lambda(G^*) < \lambda(G)$, a contradiction. It follows that $T_i \cong K_2$. □

Lemma 3.2. *The degree of each branch vertex in G is three.*

Proof. Suppose that $v \in V(G)$ with $d_G(v) \geq 4$. Let T_v be the component of $G - E(C_g)$ containing v, and w' a pendant vertex of T_v. One can easily find a path P connecting w' and v in T_v, and a vertex $w \in N(v) \setminus V(P)$ such that $d(w, C_g) > d(v, C_g)$. Suppose without loss of generality that $d(w, C_g) = d(w, v_i)$. By Lemma 3.1, $x_{v_i} > 0$. By Lemma 2.3(iii), $x'_w > x_v > 0$. Let $G' = G - (v, w) + (w', w)$ with (w', w) being oriented. Obviously, $G' \in \mathbb{UM}(n,k)$. By Lemma 2.5, $\lambda(G') < \lambda(G)$, a contradiction. □

Lemma 3.3. *If there are branch vertices outside the cycle, then all the branch vertices outside the cycle lie on a path which contains a unique vertex on the cycle as a terminal vertex, and they induce a path.*

Proof. Let u and v be two distinct branch vertices not on the cycle of G. By Lemmas 3.1 and 2.3(iii), $x_u, x_v > 0$. Suppose without loss of generality that $x_u \geq x_v$. Let $v' \in N_G(v)$ with $d(v', C_g) < d(v, C_g)$, and T_v be the component of $G - v'$ containing v.

Suppose that $u \notin V(T_v)$. Let $P = u \cdots w$ be a shortest path connecting u and a pendant vertex w (not passing v) such that $d(z, C_g) > d(u, C_g)$ for $z \in V(P) \setminus \{u\}$. By Lemma 2.3(iii), $x_w > x_u \geq x_v$. Let G' be the mixed graph obtained from G by moving T_v from v to w. Obviously, $G' \in \mathbb{UM}(n,k)$. By Lemma 2.5, $\lambda(G') < \lambda(G)$, a contradiction. It follows that $u \in V(T_v)$. Let $u_1, \ldots, u_s$ be all the branch vertices outside the cycle such that $x_{u_1} \leq \cdots \leq x_{u_s}$. Then $u_1, \ldots, u_s$ lie on a path P which contains a unique vertex, say w on the cycle as a terminal vertex such that $d(w, u_i) < d(w, u_{i+1})$ for $i = 1, \ldots, s-1$. By Lemma 3.2, all these vertices are of degree 3. Suppose that they do not induce a path. Then for some i with $i = 1, \ldots, s-1$, the neighbor z of u_i in the sub-path of P between u_i and u_{i+1} is of degree 2. Let G'' be the mixed graph obtained from G by moving a pendant path from u_i to z. Obviously, $G'' \in \mathbb{UM}(n,k)$. By Lemmas 3.1 and 2.3(iii), $x_z > x_{u_i} > 0$. By Lemma 2.5, $\lambda(G'') < \lambda(G)$, a contradiction. Thus all these branch vertices induce a path. □

Lemma 3.4. *For $k \geq 2$, each pendant path is of length one in G.*

Proof. Suppose that $Q = uw_1w_2 \cdots w_t$ is a pendant path with length at least two, where $d(u) = 3$ and $t \geq 2$. Let v be another branch vertex and $v \cdots z$ a pendant path with z being a pendant vertex, where $z \neq w_t$. Let G' be the mixed graph obtained from G by deleting (w_{t-1}, w_t) and adding an oriented edge (z, w_t). Let G'' be the mixed graph obtained from G by moving the path $v \cdots z$ from v to w_{t-1}. Obviously, $G', G'' \in \mathbb{UM}(n, k)$. If $x_{w_{t-1}} \leq x_v$, then by Lemma 2.3(iii), $x_z > x_{w_{t-1}}$, and thus by Lemma 2.5, $\lambda(G') < \lambda(G)$, a contradiction. If $x_{w_{t-1}} > x_v$, then by Lemma 2.5, $\lambda(G'') < \lambda(G)$, also a contradiction. □

Lemma 3.5. *Suppose that $k \geq 3$ and there is at least one branch vertex outside the cycle. If there are at least two branch vertices on the cycle, then no vertex outside the cycle is of degree 2.*

Proof. Let u and v be two branch vertices on the cycle. By contradiction, suppose that w_1 is a vertex of degree 2 outside C_g such that $d(w_1, C_g)$ is as small as possible. By Lemma 3.3, there is exactly one path P of length at least 2, which contains all branch vertices outside C_g and a unique vertex, say v on C_g as a terminal vertex. By Lemma 3.4, $w_1 \in V(P)$, and $(v, w_1) \in E(G)$. Let $P = vw_1 \cdots w_l$, where w_l is a pendant vertex. Let u' be the pendant neighbor of u. Let $G' = G - (w_1, w_2) + (u, w_2)$ and $G'' = G - (u, u') + (u', w_1)$ with (u, w_2) and (u', w_1) being oriented in G' and G'', respectively. Obviously, $G', G'' \in \mathbb{UM}(n, k)$. If $x_u > x_{w_1}$, then by Lemma 2.5, $\lambda(G') < \lambda(G)$, a contradiction. If $x_u < x_{w_1}$, then by Lemma 2.5, $\lambda(G'') < \lambda(G)$, also a contradiction. Suppose that $x_u = x_{w_1}$. By Lemma 2.3(i), $x_u > 0$, and thus by Lemma 2.3(iii), $x_u < x_{u'}$. By Lemma 2.5, $\lambda(G'') < \lambda(G)$, a contradiction. □

Lemma 3.6. $g = 3$.

Proof. Suppose that $g \geq 4$.

Let T_i be the component of $G - E(C_g)$ containing v_i for $i = 1, \ldots, g$. If there are branch vertices outside the cycle, then by Lemma 3.3, all these branch vertices lie on a path which contains a unique vertex, say v_1 on the cycle as a terminal vertex, and they induce a path.

For any i and j with $i \neq j$ such that $d(v_i) > d(v_j) = 2$, we have $x_{v_i} > x_{v_j}$. Otherwise, $x_{v_i} \leq x_{v_j}$. Let G^* be the mixed graph obtained from G by moving T_i from v_i to v_j. Obviously, $G^* \in \mathbb{UM}(n, k)$. By Lemma 2.5, $\lambda(G^*) < \lambda(G)$, a contradiction.

Case 1. v_1 is the only branch vertex on the cycle.

For $i \neq 1$, $x_{v_1} > x_{v_i} \geq 0$. Note that $\lambda(G) < 1$. If (v_1, v_2) is unoriented, then by eigenequation at v_2, we have $x_{v_2} = \frac{x_{v_1} - x_{v_3}}{\lambda(G) - 2} < 0$, a contradiction. Thus (v_1, v_2) is oriented. Similarly, (v_1, v_g) is oriented.

Suppose without loss of generality that $x_{v_g} \le x_{v_2}$. Let $G' = G - (v_1, v_g) + (v_2, v_g)$, where (v_2, v_g) is oriented. Obviously, $G' \in \mathbb{UM}(n,k)$ with girth $g-1$. Then

$$\begin{aligned}\lambda(G) - \lambda(G') &\ge x^T L(G)x - x^T L(G')x = (x_{v_1} - x_{v_g})^2 - (x_{v_2} - x_{v_g})^2 \\ &= (x_{v_1} + x_{v_2} - 2x_{v_g})(x_{v_1} - x_{v_2}) > 0,\end{aligned}$$

a contradiction. Hence $g = 3$.

Case 2. There are at least two branch vertices and at least one vertex of degree 2 on the cycle.

There exist branch vertices u and v and a path $Q = uw_1 \cdots w_t v$ in the cycle such that $d(w_i) = 2$ for $i = 1, \ldots, t$, where $t \ge 1$. Then $x_v > x_{w_i}$.

Suppose that Q is all-oriented. Suppose without loss of generality that $x_u \ge x_v$. If $(u,v) \in E(G)$, then by letting $G' = G - (u,v) + (v,w_1)$ with (v,w_1) being unoriented, we have $G' \in \mathbb{UM}(n,k)$ with girth $g-1$, and

$$\begin{aligned}\lambda(G) - \lambda(G') &\ge x^T L(G)x - x^T L(G')x = (x_u + x_v)^2 - (x_v + x_{w_1})^2 \\ &= (x_u + 2x_v + x_{w_1})(x_u - x_{w_1}) > 0,\end{aligned}$$

a contradiction. If $(u,v) \notin E(G)$, then by letting $G'' = G - (u,w_1) + (u,v)$ with (u,v) being oriented, we have $G'' \in \mathbb{UM}(n,k)$ with girth $g-t$ for $g-t \ge 3$, and

$$\begin{aligned}\lambda(G) - \lambda(G'') &\ge x^T L(G)x - x^T L(G'')x = (x_u - x_{w_1})^2 - (x_u - x_v)^2 \\ &= (2x_u - x_v - x_{w_1})(x_v - x_{w_1}) > 0,\end{aligned}$$

a contradiction.

Suppose that Q has an unoriented edge. If there exists a vertex of degree 2 outside Q on the cycle, then we may find another path connecting two branch vertices in the cycle with all internal vertices of degree 2 such that the edges of this path are all-oriented and thus by similar argument as above, we arrive at a contradiction.

Now suppose that each vertex on the cycle but not on Q is branch vertex. Suppose first that $t \ge 2$. If (u,w_1) is unoriented, then by the eigenequation at w_1, we have $x_{w_1} = \frac{x_u - x_{w_2}}{\lambda(G)-2} < 0$, a contradiction. Thus (u,w_1) is oriented.

Let $v' \notin V(C_g)$ be a neighbor of v, and let $G' = G - (u,w_1) + (v,w_1) - (v,v') + (u,v')$, where (v,w_1) and (u,v') are oriented. Obviously, $G' \in \mathbb{UM}(n,k)$ with girth $t+1$ for $3 \le t+1 < g$. By Lemma 2.3(iii), $x_{v'} > x_v > x_{w_1}$. We have

$$\begin{aligned}\lambda(G) - \lambda(G') &\ge x^T L(G)x - x^T L(G')x \\ &= (x_u - x_{w_1})^2 - (x_v - x_{w_1})^2 + (x_{v'} - x_v)^2 - (x_{v'} - x_u)^2 \\ &= (x_u + x_v - 2x_{w_1})(x_u - x_v) + (2x_{v'} - x_u - x_v)(x_u - x_v) \\ &= (2x_{v'} - 2x_{w_1})(x_u - x_v) \\ &\ge 0.\end{aligned}$$

If $\lambda(G) = \lambda(G')$, then $x_u = x_v$ and x is also a first eigenvector of G'. But by applying Lemma 2.3(iii) to G', we have $x_v > x_u$. Thus $\lambda(G) > \lambda(G')$, a contradiction.

Next suppose that $t = 1$. Then v has a branch neighbor w different from u. Let w' be the neighbor of w outside the cycle. Then $x_w > x_{w_1} \geq 0$, and thus by Lemma 2.3(iii), $x_{w'} > x_w$. Since $Q = uw_1v$ has an unoriented edge, we have $\operatorname{sgn}(v, w_1) = -\operatorname{sgn}(u, w_1)$, and by the eigenequation at w_1, $\operatorname{sgn}(u, w_1)(x_u - x_v) = (\lambda(G) - 2)x_{w_1} \leq 0$. If $x_u > x_v$, then $\operatorname{sgn}(u, w_1) = -1$, and thus (u, w_1) is oriented. If $x_u = x_v$, then one of (u, w_1), (w_1, v), say (u, w_1) is oriented.

Let u' be a neighbor of u outside the cycle. By Lemma 2.3(iii), $x_{u'} > x_u \geq x_v$. If $x_w < x_u$, then by letting $G' = G - (u, w_1) + (w, w_1) - (w, w') + (u, w')$ with (w, w_1) and (u, w') being oriented, we have $G' \in \mathbb{UM}(n, k)$ with girth 3, and

$$\lambda(G) - \lambda(G') \geq x^T L(G)x - x^T L(G')x = (x_u - x_w)(2x_{w'} - 2x_{w_1}) > 0,$$

a contradiction.

Suppose that $x_w \geq x_u$. Let $G' = G - (v, w) + (u, v) - (u, u') + (u', w)$ with (u, v) and (u', w) being oriented. Then $G' \in \mathbb{UM}(n, k)$ with girth 3, and

$$\lambda(G) - \lambda(G') \geq x^T L(G)x - x^T L(G')x = (x_w - x_u)(2x_{u'} - 2x_v) \geq 0.$$

If $\lambda(G) = \lambda(G')$, then $x_w = x_u$ and x is also a first eigenvector of G'. But by applying Lemma 2.3(iii) to G', we have $x_w > x_u$. It follows that $\lambda(G) > \lambda(G')$, also a contradiction. Thus $g = 3$.

Case 3. Each vertex on the cycle is a branch vertex.

By our choice of v_1 and by Lemma 3.4, $T_i \cong K_2$ for $i \neq 1$. For $i = 2, \ldots, g$, let u_i be the unique pendant neighbor of v_i. Let $\lambda = \lambda(G)$.

Subcase 3.1. $T_1 \ncong K_2$.

Suppose that λ is not a simple eigenvalue. We may find two linearly independent first eigenvectors x' and x'' of G. If $T_1 \ncong K_2$, then for the first eigenvector $x^* = x''_{v_1} x' - x'_{v_1} x''$, $x^*_{v_1} = 0$, which, together with Lemma 2.2, implies that for some signature matrix S, the nonnegative first eigenvector Sx^* have zero entry at v_1, a contradiction to Lemma 3.1. Thus λ is simple.

Since $T_1 \ncong K_2$, we have by Lemma 3.1 that $x_{v_1} > 0$. Let G' be a mixed graph in $\mathcal{U}$ such that $\widetilde{G'} = \widetilde{G}$ and (v_1, v_g) is the unique unoriented edge of G'. Obviously, $G' \in \mathbb{UM}(n, k)$. By Lemma 2.4, there exists a signature matrix S such that $L(G') = L(^S G)$. Let $x' = Sx$. Then $x'_{v_1} > 0$ and it is easy to see that x' is a first eigenvector of G'.

Define $y \in \mathbb{R}^n$ as $y_{v_i} = -x'_{v_{g+2-i}}$, $y_{u_i} = -x'_{u_{g+2-i}}$ for $i = 2, \ldots, g$, and $y_v = x'_v$ otherwise. It is easy to check by the eigenequations that y is a first eigenvector of G'. Since $L(G') = L(^S G) = S^T L(G)S$, λ is also a simple first eigenvalue of $L(G')$, and thus $y = x'$. Then $x'_{v_i} = -x'_{v_{g+2-i}}$, which implies that $x' \neq x$ and thus $S \neq I_n$.

By the eigenequations at v_1 and u_2 of ${}^SG$, we have

$$(\lambda-3)x'_{v_1} = -x'_{v_2} + x'_{v_g} - x'_{u_1} \quad \text{and} \quad (\lambda-1)x'_{u_2} = -x'_{v_2}.$$

Let $a = x'_{v_2} = -x'_{v_g}$ and $b = \frac{x'_{u_1}}{x'_{v_1}}$. Note that $x'_{v_1} > 0$ and $S \neq I_n$. By the argument of Lemma 2.4, we have $S_{v_g v_g} = -1$, which implies that $a = -x'_{v_g} = x_{v_g} \geq 0$. By Lemma 2.3(ii) and (iii), $a > 0$ and $b > 1$. Then $x'_{v_1} = \frac{2a}{3-\lambda-b} > 0$ and thus $3-\lambda-b > 0$.

Let $G'' = G' - (v_1, v_g) + (v_2, v_g) - (u_2, v_2) + (u_2, v_1)$, where (v_2, v_g) is unoriented and (u_2, v_1) is oriented. Obviously, $G'' \in \mathbb{UM}(n,k)$ with girth $g-1$. We have

$$\begin{aligned}
\lambda - \lambda(G'') &\geq x'^T L(G')x' - x'^T L(G'')x' \\
&= (x'_{v_1} + x'_{v_g})^2 - (x'_{v_2} + x'_{v_g})^2 + (x'_{u_2} - x'_{v_2})^2 - (x'_{u_2} - x'_{v_1})^2 \\
&= (x'_{v_1} - a)^2 + \left(\frac{a}{1-\lambda} - a\right)^2 - \left(\frac{a}{1-\lambda} - x'_{v_1}\right)^2 \\
&= 2a(x'_{v_1} - a)\frac{\lambda}{1-\lambda} \\
&= 2a\left(\frac{2a}{3-\lambda-b} - a\right)\frac{\lambda}{1-\lambda} \\
&= 2\lambda a^2 \frac{(b+\lambda-1)}{(1-\lambda)(3-\lambda-b)} \\
&> 0,
\end{aligned}$$

a contradiction. Thus $g = 3$.

Subcase 3.2. $T_1 \cong K_2$.

Let u_1 be the unique pendant neighbor of v_1. Considering the symmetry of $\widetilde{G}$, we may assume that (v_1, v_g) is the unique unoriented edge of G. Define $y \in \mathbb{R}^n$ as $y_{v_i} = x_{v_{g+1-i}}$ and $y_{u_i} = x_{u_{g+1-i}}$ for $i = 1, \ldots, g$. It is easy to check that y is a first eigenvectors of G. Let $z = x + y$. Then z is also a first eigenvector of G and for each i, $z_{v_i} = x_{v_i} + y_{v_i} = y_{v_{g+1-i}} + x_{v_{g+1-i}} = z_{v_{g+1-i}}$.

Let $G' = G - (v_1, v_2) + (v_1, v_{g-1}) - (u_{g-1}, v_{g-1}) + (u_{g-1}, v_2)$, where (v_1, v_{g-1}) and (u_{g-1}, v_2) are oriented. Then $G' \in \mathbb{UM}(n,k)$ with girth 3. Since $z_{v_2} = z_{v_{g-1}}$, we have

$$\begin{aligned}
\lambda - \lambda(G') &\geq z^T L(G)z - z^T L(G')z \\
&= (z_{v_1} - z_{v_2})^2 - (z_{v_1} - z_{v_{g-1}})^2 + (z_{u_{g-1}} - z_{v_{g-1}})^2 - (z_{u_{g-1}} - z_{v_2})^2 \\
&= 0,
\end{aligned}$$

and equality implies that z is also a first eigenvector of G'. This is impossible, because applying Lemma 2.3(iii) to G', we have $z_{v_{g-1}} < z_{v_2}$. Hence $\lambda > \lambda(G')$, a contradiction. Thus $g = 3$. $\square$

For $k = 1, \ldots, \lfloor \frac{n}{2} \rfloor$, let Δ_n^k be a mixed graph in $\mathbb{UM}(n,k)$ such that the underlying graph $\widetilde{\Delta}_n^k$ is an n-vertex unicyclic graph with girth 3 and k branch vertices (all of degree three) as displayed in Figure 3.1.

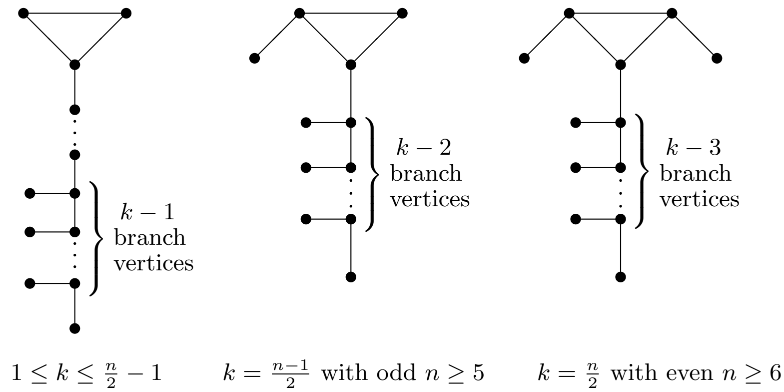

Figure 3.1: The graph $\widetilde{\Delta}_n^k$, where $(n,k) = (4,1)$, or $n \geq 5$ and $1 \leq k \leq \lfloor \frac{n}{2} \rfloor$.

Theorem 3.7. *Let $G \in \mathcal{UM}(n,k)$, where $(n,k) = (4,1)$, or $n \geq 5$ and $1 \leq k \leq \lfloor \frac{n}{2} \rfloor$. Then $\lambda(G) \geq \lambda(\Delta_n^k)$ with equality if and only if, up to a signature matrix, $G \cong \Delta_n^k$.*

Proof. Let G be a mixed graph in $\mathcal{UM}(n,k)$ with minimum first eigenvalue. By the discussion at the beginning of Section 3, up to a signature matrix, $G \in \mathbb{UM}(n,k)$, and by Lemmas 3.2–3.6, we have:

(i) the degree of each branch vertex is 3;

(ii) all branch vertices outside C_g (if any exists) induce a path;

(iii) for $k \geq 2$, the length of each pendant path is 1;

(iv) for $k \geq 3$, if there is at least one branch vertex outside C_g, and there is at least 2 branch vertices on the cycle, then no vertex outside C_g is of degree 2;

(v) the girth G is 3.

From (i), (ii) and (iii), we find that besides k branch vertices of degree 3, G has k pendant vertices and $n-2k$ vertices of degree 2. If $k = 1$, then from (i) and (v), the only one branch vertex is of degree 3 and the length of the unique cycle is 3, and thus, up to a signature matrix, $G \cong \Delta_n^1$. If $k \geq 2$, then by considering the number of vertices of degree 2, and from (i)–(v), up to a signature matrix, $G \cong \Delta_n^k$. □

Recall that for a connected nonbipartite graph G on $n \geq 3$ vertices, $\lambda(G) \geq \lambda(\widetilde{\Delta}_n^1)$ with equality if and only if $G \cong \widetilde{\Delta}_n^1$, see [3].

Corollary 3.8. *Let G be a nonbipartite unicyclic graph with n vertices and k branch vertices, where $(n,k) = (4,1)$, or $n \geq 5$ and $1 \leq k \leq \lfloor \frac{n}{2} \rfloor$. Then $\lambda_n(G) \geq \lambda_n(\widetilde{\Delta}_n^k)$ with equality if and only if $G \cong \widetilde{\Delta}_n^k$.*

Proof. By Lemma 1.1, G and $\widetilde{\Delta}_n^k$ are nonsingular mixed graphs. By Lemma 2.1, there exist signature matrices S_1, S_2 such that ${}^{S_1}G, {}^{S_2}\widetilde{\Delta}_n^k \in \mathbb{UM}(n,k)$. By Theorem 3.7, we have $\lambda(G) = \lambda({}^{S_1}G) \geq \lambda(\Delta_n^k) = \lambda(\widetilde{\Delta}_n^k)$ with equality if and only if ${}^{S_1}G \cong {}^{S_2}\widetilde{\Delta}_n^k$, i.e., $G \cong \widetilde{\Delta}_n^k$. □

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