# Spectra of closeness Laplacian and closeness signless Laplacian of graphs

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**Abstract**

For a graph $G$ with vertex set $V(G)$ and $u, v \in V(G)$, the distance between vertices $u$ and $v$ in $G$, denoted by $d_G(u, v)$, is the length of a shortest path connecting them and it is $\infty$ if there is no such a path, and the closeness of vertex $u$ in $G$ is $c_G(u) = \sum_{w \in V(G)} 2^{-d_G(u,w)}$. Given a graph $G$ that is not necessarily connected, for $u, v \in V(G)$, the closeness matrix of $G$ is the matrix whose $(u, v)$-entry is equal to $2^{-d_G(u,v)}$ if $u \neq v$ and 0 otherwise, the closeness Laplacian is the matrix whose $(u, v)$-entry is equal to

$$\begin{cases} -2^{-d_G(u,v)} & \text{if } u \neq v, \\ c_G(u) & \text{otherwise} \end{cases}$$

and the closeness signless Laplacian is the matrix whose $(u, v)$-entry is equal to

$$\begin{cases} 2^{-d_G(u,v)} & \text{if } u \neq v, \\ c_G(u) & \text{otherwise.} \end{cases}$$

We establish relations connecting the spectral properties of closeness Laplacian and closeness signless Laplacian and the structural properties of graphs. We give tight upper bounds for all nontrivial closeness Laplacian eigenvalues and characterize the extremal graphs, and determine all trees and unicyclic graphs that maximize the second smallest closeness Laplacian eigenvalue. Also, we give tight upper bounds for the closeness signless Laplacian eigenvalues and determine the trees whose largest closeness signless Laplacian eigenvalues achieve the first two largest values.

**Keywords:** Closeness Laplacian spectrum, Closeness signless Laplacian spectrum, Distances in graphs, Extremal graphs

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# 1 Introduction

We consider simple and undirected graphs. Let $G$ be a graph with vertex set $V(G)$ and edge set $E(G)$. For $u, v \in V(G)$, the distance between $u$ and $v$ in $G$, denoted by $d_G(u, v)$, is the length of a shortest path from $u$ to $v$ in $G$. Particularly, $d_G(u, u) = 0$ for any $u$ and $d_G(u, v) = \infty$ if there is no path from $u$ to $v$ in $G$.

For a graph $G$ that is not necessarily connected, the closeness matrix of $G$ is defined as [16] $C(G) = (c_G(u, v))_{u,v\in V(G)}$, where

$$c_G(u, v) = \begin{cases} 2^{-d_G(u,v)} & \text{if } u \neq v, \\ 0 & \text{otherwise.} \end{cases}$$

A general version has been considered, which is called the exponential distance matrix in [3] and the $q$-distance matrix in [15], where, for any real number $q \in (0, 1)$, the $(u, v)$-entry of the general version is $q^{d_G(u,v)}$ if $u \neq v$ and 0 otherwise. The closeness matrix of a graph deserves investigation because it combines some merits of the adjacency matrix and the distance matrix. It behalves as the adjacency matrix as both spectra are the union of the spectra of the corresponding matrices of the components of a graph. Moreover, it contains information of distances between different vertices. Note that distance matrix means only for connected graphs. Another motivation to consider the closeness matrix of a graph is the work of Dangalchev, who introduced in [6] the closeness of a graph $G$, defined as $c(G) = \sum_{v\in V(G)} c_G(v)$ with $c_G(v) = \sum_{w\in V(G)\setminus\{v\}} 2^{-d_G(v,w)}$. Closeness is a measure of centrality, an important feature of communication and social networks. Rupnik Poklukar and Žerovnik [13] discussed the connection between the closeness of a graph and the early studied Hosoya polynomial (see also [2, 10]), and they determined the graphs that minimize and maximize the closeness among several classes of graphs including trees and cacti. It is evident that for a graph $G$, $C(G)$ is a symmetric nonnegative matrix. Moreover, $C(G)$ is irreducible if and only if $G$ is connected. As $C(G)$ is symmetric, its eigenvalues are all real. We call them the closeness eigenvalues of $G$. The largest closeness eigenvalue of a graph is called the spectral closeness used as a measure for networks [16], and the extremal values (minimum and maximum values) and the extremal graphs of spectral closeness have been determined there over various classes of graphs. Properties of other closeness eigenvalues, especially the second largest and the smallest closeness eigenvalues were explored in [17]. Some results on the spectral properties of exponential distance matrix have been obtained in [5, 11].

Let $\mathrm{Dc}(G)$ be the diagonal matrix with $(u, u)$-entry to be $c_G(u)$ for each $u \in V(G)$. Motivated by [1], the closeness Laplacian is defined as the matrix $\mathbb{L}(G) = \mathrm{Dc}(G) - C(G)$, and the closeness signless Laplacian is defined as the matrix $\mathbb{Q}(G) = \mathrm{Dc}(G) + C(G)$. That is, for $u, v \in V(G)$, the $(u, v)$-entry of $\mathbb{L}(G)$ is equal to

$$\begin{cases} -2^{-d_G(u,v)} & \text{if } u \neq v, \\ c_G(u) & \text{otherwise} \end{cases}$$

and the $(u,v)$-entry of $\mathbb{Q}(G)$ is equal to

$$\begin{cases} 2^{-d_G(u,v)} & \text{if } u \neq v, \\ c_G(u) & \text{otherwise.} \end{cases}$$

Denote by $\rho_1^{\mathbb{L}}(G) \geq \cdots \geq \rho_n^{\mathbb{L}}(G)$ the eigenvalues of $\mathbb{L}(G)$, which are called the closeness Laplacian eigenvalues of $G$, and $\rho_1^{\mathbb{Q}}(G) \geq \cdots \geq \rho_n^{\mathbb{Q}}(G)$ the eigenvalues of $\mathbb{Q}(G)$, which are called the closeness signless Laplacian eigenvalues of $G$.

For $\rho \in \{\rho_n^{\mathbb{L}}(G), \rho_n^{\mathbb{Q}}(G)\}$, we have by the well known Geršgorin discs theorem (Theorem 6.1.1 in [9]) that $|\rho - c_G(v)| \leq c_G(v)$ and so $\rho \geq 0$ for some $v \in V(G)$. That is, both $\mathbb{L}(G)$ and $\mathbb{Q}(G)$ are positive semi-definite. Denote by $\mathbf{1}_n$ the $n$-dimensional column vector of all ones. Then $\mathbb{L}(G)\mathbf{1}_n = 0$, so $\rho_n^{\mathbb{L}}(G) = 0$.

If $n \geq 2$ and $G$ is connected, then each entry of $\mathbb{L}(G)$ is not zero, so the matrix $B$ obtained from $\mathbb{L}(G)$ by the deletion of, say, the last row and the last column is strictly diagonally dominant, implying that zero is not an eigenvalue of $B$, from which it follows that the multiplicity of $\rho_n^{\mathbb{L}}(G) = 0$ is one by the interlacing theorem (Theorem 4.3.17 in [9]). So the number of 0 as a closeness Laplacian eigenvalue of a graph is equal to the number of components of the graph. Consequently, a graph $G$ on $n \geq 2$ vertices is connected if and only if $\rho_{n-1}^{\mathbb{L}}(G) > 0$. This fact shows that the second smallest closeness Laplacian eigenvalue may be viewed as a distance-based 'algebraic connectivity' of a graph. Any closeness Laplacian eigenvalue that is not equal to zero is called a nontrivial one.

On the other hand, let $\mathbf{x}$ be a unit eigenvector of $\mathbb{Q}(G)$ associated to $\rho_n^{\mathbb{Q}}(G)$. Then $\rho_n^{\mathbb{Q}}(G) = \sum_{\{u,v\} \subseteq V(G)} c_G(u,v)(x_u + x_v)^2$. So $\rho_n^{\mathbb{Q}}(G) = 0$ if and only if $n = 1$ or $x_u + x_v = 0$ for any $\{u, v\}$ in a component of $G$ if $n \geq 2$, equivalently, $G$ has at least a component with one or two vertices. Thus, if $G$ is a connected graph with $n \geq 3$ vertices, then $\rho_n^{\mathbb{Q}}(G) > 0$.

We establish some connections between the closeness Laplacian eigenvalues (closeness signless Laplacian eigenvalues, respectively) and the structural properties of graphs. On one hand, we give tight upper bounds for all nontrivial closeness Laplacian eigenvalues and characterize the extremal graphs and determine all trees and unicyclic graphs that maximize the second smallest closeness Laplacian eigenvalue. On the other hand, we give tight upper bounds for the closeness signless Laplacian eigenvalues and determine the trees whose largest closeness signless Laplacian eigenvalues achieve the first two largest values.

## 2 Preliminaries

For $S \subset V(G)$, let $G - S$ denote the graph obtained by removing each vertex of $S$ (and all associated incident edges), and we write $G - v$ for $G - \{v\}$ for $v \in V(G)$. For $E \subseteq E(G)$, $G - E$ denotes the graph obtained from $G$ by removing all edges of $E$, and we write $G - e$ for $G - \{e\}$ for $e \in E(G)$. Denote by $\overline{G}$ the complement of a graph $G$. For a set $E \subseteq E(\overline{G})$, $G + E$ denotes the graph obtained from $G$ by adding all elements of $E$ as edges, and we write $G + uv$ for $G + \{uv\}$ for $uv \notin E(G)$.

For vertex disjoint graphs $G_1$ and $G_2$, let $G_1 \cup G_2$ be the (vertex disjoint) union of $G_1$ and $G_2$, and $G_1 \vee G_2$ the join of $G_1$ and $G_2$ with $G_1 \vee G_2 = (G_1 \cup G_2) + \{uv : u \in V(G_1), v \in V(G_2)\}$.

Let $K_n$ and $P_n$ be the $n$-vertex complete graph and path, respectively. Let $K_{n_1,\dots,n_k}$ be the complete $k$-partite graph with $n_i$ vertices in the $i$th partite set for $i = 1, \dots, k$, where $k \geq 2$ and $n_i \geq 1$. For positive integers $n$ and $a$ with $1 \leq a \leq \frac{n-2}{2}$, let $D_{n,a}$ be the tree on $n$ vertices obtained from a path on two vertices by attaching $a$ and $n - a - 2$ pendant vertices to its end vertices, respectively.

The degree of a vertex $v$ in a graph $G$ is the number of vertices that are adjacent to $v$ in $G$, denoted by $\delta_G(v)$. A vertex $v$ is called a pendant vertex if $\delta_G(v) = 1$. For a graph $H$ with $u \in V(H)$ and $v \notin V(H)$, we say that the graph $G$ with $V(G) = V(H) \cup \{v\}$ and $E(G) = E(H) \cup \{uv\}$ is obtained from $H$ by attaching a pendant vertex at $u$.

For an $n \times n$ matrix $M$ with $n$ real eigenvalues, we denote by $\rho_1(M) \geq \cdots \geq \rho_n(M)$ the eigenvalues of $M$. So, for a graph $G$ on $n$ vertices and $i = 1, \dots, n$,

$$\rho_i^{\mathbb{L}}(G) = \rho_i(\mathbb{L}(G)) \text{ and } \rho_i^{\mathbb{Q}}(G) = \rho_i(\mathbb{Q}(G)).$$

**Proposition 2.1.** *Let $G$ be a connected graph on $n \geq 3$ vertices that is not complete. Suppose that $uv \notin E(G)$ for $\{u, v\} \subset V(G)$. Then*

$$\rho_i^{\mathbb{L}}(G + uv) \geq \rho_i^{\mathbb{L}}(G) \text{ for } i = 1, \dots, n - 1$$

*and*

$$\rho_i^{\mathbb{Q}}(G + uv) \geq \rho_i^{\mathbb{Q}}(G) \text{ for } i = 1, \dots, n.$$

*Moreover, $\rho_1^{\mathbb{Q}}(G + uv) > \rho_1^{\mathbb{Q}}(G)$.*

*Proof.* Let

$$M = \mathbb{L}(G + uv) - \mathbb{L}(G).$$

The diagonal entry $M_{ww}$ of $M$ for $w \in V(G)$ is $c_{G+uv}(w) - c_G(w) \geq 0$, and the sum of non-diagonal entries of $M$ corresponding to vertex $w$ is $-c_{G+uv}(w) + c_G(w)$. So $M$ is diagonally dominant with nonnegative diagonal entries, so it is a positive semi-definite matrix. As $M\mathbf{1}_n = 0$, we have $\rho_n(M) = 0$. So by the Weyl inequalities (Theorem 4.3.1 in [9]), we have

$$\rho_i^{\mathbb{L}}(G + uv) = \rho_i(\mathbb{L}(G) + M) \geq \rho_i(\mathbb{L}(G)) + \rho_n(M) = \rho_i^{\mathbb{L}}(G)$$

for $i = 1, \dots, n - 1$. Similarly, we have $\rho_i^{\mathbb{Q}}(G + uv) \geq \rho_i^{\mathbb{Q}}(G)$ for $i = 1, \dots, n$. As $\mathbb{Q}(G + uv) - \mathbb{Q}(G)$ is nonzero nonnegative and $\mathbb{Q}(G)$ is irreducible, we have by the Perron-Frobenius theorem (Theorem 8.4.4 in [9]) that $\rho_1^{\mathbb{Q}}(G + uv) > \rho_1^{\mathbb{Q}}(G)$. □

Usually, we use a multiset to denote the spectrum of some matrix, in which $a^{[k]}$ means that the multiplicity of $a$ is $k$.

Given a graph $G$, denote by $\mathrm{Deg}(G)$ the vertex degree diagonal matrix of a graph $G$. The adjacency matrix of $G$ is the matrix $A(G) = (a_{uv})_{u,v \in V(G)}$ with $a_{uv} = 1$ if $u$ and $v$ are adjacent and 0 otherwise. Then the Laplacian of $G$ is the matrix $L(G) = \mathrm{Deg}(G) - A(G)$

and the signless Laplacian of $G$ is $Q(G) = \mathrm{Deg}(G) + A(G)$. Both Laplacians have been extensively studied [4].

For a graph $G$ with $V(G) = \{v_1, \dots, v_n\}$, a vector $\mathbf{x} = (x_{v_1}, \dots, x_{v_n})^\top$ can be viewed as a function defined on $V(G)$ that maps $v_i$ to $x_{v_i}$. In this case, $x_u$ is said to be the entry of $\mathbf{x}$ at $u \in V(G)$.

# 3 Closeness Laplacian eigenvalues

Firstly, we recall some facts on the Laplacian eigenvalues of a graph. Let $G$ be a connected graph on $n$ vertices. Let $\lambda_1^L(G) \geq \dots \geq \lambda_{n-1}^L(G) > \lambda_n^L(G) = 0$ be the Laplacian eigenvalues of $G$. Then the Laplacian eigenvalues of $\overline{G}$ are $n - \lambda_{n-1}^L(G) \geq \dots \geq n - \lambda_1^L(G) \geq \lambda_n^L(\overline{G}) = 0$. From this, it follows that $\lambda_1^L(G) \leq n$ with equality if and only if $\lambda_{n-1}^L(\overline{G}) = 0$, i.e., $\overline{G}$ is disconnected.

**Proposition 3.1.** *Let $G$ be a connected graph on $n \geq 2$ vertices with diameter at most two. Let $\lambda_1^L \geq \dots \geq \lambda_{n-1}^L > \lambda_n^L = 0$ be the Laplacian eigenvalues of $G$. Then the closeness Laplacian eigenvalues of $G$ are*

$$\frac{1}{4}(n + \lambda_1^L) \geq \dots \geq \frac{1}{4}(n + \lambda_{n-1}^L) > \lambda_n^L = 0.$$

*Proof.* If the diameter of $G$ is one, then $G \cong K_n$, $\lambda_1^L = \dots = \lambda_{n-1}^L = n$ and $\mathbb{L}(G) = \frac{1}{2}L(K_n)$, so $\rho_1^{\mathbb{L}}(G) = \dots = \rho_{n-1}^{\mathbb{L}}(G) = \frac{n}{2}$.

Suppose that the diameter of $G$ is two. Then $C(G) = \frac{1}{2}A(G) + \frac{1}{4}(J_n - I_n - A(G)) = \frac{1}{4}(J_n - I_n + A(G))$ and $\mathrm{Dc}(G) = \frac{n-1}{4}I_n + \frac{1}{4}\mathrm{Deg}(G)$, so

$$\begin{aligned}\mathbb{L}(G) &= \frac{n-1}{4}I_n + \frac{1}{4}\mathrm{Deg}(G) - \frac{1}{4}(J_n - I_n + A(G)) \\ &= \frac{n}{4}I_n - \frac{1}{4}J_n + \frac{1}{4}L(G).\end{aligned}$$

For any $i$ with $1 \leq i \leq n-1$, assume that $\mathbf{x}_i$ is an eigenvector of $L(G)$ associated to $\lambda_i^L$. As $L\mathbf{1}_n = 0$, we have $\mathbf{1}_n^\top \mathbf{x}_i = 0$, so $J_n \mathbf{x}_i = 0$. It follows that

$$\begin{aligned}\mathbb{L}(G)\mathbf{x}_i &= \left(\frac{n}{4}I_n - \frac{1}{4}J_n + \frac{1}{4}L(G)\right)\mathbf{x}_i \\ &= \frac{n}{4}\mathbf{x}_i + \frac{1}{4}\lambda_i^L \mathbf{x}_i \\ &= \frac{1}{4}(n + \lambda_i^L)\mathbf{x}_i.\end{aligned}$$

That is, $\frac{1}{4}(n + \lambda_i^L)$ is the $i$-th largest closeness Laplacian eigenvalue of $G$ for $i = 1, \dots, n-1$. □

**Theorem 3.1.** *Let $G$ be a connected graph on $n \geq 2$ vertices. For $i = 1, \dots, n-1$,*

$$\rho_i^{\mathbb{L}}(G) \leq \frac{n}{2}$$

*with equality for all $i = 1, \dots, r$ with $r \leq n-1$ if $G$ is a complete $k$-partite graph for any $k$ with $r+1 \leq k \leq n$.*

*Proof.* By Proposition 2.1, we have $\rho_i^{\mathbb{L}}(G) \leq \rho_i^{\mathbb{L}}(K_n) = \frac{n}{2}$.

If $G$ is a complete $k$-partite graph, say $G = K_{n_1,\dots,n_k}$, then the Laplacian spectrum of $\overline{G} = \cup_{i=1}^k K_{n_i}$ is $\left\{n_1^{[n_1-1]}, \dots, n_k^{[n_k-1]}, 0^{[k]}\right\}$, so the Laplacian spectrum of $G$ is

$$\left\{n^{[k-1]}, n - n_1^{[n_1-1]}, \dots, n - n_k^{[n_k-1]}, 0\right\},$$

which, together with Proposition 3.1, implies that the closeness Laplacian spectrum of $G$ is

$$\left\{\frac{n}{2}^{[k-1]}, \frac{n}{2} - \frac{n_1}{4}^{[n_1-1]}, \dots, \frac{n}{2} - \frac{n_k}{4}^{[n_k-1]}, 0\right\}.$$

This completes the proof. □

**Lemma 3.1.** *Let $G$ be a connected graph on $n \geq 2$ vertices. Then there is a nonzero closeness Laplacian eigenvalue with multiplicity $n-1$ if and only if $G \cong K_n$.*

*Proof.* If $G \cong K_n$, then it is obvious that $\frac{n}{2}$ is a nonzero closeness Laplacian eigenvalue with multiplicity $n-1$.

Suppose that $a$ is a nonzero closeness Laplacian eigenvalue with multiplicity $n-1$. Then $\mathbb{L}(G)$ has eigenvalues $a$ with multiplicity $n-1$ and 0 with multiplicity one. So for some $n \times n$ orthonormal matrix $P$, $P^\top \mathbb{L}(G) P$ is a diagonal matrix with $(i,i)$-entry to be $a$ for $i = 1, \dots, n-1$ and 0 for $i = n$. Let $\mathbf{x} = (x_1, \dots, x_n)$ be the last row vector of $P^\top$. So

$$\mathbb{L}(G) - aI_n = -aP(0, \dots, 0, 1)^\top (0, \dots, 0, 1) P^\top = -a\mathbf{x}^\top \mathbf{x}.$$

That is, $\mathbb{L}(G) = aI_n - a\mathbf{x}^\top \mathbf{x}$. For $i = 1, \dots, n$, considering the sum of entries of the $i$th row of $\mathbb{L}(G)$, we have

$$ax_i \left(\sum_{j=1}^n x_j - x_i\right) = a(1 - x_i^2),$$

so

$$x_i \left(\sum_{j=1}^n x_j - x_i\right) = 1 - x_i^2,$$

i.e.,

$$x_i \sum_{j=1}^n x_j = 1,$$

implying that $x_1 = \cdots = x_n := c$. This forces that the entries of $\mathbb{L}(G)$ outside the main diagonal are all equal, implying that $G \cong K_n$. □

By Theorem 3.1 and Lemma 3.1, we immediately have the following consequence.

**Corollary 3.1.** *Let $G$ be a connected graph on $n \geq 2$ vertices. Then*

$$\rho_{n-1}^{\mathbb{L}}(G) \leq \frac{n}{2}$$

*with equality if and only if $G \cong K_n$.*

Rupnik Poklukar and Žerovnik [13] noted that if $G$ is a tree on $n \geq 2$ vertices, then $c(G) \leq c(K_{1,n-1}) = \frac{(n-1)(n+2)}{4}$ with equality if and only if $G \cong K_{1,n-1}$.

For a graph $G$ with $u \in V(G)$, we denote by $N_G(u)$ the neighborhood of $u$ in $G$ (that is, the set of vertices that are adjacent to $u$ in $G$). The following is Corollary 3.1 in [13].

**Lemma 3.2.** *Let $G$ be a connected graph with a cut edge $uv$. Suppose that $uv$ is not a pendant edge. Let $G_{uv} = G - \{vw : w \in N_G(v) \setminus \{u\}\} + \{uw : w \in N_G(v) \setminus \{u\}\}$, see Fig. 1. Then $c(G_{uv}) > c(G)$.*

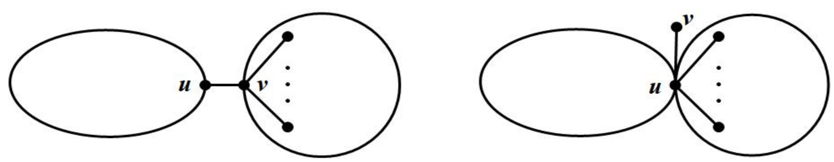


Fig. 1: Graphs $G$ (left) and $G_{uv}$ (right) in Lemma 3.2.

Let $H$ be a nontrivial connected graph. Let $u$ and $v$ be two vertices of $H$. Let $H_{u,v}(s,t)$ be the graph obtained from $H$ by attaching $s$ pendant vertices at $u$ and $t$ pendant vertices at $v$, where $s, t \geq 0$, see Fig. 2. Particularly, $H_{u,v}(0,0) = H$.


Fig. 2: Graphs $H_{u,v}(s,t)$ for $s,t > 0$ (left) and $H_{u,v}(s,0)$ for $s > 0$ (right).

The following is Corollary 3.2 in [13].

**Lemma 3.3.** *Let $H$ be a nontrivial connected graph. Let $u$ and $v$ be two vertices of $H$. For positive integers $s$ and $t$, $c(H_{u,v}(s+t,0)) > c(H_{u,v}(s,t))$ or $c(H_{u,v}(0,s+t)) > c(H_{u,v}(s,t))$.*

**Lemma 3.4.** *Suppose that $G$ is a tree on $n \geq 4$ vertices and $G \ncong K_{1,n-1}$. Then $c(G) \leq \frac{n^2+1}{4}$ with equality if and only if $G \cong D_{n,1}$. Moreover, if $G \ncong D_{n,1}$ with $n \geq 6$, then $c(G) \leq \frac{n^2-n+6}{4}$ with equality if and only if $G \cong D_{n,2}$.*

*Proof.* Denote by $d$ the diameter of $G$. As $G \ncong K_{1,n-1}$, one has $d \geq 3$.

Suppose that $d = 3$. Then $G \cong D_{n,a}$ with $1 \leq a \leq \frac{n-2}{2}$. Let $b = n-2-a$. It is easy to see that

$$\begin{aligned}\frac{1}{2}c(G) &= \frac{1}{2}(n-1) + \frac{1}{4}\left(\binom{a+1}{2} + \binom{b+1}{2}\right) + \frac{1}{8}ab \\ &= \frac{n-1}{2} + \frac{(n-1)(n-2)}{8} - \frac{ab}{8} \\ &\leq \frac{n-1}{2} + \frac{(n-1)(n-2)}{8} - \frac{n-3}{8} \\ &= \frac{n^2+1}{8},\end{aligned}$$

so $c(G) \leq \frac{n^2+1}{4}$ with equality if and only if $a = 1$ and $b = n-3$, that is $G \cong D_{n,1}$. Suppose that $G \ncong D_{n,1}$ with $n \geq 6$. Then

$$\frac{1}{2}c(G) \leq \frac{n-1}{2} + \frac{(n-1)(n-2)}{8} - \frac{2(n-4)}{8}$$

so $c(G) \leq \frac{n^2-n+6}{4}$ with equality if and only if $a = 2$ and $b = n-4$, that is $G \cong D_{n,2}$.

Suppose that $d \geq 4$. It suffices to show that $c(G) < \frac{n^2-n+6}{4}$. By Lemma 3.2, there is a caterpillar $G'$ on $n$ vertices with diameter four so that $c(G) \leq c(G')$ with equality if and only if $G \cong G'$. Let $T_{n,4}^1$ be the caterpillar on $n$ vertices of diameter four obtained from the path $v_1 \dots v_5$ by attaching $n-5$ pendant vertices at $v_3$ and $T_{n,4}^2$ be the caterpillar on $n$ vertices of diameter four obtained from the path $v_1 \dots v_5$ by attaching $n-5$ pendant vertices at $v_4$. By Lemma 3.3, $c(G') \leq c(T_{n,4}^1)$ or $c(G') \leq c(T_{n,4}^2)$. By an easy direct calculation, one has

$$\frac{1}{2}c(T_{n,4}^1) = \frac{n-1}{2} + \frac{\binom{n-5}{2} + 2(n-5) + 3}{4} + \frac{2(n-5)+2}{8} + \frac{1}{16}$$

and

$$\frac{1}{2}c(T_{n,4}^2) = \frac{n-1}{2} + \frac{\binom{n-5}{2} + 2(n-5) + 3}{4} + \frac{(n-5)+2}{8} + \frac{n-4}{16},$$

so $c(T_{n,4}^1) = \frac{2n^2-2n+9}{8} > c(T_{n,4}^2) = \frac{2n^2-3n+14}{8}$. Therefore, $c(G') \leq c(T_{n,4}^1) = \frac{2n^2-2n+9}{8}$. It follows that $c(G) \leq \frac{2n^2-2n+9}{8} < \frac{n^2-n+6}{4}$, as desired. □

**Theorem 3.2.** *Let $G$ be a tree on $n \geq 3$ vertices. Then*

$$\rho_{n-1}^{\mathbb{L}}(G) \leq \frac{n+1}{4}$$

*with equality if and only if $G \cong K_{1,n-1}$.*

*Proof.* The result is trivial if $n = 3$, and it follows easily if $n = 4$ as $\rho_{n-1}^{\mathbb{L}}(P_4) = \frac{11-\sqrt{13}}{8} < \frac{5}{4}$.

Suppose in the following that $n \geq 5$ and $G \ncong K_{1,n-1}$. As $\rho_{n-1}^{\mathbb{L}}(K_{1,n-1}) = \frac{n+1}{4}$, it suffices to show that $\rho_{n-1}^{\mathbb{L}}(G) < \frac{n+1}{4}$.

If $G \ncong D_{n,1}$, then, by Lemma 3.4, one has $c(G) \leq \frac{n^2-n+6}{4}$. As $\rho_n^L(G) = 0$ and $G \ncong K_n$, one has by Lemma 3.1 that

$$\rho_{n-1}^{\mathbb{L}}(G) < \frac{c(G)}{n-1} \leq \frac{n^2-n+6}{4(n-1)} \leq \frac{n+1}{4},$$

as desired.

Assume that $G = D_{n,1}$. Label the vertices od $D_{n,1}$ so that $v_1v_2v_3v_i$ is a path for reach $i = 4, \ldots, n$. Denote by $\mathbf{x}$ the eigenvector of $\mathbb{L}(G)$ associated with $\rho = \rho_{n-1}^{\mathbb{L}}(G)$. Let $x_i = x_{v_i}$ for $i = 1, \ldots, n$. Note that $\rho > 0$ and $\mathbf{x}^\top \mathbf{1}_n = 0$, i.e., $x_1 + \cdots + x_n = 0$. For each $i = 4, \ldots, n$, as $\rho\mathbf{x} = \mathbb{L}(G)\mathbf{x}$, we have

$$\rho x_i = -\frac{1}{8}x_1 - \frac{1}{4}x_2 - \frac{1}{2}x_3 + \frac{2n-1}{8}x_i - \frac{1}{4}\left(\sum_{j=4}^{n} x_j - x_i\right),$$

i.e.,

$$\begin{aligned}\left(\rho - \frac{2n+1}{8}\right)x_i &= -\frac{1}{8}x_1 - \frac{1}{4}x_2 - \frac{1}{2}x_3 - \frac{1}{4}\sum_{j=4}^{n} x_j \\ &= -\frac{1}{8}x_1 - \frac{1}{4}x_2 - \frac{1}{2}x_3 + \frac{1}{4}(x_1 + x_2 + x_3) \\ &= \frac{1}{8}x_1 - \frac{1}{4}x_3.\end{aligned}$$

If $\rho = \frac{2n+1}{8}$, then $\rho < \frac{n+1}{4}$. Suppose that $\rho \neq \frac{2n+1}{8}$. It then follows that $x_4 = \cdots = x_n$. Recall that $x_1 + \cdots + x_n = 0$. From $\rho\mathbf{x} = \mathbb{L}(G)\mathbf{x}$, one has

$$\rho x_1 = \frac{n+4}{8}x_1 - \frac{3}{8}x_2 - \frac{1}{8}x_3,$$

$$\rho x_2 = -\frac{1}{4}x_1 + \frac{n+2}{4}x_2 - \frac{1}{4}x_3$$

and

$$\rho x_3 = \frac{1}{4}x_1 + \frac{2n-1}{4}x_3.$$

The above homogeneous linear system in the variables $x_1, x_2, x_3$ has a nonzero solution. So the determinant of its coefficient matrix is zero. That is,

$$\det \begin{pmatrix} \rho - \frac{n+4}{8} & \frac{3}{8} & \frac{1}{8} \\ \frac{1}{4} & \rho - \frac{n+2}{4} & \frac{1}{4} \\ -\frac{1}{4} & 0 & \rho - \frac{2n-1}{4} \end{pmatrix} = 0.$$

By a direct calculation, the above determinant is equal to $f(\rho)$, where

$$f(\rho) = \rho^3 - \frac{7n+6}{8}\rho^2 + \frac{7n^2+19n-2}{32}\rho - \frac{2n^3+11n^2+5n}{128}.$$

It thus follows that $\rho$ is the smallest root if $f(t) = 0$. As $f\left(\frac{n+1}{4}\right) = \frac{n^2-n-6}{128} > 0$ and $f\left(\frac{3n}{8}\right) = -\frac{n(n-4)^2}{256} < 0$, we have $\rho < \frac{n+1}{4}$, as desired. □

Denote by $U_{n,r}$ with $3 \le r \le n$ the unicyclic graph on $n$ vertices obtained from the cycle $C_r$ by attaching $n-r$ pendant vertices at a vertex. Denote by $U^*_{n,r}$ with $3 \le r \le n-2$ the unicyclic graph on $n$ vertices obtained from $U_{r+1,r}$ by attaching $n-r-1$ pendant vertices at the pendant vertex, see Fig. 3.

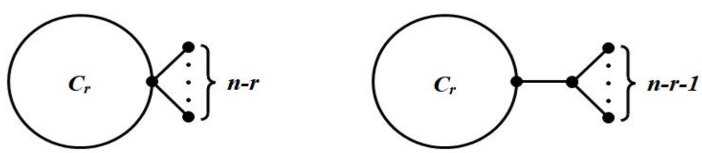


Fig. 3: Graphs $U_{n,r}$ (left) and $U^*_{n,r}$ (right).

Let $S^1_n$ be the unicyclic graph with $n \ge 5$ vertices obtained from $U_{n-1,3}$ by attaching a pendant vertex at a vertex of degree two. Let $S^2_n$ be the unicyclic graph with $n \ge 7$ vertices obtained from $S^1_{n-1}$ by attaching a pendant vertex at the vertex of degree three. Let $S^+_n$ be the unicyclic graph with $n \ge 5$ vertices obtained from $U_{n-1,3}$ by attaching a pendant vertex at the vertex of degree one, see Fig. 4.

**Lemma 3.5.** *Among unicyclic graphs on $n$ vertices with girth three, $U_{n,3}$ with $n \ge 4$, $S^1_n$ with $n \ge 5$, $S^+_n$ and $S^2_n$ with $n \ge 8$ are the only ones that have the first, the second, the third and the fourth largest closeness, which are equal to $\frac{n^2+n}{4}$, $\frac{n^2+4}{4}$, $\frac{n^2+3}{4}$ and $\frac{n^2-n+10}{4}$, respectively.*

*Proof.* Let $\mathcal{U}(n)$ be the set of unicyclic graphs on $n$ vertices with girth three.

The fact that $U_{n,3}$ is the only graph in $\mathcal{U}(n)$ that has the largest closeness follows from Lemmas 3.2 and 3.3, and by a direct calculation, $c(U_{n,3}) = \frac{n^2+n}{4}$.

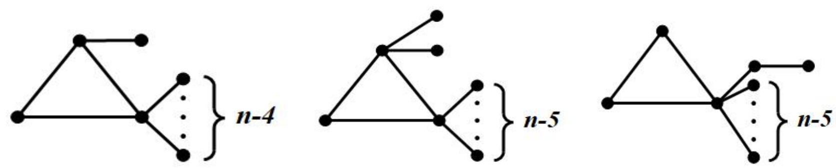



Fig. 4: Graphs $S_n^1$ (left), $S_n^2$ (middle) and $S_n^+$ (right).

Let $G \in \mathcal{U}(n) \setminus \{U_{n,3}\}$. By Lemmas 3.2 and 3.3, the maximum values of $c(G)$ is achieved only by one of $S_n^1$, $S_n^+$ and $U_{n,3}^*$. By a direct calculation, we have

$$c(S_n^1) = n + \frac{1}{2}\left(\binom{n-4}{2} + 2(n-4) + 2\right) + \frac{1}{4}(n-4) = \frac{n^2+4}{4},$$

$$c(S_n^+) = n + \frac{1}{2}\left(\binom{n-4}{2} + 2(n-4) + 1\right) + \frac{1}{4}(n-3) = \frac{n^2+3}{4}$$

and

$$c(U_{n,3}^*) = n + \frac{1}{2}\left(\binom{n-4}{2} + (n-4) + 2\right) + \frac{1}{4}(2n-8) = \frac{n^2-n+8}{4}.$$

So it is evident that $S_n^1$ with $n \geq 5$ is the only graph in $\mathcal{U}(n)$ that has the second largest closeness, which is equal to $\frac{n^2+4}{4}$.

Next, let $G \in \mathcal{U}(n) \setminus \{U_{n,3}, S_n^1\}$ with $n \geq 8$. By Lemmas 3.2 and 3.3, the maximum values of $c(G)$ is achieved only by one of $S_n^+$, $S_n^2$ and $U_{n,3}^*$. As

$$\begin{aligned} c(S_n^2) &= n + \frac{1}{2}\left(\binom{n-5}{2} + 1 + 2(n-5) + 4\right) + \frac{1}{2}(n-5) \\ &= \frac{n^2-n+10}{4} \\ &< \frac{n^2+3}{4} \end{aligned}$$

for $n \geq 8$, we see that $S_n^+$ with $n \geq 8$ is the only graph in $\mathcal{U}(n)$ that has the third largest closeness, which is equal to $\frac{n^2+3}{4}$.

Finally, let $G \in \mathcal{U}(n) \setminus \{U_{n,3}, S_n^1, S_n^+\}$ with $n \geq 8$. By Lemmas 3.2 and 3.3, the maximum values of $c(G)$ is achieved only by one of $S_n^2$, $U_{n,3}^*$, $G'$ and $G''$, where $G'$ is obtained from $S_{n-1}^+$ by attaching a pendant vertex at the vertex with degree two that is adjacent to a pendant vertex, and $G''$ is obtained from $U_{n-1,3}^*$ by attaching a pendant vertex at vertex of degree three on the triangle. Note that

$$c(G') = n + \frac{1}{2}\left(\binom{n-5}{2} + 2(n-5) + 3\right) + \frac{1}{4}(2n-8) = \frac{n^2-n+8}{4}$$

and

$$c(G'') = n + \frac{1}{2}\left(\binom{n-5}{2} + n\right) + \frac{1}{4}(3n - 15) = \frac{n^2 - 2n + 15}{4}.$$

So $S_n^2$ with $n \geq 8$ is the only graph in $\mathcal{U}(n)$ that has the fourth largest closeness, which is equal to $\frac{n^2-n+10}{4}$. □

Let $U_n^1$ ($U_n^2$, respectively) be the graph obtained from $U_{n-1,4}$ by attaching a pendant vertex at a vertex of degree 2 that is adjacent (not adjacent, respectively) to the vertex of degree $n-3$, see Fig. 5.

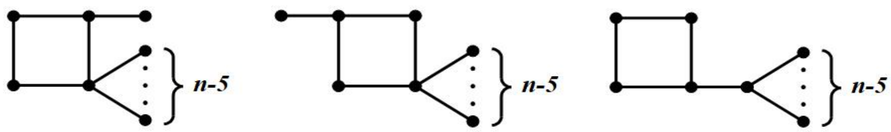


Fig. 5: Graphs $U_n^1$ (left), $U_n^2$ (middle) and $U_{n,4}^*$ (right).

**Lemma 3.6.** *Among unicyclic graphs on $n$ vertices with girth four, $U_{n,4}$ with $n \geq 5$ and $U_n^1$ or $U_{n,4}^*$ with $n \geq 6$ are the only ones that have the first and the second largest closeness, which are equal to $\frac{n^2+4}{4}$, $\frac{n^2-n+9}{4}$, respectively.*

*Proof.* By Lemmas 3.2 and 3.3, $U_{n,4}$ is the only unicyclic graph on $n$ vertices with girth four that has the largest closeness, and it is easy to see that $c(U_{n,4}) = \frac{n^2+4}{4}$.

Let $G$ be a unicyclic graphs on $n \geq 6$ vertices and the girth is four such that $G \ncong U_{n,4}$. By Lemmas 3.2 and 3.3, the maximum values of $c(G)$ is achieved only by one of $U_{n,4}^*$, $U_n^1$, $G'$ and $U_n^2$, where $G'$ is obtained from $U_{n-1,4}$ by attaching a pendant vertex at some pendant vertex. Then by a direct calculation, we have

$$c(U_n^1) = \frac{n^2 - n + 9}{4},$$

$$c(U_{n,4}^*) = \frac{2n^2 - 5n + 33}{8} < \frac{n^2 - n + 9}{4},$$

$$c(G') = \frac{2n^2 - 2n + 15}{8} < \frac{n^2 - n + 9}{4}$$

and

$$c(U_n^2) = \frac{2n^2 - 3n + 23}{8} < \frac{n^2 - n + 9}{4}$$

for $n \geq 6$. So $U_n^1$ with $n \geq 6$ is the only unicyclic graph on $n$ vertices with girth four that have the second largest closeness, which is equal to $\frac{n^2-n+9}{4}$. □

**Lemma 3.7.** *Let $G$ be a unicyclic graph on $n$ vertices. If $n \geq 8$ and $G \ncong U_{n,3}, U_{n,4}, S_n^1, S_n^+$, then*

$$c(G) \leq \frac{n^2 - n + 10}{4}$$

*with equality if and only if $G \cong S_n^2, U_{n,5}$. Moreover, we have*

$$c(U_{n,3}) = \frac{n^2 + n}{4},$$

$$c(S_n^1) = c(U_{n,4}) = \frac{n^2 + 4}{4}$$

*and*

$$c(S_n^+) = \frac{n^2 + 3}{4}.$$

*Proof.* Let $r$ be the girth of $G$. By Lemmas 3.2 and 3.3, $c(G) \leq c(U_{n,r})$ with equality if and only if $G \cong U_{n,r}$. Note that

$$c(C_r) = \begin{cases} 2r\left(1 - 2^{-\frac{r-1}{2}}\right) & \text{if } r \text{ is odd,} \\ r\left(2 - 3 \cdot 2^{-\frac{r}{2}}\right) & \text{if } r \text{ is even.} \end{cases}$$

Let $a = \frac{c(C_r)}{r}$. Then

$$\begin{aligned} c(U_{n,r}) &= c(C_r) + 2^{-1}\binom{n-r}{2} + 2(n-r)(2^{-1} + 2^{-1}a) \\ &= \frac{n^2 + 11n + r^2 - 3r - 2rn}{4} - \begin{cases} 2^{-\frac{r-3}{2}} n & \text{if } r \text{ is odd,} \\ 3 \cdot 2^{-\frac{r}{2}} n & \text{if } r \text{ is even.} \end{cases} \end{aligned}$$

Suppose that $r + 1 \leq n$. Then

$$c(U_{n,r+1}) - c(U_{n,r}) = \frac{r-1}{2} + \begin{cases} (2^{-\frac{r+1}{2}} - 2^{-1})n & \text{if } r \text{ is odd,} \\ (2^{-\frac{r}{2}} - 2^{-1})n & \text{if } r \text{ is even.} \end{cases}$$

Let $g(t) = -1 + 2^{-\frac{t}{2}}t$. As $g'(t) = 2^{-\frac{t}{2}}(1 - t\log\sqrt{2}) < 0$ for $t \geq 4$, $g(t)$ is strictly decreasing for $t \geq 4$. If $r$ is odd with $r \geq 5$, then

$$\begin{aligned} c(U_{n,r+1}) - c(U_{n,r}) &= \frac{r-1}{2} + (2^{-\frac{r+1}{2}} - 2^{-1})n \\ &\leq \frac{r-1}{2} + (2^{-\frac{r+1}{2}} - 2^{-1})(r+1) \\ &= g(r+1) \\ &< g(4) = 0, \end{aligned}$$

so $c(U_{n,r+1}) < c(U_{n,r})$. Suppose that $r$ is even with $r \geq 6$,

$$\begin{aligned} c(U_{n,r+1}) - c(U_{n,r}) &= \frac{r-1}{2} + (2^{-\frac{r}{2}} - 2^{-1})n \\ &\leq \frac{r-1}{2} + (2^{-\frac{r}{2}} - 2^{-1})(r+1) \\ &= g(r) + 2^{-\frac{r}{2}} \\ &\leq g(6) + 2^{-\frac{r}{2}} = -2^{-2} + 2^{-\frac{r}{2}} < 0, \end{aligned}$$

so $c(U_{n,r+1}) < c(U_{n,r})$. Thus, we conclude that among unicyclic graphs on $n$ vertices with girth at least five, $U_{n,5}$ is the unique one with the largest closeness, which is equal to $\frac{n^2-n+10}{4}$. Now the result follows by Lemmas 3.5 and 3.6. □

**Theorem 3.3.** *Let $G$ be a unicyclic graph on $n \geq 11$ vertices. Then*

$$\rho^{\mathbb{L}}_{n-1}(G) \leq \frac{n+1}{4}$$

*with equality if and only if $G \cong U_{n,3}$.*

*Proof.* Suppose that $G \ncong U_{n,3}, S^1_n, U_{n,4}, S^+_n$. By Lemma 3.7, $c(G) \leq \frac{n^2-n+10}{4}$. As $n \geq 11$, $\rho^{\mathbb{L}}_n(G) = 0$ and $G \ncong K_n$, one has by Lemma 3.1 that

$$\rho^{\mathbb{L}}_{n-1}(G) < \frac{c(G)}{n-1} \leq \frac{n^2-n+10}{4(n-1)} \leq \frac{n+1}{4}.$$

By Proposition 3.1, it is easy to see that $\rho^{\mathbb{L}}_{n-1}(U_{n,3}) = \frac{n+1}{4}$. It suffices to show that $\rho(G) < \frac{n+1}{4}$ if $G$ is one of $S^1_n, U_{n,4}, S^+_n$.

Note that $S^1_n$ is the unicyclic graph with $n \geq 5$ vertices obtained from the cycle $C_3 := v_1v_2v_3$ by attaching $n-4$ pendant vertices $v_5, \dots, v_n$ at $v_1$ and a pendant vertex $v_4$ at $v_2$. Denote by $\mathbf{x}$ an eigenvector of $\mathbb{L}(S^1_n)$ associated with $\rho = \rho^{\mathbb{L}}_{n-1}(S^1_n)$. Let $x_i = x_{v_i}$ for $i = 1, \dots, n$. Note that $\rho > 0$. As $\mathbb{L}(S^1_n)$ is symmetric, we have $\mathbf{x}^\top \mathbf{1}_n = 0$, that is, $x_1 + \cdots + x_n = 0$. Note that for any $i = 5, \dots, n$,

$$\rho x_i = -\frac{1}{2}x_1 - \frac{1}{4}x_2 - \frac{1}{4}x_3 - \frac{1}{8}x_4 + \frac{2n-1}{8}x_i - \frac{1}{4}\left(\sum_{j=5}^{n} x_j - x_i\right),$$

i.e.,

$$\left(\rho - \frac{2n+1}{8}\right)x_i = -\frac{1}{4}x_1 + \frac{1}{8}x_4.$$

If $\rho = \frac{2n+1}{8}$, then $\rho^{\mathbb{L}}_{n-1} = \rho < \frac{n+1}{4}$, as desired. Suppose that $\rho \neq \frac{2n+1}{8}$. It then follows that $x_5 = \cdots = x_n$. Note that $x_1 + \cdots + x_n = 0$. Then

$$\rho x_1 = \frac{2n-1}{4}x_1 + \frac{1}{4}x_4,$$

$$\rho x_2 = -\frac{1}{4}x_1 + \frac{n+3}{4}x_2 - \frac{1}{4}x_3 - \frac{1}{4}x_4,$$

$$\rho x_3 = -\frac{1}{4}x_1 - \frac{1}{4}x_2 + \frac{n+2}{4}x_3$$

and

$$\rho x_4 = -\frac{1}{8}x_1 - \frac{3}{8}x_2 - \frac{1}{8}x_3 + \frac{n+5}{8}x_4.$$

So

$$\det \begin{pmatrix} \rho - \frac{2n-1}{4} & 0 & 0 & -\frac{1}{4} \\ \frac{1}{4} & \rho - \frac{n+3}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \rho - \frac{n+2}{4} & 0 \\ \frac{1}{8} & \frac{3}{8} & \frac{1}{8} & \rho - \frac{n+5}{8} \end{pmatrix} = 0,$$

i.e.,

$$f(\rho) = 0,$$

where

$$f(t) = t^4 - \frac{9n+13}{8}t^3 + \frac{7n^2+25n+9}{16}t^2 - \frac{9n^3+56n^2+68n-5}{128}t + \frac{2n^4+19n^3+45n^2+18n}{512}.$$

It follows that $\rho$ is the smallest root of $f(t) = 0$. As $f(\frac{n+1}{4}) = -\frac{(n+3)(n-4)}{512} < 0$, we have $\rho < \frac{n+1}{4}$, as desired.

Note that $U_{n,4}$ is the unicyclic graph with $n \geq 5$ vertices obtained from the cycle $C_4 := v_1v_2v_3v_4$ by attaching $n-4$ pendant vertices $v_5, \dots, v_n$ at $v_1$. Denote by $\mathbf{y}$ an eigenvector of $\mathbb{L}(U_{n,4})$ associated with $\rho' = \rho^{\mathbb{L}}_{n-1}(U_{n,4})$. Let $y_i = y_{v_i}$ for $i = 1, \dots, n$. Then $\rho' > 0$. As $\mathbb{L}(U_{n,4})$ is symmetric, we have $y_1 + \cdots + y_n = 0$. Note that for any $i = 5, \dots, n$,

$$\rho' y_i = -\frac{1}{2}y_1 - \frac{1}{4}y_2 - \frac{1}{8}y_3 - \frac{1}{4}y_4 + \frac{2n-1}{8}y_i - \frac{1}{4}\left(\sum_{j=5}^{n} y_j - y_i\right),$$

i.e.,

$$\left(\rho' - \frac{2n+1}{8}\right) y_i = -\frac{1}{4}y_1 + \frac{1}{8}y_3.$$

If $\rho' = \frac{2n+1}{8}$, then $\rho^{\mathbb{L}}_{n-1}(U_{n,4}) = \rho' < \frac{n+1}{4}$, as desired. Suppose that $\rho' \neq \frac{2n+1}{8}$. It then follows that $y_5 = \cdots = y_n$. Note that $y_1 + \cdots + y_n = 0$. Then

$$\rho' y_1 = \frac{2n-1}{4}y_1 + \frac{1}{4}y_3,$$

$$\rho' y_2 = -\frac{1}{4}y_1 + \frac{n+2}{4}y_2 - \frac{1}{4}y_3,$$

$$\rho' y_3 = -\frac{1}{8}y_1 - \frac{3}{8}y_2 + \frac{n+7}{8}y_3 - \frac{3}{8}y_4$$

and

$$\rho' y_4 = -\frac{1}{4}y_1 - \frac{1}{4}y_3 + \frac{n+2}{4}y_4.$$

So $\rho'$ is the smallest root of $g(t) = 0$, where

$$\begin{aligned} g(t) &= \det \begin{pmatrix} t - \frac{2n-1}{4} & 0 & -\frac{1}{4} & 0 \\ \frac{1}{4} & t - \frac{n+2}{4} & \frac{1}{4} & 0 \\ \frac{1}{8} & \frac{3}{8} & t - \frac{n+7}{8} & \frac{3}{8} \\ \frac{1}{4} & 0 & \frac{1}{4} & t - \frac{n+2}{4} \end{pmatrix} \\ &= t^4 - \frac{9n+13}{8}t^3 + \frac{14n^2+51n+16}{32}t^2 \\ &\quad - \frac{9n^3+59n^2+62n-4}{128}t + \frac{2n^4+21n^3+42n^2+16n}{512}. \end{aligned}$$

As $g(\frac{n+1}{4}) = \frac{-n^2+n+9}{512} < 0$, we have $\rho' < \frac{n+1}{4}$, as desired.

Label the vertices of $S_n^+$ as follows: let $v_1v_2v_3v_1$ be the triangle and let $v_5, \dots, v_n$ be the pendant vertices so that $v_1v_4, v_4v_5$ are edges. Denote by $z$ an eigenvector of $\mathbb{L}(S_n^+)$ associated with $\rho'' = \rho_{n-1}^{\mathbb{L}}(S_n^+)$. Let $z_i = z_{v_i}$ for $i = 1, \dots, n$. Note that $\rho'' > 0$ and $z_1 + \cdots + z_n = 0$. For any $i = 6, \dots, n$,

$$\rho'' z_i = -\frac{1}{2}z_1 - \frac{1}{4}z_2 - \frac{1}{4}z_3 - \frac{1}{4}z_4 - \frac{1}{8}z_5 + \frac{2n-1}{8}z_i - \frac{1}{4}\left(\sum_{j=6}^{n} z_j - z_i\right),$$

i.e.,

$$\left(\rho'' - \frac{2n+1}{8}\right) z_i = -\frac{1}{4}z_1 + \frac{1}{8}z_5.$$

If $\rho'' = \frac{2n+1}{8}$, then $\rho_{n-1}^{\mathbb{L}}(S_n^+) = \rho'' < \frac{n+1}{4}$, as desired. Suppose that $\rho'' \neq \frac{2n+1}{8}$. It then follows that $z_6 = \cdots = z_n$. Thus

$$\rho'' z_1 = \frac{2n-1}{4}z_1 + \frac{1}{4}z_5, \tag{3.1}$$

$$\rho'' z_2 = -\frac{1}{4}z_1 + \frac{2n+3}{8}z_2 - \frac{1}{4}z_3 + \frac{1}{8}z_5, \tag{3.2}$$

$$\rho'' z_3 = -\frac{1}{4}z_1 - \frac{1}{4}z_2 + \frac{2n+3}{8}z_3 + \frac{1}{8}z_5, \tag{3.3}$$

$$\rho'' z_4 = -\frac{1}{4}z_1 + \frac{n+2}{4}z_4 - \frac{1}{4}z_5 \tag{3.4}$$

and

$$\rho'' z_5 = -\frac{1}{8}z_1 - \frac{3}{8}z_4 + \frac{n+4}{8}z_5. \tag{3.5}$$

Subtracting (3.2) from (3.3) yields $\left(\rho'' - \frac{2n+5}{8}\right)(z_3 - z_2) = 0$. Suppose that $\rho'' = \frac{2n+5}{8}$. Then (3.4) and (3.5) become $-\frac{1}{8}z_4 = \frac{1}{4}z_1 + \frac{1}{4}z_5$ and $-\frac{3}{8}z_4 = \frac{1}{8}z_1 + \frac{n+1}{8}z_5$, so $z_1 = \frac{n-5}{5}z_5$. From (3.1), we have $z_1 = \frac{2}{-2n+7}z_5$. It thus follows that $\frac{n-5}{5} = \frac{2}{-2n+7}$, which is a contradiction. So $\rho'' \neq \frac{2n+5}{8}$ and $z_2 = z_3$. Now (3.2) becomes

$$\rho'' z_2 = -\frac{1}{4}z_1 + \frac{2n+1}{8}z_2 + \frac{1}{8}z_5. \tag{3.6}$$

Combining (3.1), (3.6), (3.4) and (3.5), we have

$$\det\begin{pmatrix} \rho'' - \frac{2n-1}{4} & 0 & 0 & -\frac{1}{4} \\ \frac{1}{4} & \rho'' - \frac{2n+1}{8} & 0 & -\frac{1}{8} \\ \frac{1}{4} & 0 & \rho'' - \frac{n+2}{4} & \frac{1}{4} \\ \frac{1}{8} & 0 & \frac{3}{8} & \rho'' - \frac{n+4}{8} \end{pmatrix} = 0,$$

i.e.,

$$h(\rho'') = 0,$$

where

$$\begin{aligned} h(t) = t^4 - \frac{9n+7}{8}t^3 + \frac{28n^2+57n+2}{64}t^2 \\ - \frac{18n^3+67n^2+25n-2}{256}t + \frac{4n^4+24n^3+21n^2+5n}{1024}. \end{aligned}$$

So $\rho''$ is the smallest root of $h(t) = 0$. For $n \geq 8$, we have $h\left(\frac{n}{4}\right) = \frac{-2n^2+7n}{1024} < 0$ and $h\left(\frac{n+1}{4}\right) = \frac{n^2-n-6}{1024} > 0$, so $\rho'' < \frac{n+1}{4}$, as desired. □

# 4 Closeness signless Laplacian eigenvalues

Similarly to the proof of Proposition 3.1, we have the following result, where the graph is required to be regular.

**Proposition 4.1.** *Let $G$ be a regular connected graph on $n \geq 2$ vertices with diameter at most two. Let $\lambda_1^Q > \lambda_2^Q \geq \cdots \geq \lambda_n^Q$ be the signless Laplacian eigenvalues of $G$. Then the closeness signless Laplacian eigenvalues of $G$ are*

$$\frac{n-1}{2} + \frac{\lambda_1^Q}{4} > \frac{1}{4}(n-2+\lambda_2^Q) \geq \cdots \geq \frac{1}{4}(n-2+\lambda_n^Q).$$

**Theorem 4.1.** *Let $G$ be a connected graph on $n \geq 2$ vertices. For $i = 1, \ldots, n-1$,*

$$\rho_1^{\mathbb{Q}}(G) \leq n-1$$

*with equality if and only if $G \cong K_n$. Moreover, for $i = 2, \ldots, n$,*

$$\rho_i^{\mathbb{Q}}(G) \leq \frac{n-2}{2}$$

*with equality if $G \cong K_n$.*

*Proof.* By Proposition 4.1, we have

$$\rho_i^{\mathbb{Q}}(K_n) = \begin{cases} n-1 & \text{if } i = 1, \\ \frac{n-2}{2} & \text{if } i = 2, \ldots, n. \end{cases}$$

So the result follows from Proposition 2.1. □

Similarly to the proof of Lemma 3.1, we have

**Lemma 4.1.** *Let $G$ be a connected graph on $n \geq 2$ vertices. Then $\rho_2^{\mathbb{Q}}(G) = \cdots = \rho_n^{\mathbb{Q}}(G)$ if and only if $G \cong K_n$.*

By Theorem 4.1 and Lemma 4.1, we have

**Corollary 4.1.** *Let $G$ be a connected graph on $n \geq 2$ vertices. Then*

$$\rho_n^{\mathbb{Q}}(G) \leq \frac{n-2}{2}$$

*with equality if and only if $G \cong K_n$.*

If $G$ is a connected graph, then $\mathbb{Q}(G)$ is irreducible, so the Perron-Frobenius theorem implies that corresponding to $\rho_1^{\mathbb{Q}}(G)$, there is a unique unit positive eigenvector, which is called the Perron vector of $\mathbb{Q}(G)$. If $\mathbf{x}$ is the Perron vector of $\mathbb{Q}(G)$ of a connected graph $G$, and $\varphi$ is an automorphism of $G$, then, as in [16, Lemma 2.1], $\varphi(u) = v$ implies that $x_u = x_v$. In this case, we say that $x_u = x_v$ by symmetry.

**Theorem 4.2.** *Let $G$ be a connected graph with a cut edge $uv$. Suppose that $uv$ is not a pendant edge. Let $G_{uv}$ be defined as in Lemma 3.2, see Fig. 1. Then $\rho_1^{\mathbb{Q}}(G_{uv}) > \rho_1^{\mathbb{Q}}(G)$.*

*Proof.* Let $\mathbf{x}$ be the Perron vector of $\mathbb{Q}(G)$.

Let $G_1$ and $G_2$ be the components of $G - uv$ containing $u$ and $v$, respectively. As we pass from $G$ to $G_{uv}$, the distance between any vertex in $V(G_2) \setminus \{v\}$ and any vertex in $V(G_1)$ is decreased by 1, the distance between any vertex in $V(G_2) \setminus \{v\}$ and $v$ is increased by 1, and the distance between any other vertex pair remains unchanged. So, by Rayleigh's principle, we have

$$\frac{1}{2}\left(\rho_1^{\mathbb{Q}}(G_{uv}) - \rho_1^{\mathbb{Q}}(G)\right) \geq \frac{1}{2}\mathbf{x}^\top(\mathbb{Q}(G_{uv}) - \mathbb{Q}(G))\mathbf{x}$$

$$
\begin{aligned}
&= \sum_{y\in V(G_2)\setminus\{v\}} \sum_{w\in V(G_1)} \left(2^{-(d_G(w,y)-1)} - 2^{-d_G(w,y)}\right)(x_w+x_y)^2 \\
&\quad + \sum_{y\in V(G_2)\setminus\{v\}} \left(2^{-(d_G(v,y)+1)} - 2^{-d_G(v,y)}\right)(x_v+x_y)^2 \\
&= \sum_{y\in V(G_2)\setminus\{v\}} \sum_{w\in V(G_1)\setminus\{u\}} 2^{-d_G(w,y)}(x_w+x_y)^2 \\
&\quad + \sum_{y\in V(G_2)\setminus\{v\}} 2^{-d_G(u,y)}(x_u+x_y)^2 - \sum_{y\in V(G_2)\setminus\{v\}} 2^{-(d_G(v,y)+1)}(x_v+x_y)^2 \\
&= \sum_{y\in V(G_2)\setminus\{v\}} \sum_{w\in V(G_1)\setminus\{u\}} 2^{-d_G(w,y)}(x_w+x_y)^2 \\
&\quad + \sum_{y\in V(G_2)\setminus\{v\}} 2^{-d_G(u,y)}(x_u-x_v)(x_u+x_v+2x_y).
\end{aligned}
$$

Let $G' = G - \{uw : w \in N_G(u)\setminus\{v\}\} + \{vw : w \in N_G(u)\setminus\{v\}\}$, i.e., $G' = G_{vu}$. Similarly as above, we have

$$
\begin{aligned}
\frac{1}{2}\left(\rho_1^{\mathbb{Q}}(G_{vu}) - \rho_1^{\mathbb{Q}}(G)\right) &\geq \frac{1}{2}\mathbf{x}^\top(\mathbb{Q}(G_{vu}) - \mathbb{Q}(G))\mathbf{x} \\
&= \sum_{y\in V(G_2)\setminus\{v\}} \sum_{w\in V(G_1)\setminus\{u\}} 2^{-d_G(w,y)}(x_w+x_y)^2 \\
&\quad + \sum_{w\in V(G_1)\setminus\{u\}} 2^{-d_G(v,w)}(x_v-x_u)(x_u+x_v+2x_w).
\end{aligned}
$$

So, if $x_u \geq x_v$, then $\rho_1^{\mathbb{Q}}(G_{uv}) > \rho_1^{\mathbb{Q}}(G)$, and otherwise, $\rho_1^{\mathbb{Q}}(G_{vu}) > \rho_1^{\mathbb{Q}}(G)$. Note that $G_{uv} \cong G_{vu}$. So $\rho_1^{\mathbb{Q}}(G_{uv}) > \rho_1^{\mathbb{Q}}(G)$. $\square$

**Theorem 4.3.** *Let $G$ be a tree on $n \geq 3$ vertices. Then $\rho_1^{\mathbb{Q}}(G) \leq \frac{n-1+\sqrt{n-1}}{2}$ with equality if and only if $G \cong K_{1,n-1}$.*

*Proof.* Let $d$ be the diameter of $G$. Then $2 \leq d \leq n-1$. Suppose that $d \geq 3$. Then there is an edge $uv$ that is not a pendant edge. By Theorem 4.2, $\rho_1^{\mathbb{Q}}(G_{uv}) > \rho_1^{\mathbb{Q}}(G)$. So, the tree with diameter two, $K_{1,n-1}$, is the unique $n$-vertex tree that maximizes the closeness signless Laplcian spectral radius. By a direct calculation, we have $\rho_1^{\mathbb{Q}}(K_{1,n-1}) = \frac{n-1+\sqrt{n-1}}{2}$. $\square$

**Lemma 4.2.** *For integers $\ell$ and $n$ with $2 \leq \ell \leq \lfloor \frac{n-2}{2} \rfloor$, we have $\rho_1^{\mathbb{Q}}(D_{n,\ell}) < \rho_1^{\mathbb{Q}}(D_{n,\ell-1})$.*

*Proof.* Let $\mathbf{x}$ be the Perron vector of $\mathbb{Q}(D_{n,\ell})$ and let $\rho = \rho_1^{\mathbb{Q}}(D_{n,\ell})$. Let $u$ and $v$ be two vertices in $D_{n,\ell}$ so that the degree of $u$ and $v$ are $\ell+1$ and $n-\ell-1$, respectively. By symmetry, the entries of $\mathbf{x}$ at all pendant neighbors of $u$ ($v$, respectively) have the same value, which we denote by $\alpha$ ($\beta$, respectively).

By deleting a pendant edge at $u$ and adding an edge between the resulted isolated vertex and $v$ in $D_{n,\ell}$ we have a graph that is isomorphic to $D_{n,\ell-1}$. By Rayleigh's principle, we have

$$\begin{aligned}
&\frac{1}{2}\left(\rho_1^{\mathbb{Q}}(D_{n,\ell-1}) - \rho_1^{\mathbb{Q}}(D_{n,\ell})\right)\\
&\geq (\ell-1)\left(\frac{1}{8}-\frac{1}{4}\right)(\alpha+\alpha)^2 + \left(\frac{1}{4}-\frac{1}{2}\right)(\alpha+x_u)^2\\
&\quad+\left(\frac{1}{2}-\frac{1}{4}\right)(\alpha+x_v)^2 + (n-2-\ell)\left(\frac{1}{4}-\frac{1}{8}\right)(\alpha+\beta)^2\\
&=\frac{\ell-1}{8}(3\alpha+\beta)(\beta-\alpha)+\frac{1}{4}(x_v-x_u)(x_v+x_u+2\alpha)+\frac{n-2\ell-1}{8}(\alpha+\beta)^2.
\end{aligned} \tag{4.1}$$

By deleting $n-2\ell-1$ pendant edges at $v$ and adding edges between $u$ and the resulted isolated vertices, we have a graph that is isomorphic to $D_{n,\ell-1}$. Similarly as above, we have

$$\begin{aligned}
&\frac{1}{2(n-2\ell-1)}\left(\rho_1^{\mathbb{Q}}(D_{n,\ell-1}) - \rho_1^{\mathbb{Q}}(D_{n,\ell})\right)\\
&\geq \ell\left(\frac{1}{4}-\frac{1}{8}\right)(\alpha+\beta)^2 + \left(\frac{1}{2}-\frac{1}{4}\right)(x_u+\beta)^2\\
&\quad+\left(\frac{1}{4}-\frac{1}{2}\right)(x_v+\beta)^2 + (\ell-1)\left(\frac{1}{8}-\frac{1}{4}\right)(\beta+\beta)^2\\
&=\frac{1}{4}(x_u-x_v)(x_u+x_v+2\beta)+\frac{\ell-1}{8}(\alpha+3\beta)(\alpha-\beta)+\frac{1}{8}(\alpha+\beta)^2
\end{aligned} \tag{4.2}$$

**Case 1.** $x_v \geq x_u$.

Considering the entries of $\rho\mathbf{x} = \mathbb{Q}(D_{n,\ell})\mathbf{x}$ at $u$ and $v$, respectively, we have

$$\left(\rho - \frac{n+\ell+2}{8}\right)\alpha = \frac{\ell-1}{4}\alpha + \frac{1}{2}x_u + \frac{1}{4}x_v + \frac{n-\ell-2}{8}\beta$$

and

$$\left(\rho - \frac{2n-\ell}{8}\right)\beta = \frac{\ell}{8}\alpha + \frac{1}{4}x_u + \frac{1}{2}x_v + \frac{n-\ell-3}{4}\beta.$$

So

$$\left(\rho - \frac{n+2\ell}{8}\right)\alpha - \left(\rho - \frac{3n-2\ell-4}{8}\right)\beta = \frac{1}{4}(x_u-x_v) \leq 0.$$

Note that $3n-2\ell-4 \geq n+2\ell$ as $2 \leq \ell \leq \lfloor \frac{n-2}{2} \rfloor$. Then

$$\left(\rho - \frac{3n-2\ell-4}{8}\right)(\alpha-\beta) \leq 0. \tag{4.3}$$

By Interlacing theorem, we have $\rho \geq c_{D_{n,\ell}}(v) = \frac{2n-\ell-2}{4} > \frac{3n-2\ell-4}{8}$. By (4.3), we have $\alpha \leq \beta$. Now, by (4.1), we have $\rho_1^{\mathbb{Q}}(D_{n,\ell-1}) > \rho_1^{\mathbb{Q}}(D_{n,\ell})$.

**Case 2.** $x_u > x_v$.

From $\rho\mathbf{x} = \mathbb{Q}(D_{n,\ell})\mathbf{x}$ at $u$ and $v$, we have

$$\left(\rho - \frac{n+\ell}{4}\right) x_u = \frac{\ell}{2}\alpha + \frac{1}{2}x_v + \frac{n-\ell-2}{4}\beta$$

and

$$\left(\rho - \frac{2n-\ell-2}{4}\right) x_v = \frac{\ell}{4}\alpha + \frac{1}{2}x_u + \frac{n-\ell-2}{2}\beta.$$

So

$$\left(\rho - \frac{n+\ell-2}{4}\right) x_u - \left(\rho - \frac{2n-\ell-4}{4}\right) x_v = \frac{\ell}{4}\alpha - \frac{n-\ell-2}{4}\beta.$$

Note that $n-\ell-2 \geq \ell$ and $2n-\ell-4 \geq n+\ell-2$ as $2 \leq \ell \leq \lfloor \frac{n-2}{2} \rfloor$. Then

$$\left(\rho - \frac{2n-\ell-4}{4}\right)(x_u - x_v) \leq \frac{n-\ell-2}{4}(\alpha - \beta). \tag{4.4}$$

Note that $\rho \geq c_{D_{n,\ell}}(v) = \frac{2n-\ell-2}{4} > \frac{2n-\ell-4}{4}$. By (4.4), we have $\alpha \geq \beta$. Hence, by (4.2), we have $\rho_1^{\mathbb{Q}}(D_{n,\ell-1}) > \rho_1^{\mathbb{Q}}(D_{n,\ell})$. □

**Theorem 4.4.** *Let $G$ be a tree on $n \geq 3$ vertices and $G \ncong K_{1,n-1}$. Then $\rho_1^{\mathbb{Q}}(G) \leq r_n$ with equality if and only if $G \cong D_{n,1}$, where $r_n$ is the largest root of $f(t) = 0$ with*

$$\begin{aligned} f(t) = t^4 - \frac{11n-10}{8}t^3 + \frac{21n^2-39n+6}{32}t^2 - \frac{16n^3-35n^2-47n+128}{128}t \\ + \frac{2n^4-3n^3-28n^2+85n-60}{256}. \end{aligned}$$

*Proof.* Suppose that $G$ is a tree on $n \geq 3$ vertices and $G \ncong K_{1,n-1}$ that maximizes the closeness signless Laplcian spectral radius. Let $d$ be the diameter of $G$. Then $3 \leq d \leq n-1$. By Theorem 4.2, $d = 3$. So $G \cong D_{n,a}$ with $1 \leq a \leq \frac{n-2}{2}$. Then by Lemma 4.2, we have $G \cong D_{n,1}$.

In the following we compute $\rho = \rho_1^{\mathbb{Q}}(D_{n,1})$. Let $\mathbf{x}$ be the Perron vector of $\mathbb{Q}(D_{n,1})$. Let $v_2$ and $v_3$ be the two vertices so that the degree of $v_2$ and $v_3$ are 2 and $n-2$, respectively. Label the pendant vertex at $v_2$ by $v_1$, and the other pendant vertices labeled by $v_4, \ldots, v_n$, respectively. Let $x_i = x_{v_i}$ for $i = 1, \ldots, n$. By symmetry, for all $n-3$ pendant vertices at $v_3$, the corresponding entries in $\mathbf{x}$ are equal. Then

$$\left(\rho - \frac{n+3}{8}\right) x_1 = \frac{1}{2}x_2 + \frac{1}{4}x_3 + \frac{n-3}{8}x_4,$$

$$\left(\rho - \frac{n+1}{4}\right) x_2 = \frac{1}{2}x_1 + \frac{1}{2}x_3 + \frac{n-3}{4}x_4,$$

$$\left(\rho - \frac{2n-3}{4}\right) x_3 = \frac{1}{4}x_1 + \frac{1}{2}x_2 + \frac{n-3}{2}x_4,$$

and

$$\left(\rho - \frac{4n-9}{8}\right) x_4 = \frac{1}{8}x_1 + \frac{1}{4}x_2 + \frac{1}{2}x_3.$$

So

$$\det \begin{pmatrix} \rho - \frac{n+3}{8} & -\frac{1}{2} & -\frac{1}{4} & -\frac{n-3}{8} \\ -\frac{1}{2} & \rho - \frac{n+1}{4} & -\frac{1}{2} & -\frac{n-3}{4} \\ -\frac{1}{4} & -\frac{1}{2} & \rho - \frac{2n-3}{4} & -\frac{n-3}{2} \\ -\frac{1}{8} & -\frac{1}{4} & -\frac{1}{2} & \rho - \frac{4n-9}{8} \end{pmatrix} = 0.$$

By a direct calculation, this determinant is just equal to $f(\rho)$. It thus follows that $\rho$ is the largest root of $f(t) = 0$. □

# 5 Concluding remarks

In [16], a number of results have been obtained to connect the spectral properties of the closeness matrix and the structural properties of graphs. In this paper, various connections between the spectral properties of closeness Laplacian (closeness signless Laplacian, respectively) and structural properties of graphs are established, and extremal problems to minimize certain closeness Laplacian (closeness signless Laplacian, respectively) eigenvalues are investigated. The two Laplacians based on closeness may be studied for any graphs, while the distance versions applied only to connected graphs, see [1]. As compared to the ordinary Laplacian and signless Laplacian based on adjacency, the versions considered in this article also have merits as distances should be considered so as to reveal more elusive connections between spectral and structural properties. There are lots of problems to further study. For example, one may consider more extremal problems for different graph classes, and the corrections between the largest closeness Laplacian and closeness signless Laplacian eigenvalues and other distance-based graph invariants such as radius, diameter, average distance, average eccentricity, remoteness and proximity, see, e.g. [8, 14]. As in [12], one may also merge the spectral properties of closeness matrix and its signless Laplacian.

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