On the Spectral Closeness and Residual Spectral Closeness of Graphs

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Abstract

The spectral closeness of a graph G is defined as the spectral radius of the closeness matrix of G, whose (u, v)-entry for vertex u and vertex v is $2^{-d_G(u,v)}$ if $u \neq v$ and 0 otherwise, where $d_G(u, v)$ is the distance between u and v in G. The residual spectral closeness of a nontrivial graph G is defined as the minimum spectral closeness of the subgraphs of G with one vertex deleted. We propose local grafting operations that decrease or increase the spectral closeness and determine those graphs that uniquely minimize and/or maximize the spectral closeness in some families of graphs. We also discuss extremal properties of the residual spectral closeness.

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1 Introduction

A complex network is often modeled as a simple and undirected graph. Let G be a graph on n vertices 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 detail on graph distances, we refer to the book [7]. The spectral properties of some matrices associated with graphs such as the adjacency matrix (for any graph) and the distance matrix (for any connected graph) have been studied extensively, see [1, 10].

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

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

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It can be readily seen that two n-vertex graphs G_1 and G_2 are isomorphic if and only if $PC(G_1)P^\top = C(G_2)$ for some permutation matrix P of order n. That is, the vertices of G_1 may be relabeled so that its closeness matrix is just $C(G_2)$. So, a graph can be completely described by giving the closeness matrix.

The closeness matrix may be extended to the q-closeness matrix (or exponential distance matrix [6], q-distance matrix [23]) for any real number $q \in (0,1)$ by defining the (u,v)-entry to be $q^{d_G(u,v)}$ if $u \neq v$ and 0 otherwise.

Dangalchev [11] introduced a novel version of closeness as a measure of centrality [13, 14]. For a graph G with $v \in V(G)$, the closeness of vertex v in G is defined as [11]

$$c_G(v) = \sum_{w \in V(G) \setminus \{v\}} 2^{-d_G(v,w)},$$

and the closeness of a graph G is defined as [11]

$$c(G) = \sum_{v \in V(G)} c_G(v).$$

It is evident that $c(G)$ is equal to the sum of all entries of the matrix $C(G)$. Moreover, this concept of closeness is then used in [11] to define the (vertex) residual closeness of a nontrivial graph G by

$$R(G) = \min\{c(G-u) : u \in V(G)\},$$

which is used to measure the network resistance in the face of possible node destruction, see also [2–4, 12, 18].

For a graph G, $C(G)$ is a symmetric nonnegative matrix. Moreover, $C(G)$ is irreducible if and only if G is connected. The spectral radius (or principal eigenvalue) of a square nonnegative matrix M is defined as

$$\mu(M) = \max\{|\lambda| : \lambda \text{ is an eigenvalue of } M\}.$$

The *spectral closeness* of a graph G is defined as the spectral radius of its closeness matrix, denoted by $\varrho(G)$. That is, $\varrho(G) = \mu(C(G))$. As $C(G)$ is symmetric, its eigenvalues are all real, so $\rho(G)$ is equal to the greatest eigenvalue of $C(G)$. A routine connection between the spectral closeness and the closeness of an n-vertex graph G is

$$\frac{c(G)}{n} \leq \varrho(G) \leq \max_{v \in V(G)} c_G(v)$$

with either equality when G is connected if and only if $c_G(v)$ is a constant for any $v \in V(G)$. The left part follows from Rayleigh's principle and Perron-Frobenius theorem, while the right part follows from a classical result that the spectral radius of a nonnegative matrix is bounded from above by the maximum row sum (see Lemma 2.3 below). So, $\varrho(G)$ is indeed a graph invariant that is closely related the closeness of the graph G. Similarly, we propose the *residual spectral closeness* of a nontrivial graph G to be defined as

$$\varrho^R(G) = \min\{\varrho(G-v) : v \in V(G)\}.$$

with convention that $\varrho^R(K_1) = 0$. As above, for an n-vertex graph G with $n \geq 2$, one has

$$\frac{R(G)}{n-1} = \min_{v \in V(G)} \frac{c(G-v)}{n-1} \leq \varrho^R(G) \leq \min_{v \in V(G)} \max_{w \in V(G) \setminus \{v\}} c_{G-v}(w).$$

Spectral measures have long been used to quantify the robustness of networks. For example, spectral radius of the adjacency matrix of a graph is related to the effective spreading rates of dynamic processes (e.g., rumor, disease, information propagation) on networks [9, 20], and the spectral radius of distance matrix of a connected graph is used as a molecular descriptor [5, 15, 21].

For an n-vertex graph G with $n \geq 2$, we may view $\frac{R(G)}{n-1}$ as a normalized version of the residual closeness of G. In this sense, the residual spectral closeness is the spectral version of this 'normalized version of residual closeness'. Like the residual closeness, it may also serve as a network vulnerability parameter in the model where links are reliable and the nodes fail independently of each other, or it may also be viewed as a measure of graph or network structures.

As demonstrated by the example below, spectral closeness and residual spectral closeness may be used to distinguish graphs with equal closeness.

In [12], Dangalchev gave a pair of graphs W and H on 7 vertices (in Figs. 3 and 4 in [12]) with the same closeness. See Fig. 1 for W and H.

Fig. 1: Graphs W and H.

Note that W has no cut vertex and H has a cut vertex, so the two graphs are quite different. By an easy calculation, we find that they have different spectral closeness as $\varrho(W) = \frac{7+\sqrt{145}}{8} \approx 2.3802 < \varrho(H) = 2.5$. Let u be the vertex of degree 7 in W (6 in H, respectively) and v be any other vertex in W (H, respectively). Then $\varrho(W-u) = \frac{13}{8} < \varrho(W-v) \approx 2.0240$ and $\varrho(H-u) = 1 < \varrho(H-v) \approx 2.0251$, so W and H have also different residual spectral closeness as $\varrho^R(W) = \frac{13}{8} > 1 = \varrho^R(H) = 1$.

Denote by $\mathbb{G}$ a class of graph and $f(G)$ a graph invariant. Often, it is of interest to study the extremal problem to determine

$$\min\{f(G) : G \in \mathbb{G}\}$$

and

$$\max\{f(G) : G \in \mathbb{G}\}.$$

Moreover, we want to identify those graphs in $\mathbb{G}$ for which the above minimum and maximum are achieved, respectively.

The rest of this article is organized as follows. Section 2 introduces preliminaries including concepts and lemmas that are needed in subsequent proofs. In Section 3, we propose some local grafting operations that decrease or increase the spectral closeness. In Section 4, we study the above extremal problem to identify the graphs that minimize and/or maximize the spectral closeness in some well known classes of graphs by exploiting the results established in Section 3. In particular, we identify the unique trees, unicyclic graphs, graphs with given number of pendant vertices and graphs with given connectivity that maximize the spectral closeness, respectively. In Section 5, we give some preliminary results for the residual spectral closeness and discuss further study in the future.

2 Preliminaries

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, obtained from $G_1 \cup G_2$ by adding all possible edges between vertices in G_1 and vertices in G_2. 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 $e \in E(G)$. Let $\overline{G}$ be 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 edges of E', and we write $G + uv$ for $G + \{uv\}$ for $uv \in E(\overline{G})$. For a graph G with $v \in V(G)$, denote by $N_G(v)$ the set of vertices that are adjacent to v in G.

Let K_n, P_n and S_n be the n-vertex complete graph, path and star, respectively. Let $K_{a,b}$ be the complete bipartite graph with a and b vertices in the two partite sets, respectively. Let S_n^+ be the graph obtained from S_n by adding an edge. Let $D_{n,\ell}$ be the n-vertex tree of diameter 3 such that its two center vertices have degrees $\ell + 1$ and $n - \ell - 1$, respectively.

Let v be a vertex of a graph G. The degree of v in G is the number of edges that are incident to v in G. The vertex v is called a *pendant vertex* if its degree in G is one. An edge in a graph G is called a *pendant edge* if it is incident to a pendant vertex in G.

Let G be a graph with $V(G) = \{v_1, \ldots, v_n\}$. Let $\mathbf{x} = (x_{v_1}, \ldots, x_{v_n})^\top$ be a real vector. Then

$$\mathbf{x}^\top C(G)\mathbf{x} = \sum_{u,v \in V(G)} 2^{-d_G(u,v)} x_u x_v.$$

If G is connected, then $C(G)$ is irreducible, so, by Perron-Frobenius theorem, $\varrho(G)$ is a simple eigenvalue of $C(G)$, and associated with $\varrho(G)$, there is a unique positive unit eigenvector, which we call the *closeness Perron vector* of G.

If G is connected and $\mathbf{x}$ is the closeness Perron vector of G, then, for any vertex

$v \in V(G)$, from $\varrho(G)\mathbf{x} = C(G)\mathbf{x}$, we have

$$\varrho(G)x_u = \sum_{v \in V(G) \setminus \{u\}} 2^{-d_G(u,v)} x_v. \tag{2.1}$$

We call (2.1) the *closeness equation* of G at u.

Let G be a graph of order n. By Rayleigh's principle, for any n-dimensional unit (column) vector $\mathbf{x}$, we have $\varrho(G) \geq \mathbf{x}^\top C(G)\mathbf{x}$ with equality if and only if $\mathbf{x}$ is an eigenvector associated with $\varrho(G)$.

Lemma 2.1. *Let G be a connected graph and $\mathbf{x}$ the closeness Perron vector of G. Let φ be an automorphism of G. If $\varphi(u) = v$, then $x_u = x_v$.*

Proof. Denote by $P = (P_{uv})_{u,v \in V(G)}$ the permutation matrix such that $P_{uv} = 1$ if $\varphi(u) = v$ and 0 otherwise. Then $C(G) = PC(G)P^\top$. So $\varrho(G) = \mathbf{x}^\top C(G)\mathbf{x} = \mathbf{x}^\top PC(G)P^\top \mathbf{x} = (P^\top \mathbf{x})^\top C(G)(P^\top \mathbf{x})$. By Rayleigh's principle and Perron-Frobenius theorem, $P^\top \mathbf{x} = \mathbf{x}$. This implies that $x_u = x_v$ provided that $P_{uv} = 1$, or equivalently, $\varphi(u) = v$. $\square$

Recall that, for a square nonnegative matrix M, $\mu(M)$ is the spectral radius of M. Combining Corollaries 2.1 and 2.2 in [17, p. 38], we have the following lemma.

Lemma 2.2. *[17] Let B_1 and B_2 be $n \times n$ nonnegative matrices such that $B_1 - B_2$ is nonnegative. Then $\mu(B_1) \geq \mu(B_2)$. Furthermore, if B_1 is irreducible and $B_1 \neq B_2$, then $\mu(B_1) > \mu(B_2)$.*

For a principal matrix M of $C(G)$ for a graph G, we have $\varrho(G) \geq \mu(M)$. This follows from Lemma 2.2 (by noting that $\mu(M) = \mu(M')$ with M' being the matrix obtained from $C(G)$ by replacing any entry not in M by 0), and it is part of the well known Interlacing Theorem (see, e.g., Theorem 4.3.28 in [16, p. 246]). For any graph G with two nonadjacent vertices u and v, by Lemma 2.2, we have $\varrho(G+uv) \geq \varrho(G)$, and it is strict if $G + uv$ is connected.

The following lemma is well known, see, e.g., Theorem 1.1 in [17, p. 24].

Lemma 2.3. *[17] Let B be a nonnegative matrix of order n with the i-th row sum $r_i(B)$ for $i = 1, \ldots, n$. Then*

$$\min\{r_i(B) : i = 1, \ldots, n\} \leq \mu(B) \leq \max\{r_i(B) : i = 1, \ldots, n\}$$

with either equality when B is irreducible if and only if $r_1(B) = \cdots = r_n(B)$.

3 Effect of local grafting operations on the spectral closeness

In this section, we propose some local grafting operations that decrease or increase the spectral closeness. By a local grafting operation, we mean to remove and add some edge(s) to form a new graph with certain desired structure.

A path $P := u_0 \dots u_k$ in a graph G is called a *pendant path* of length k at u_0 if the degree of u_k is one, the degree of u_0 is at least two, and if $k > 1$, the degree of u_i is two for all $i = 1, \dots, k-1$. In particular, a pendant path of length one is a pendant edge. If $P := u_0 \dots u_k$ is a pendant path of G at u_0, we also say G is obtained from $H - \{u_1, \dots, u_k\}$ by attaching a pendant path of length k at u_0. For positive integers k and r, let $G_u(k,r)$ be the graph obtained from G by attaching two pendant paths of length k and r respectively at u, and let $G_u(k,0)$ be the graph obtained from G by attaching a pendant path of length k at u, see Fig. 2, where the pendant paths are $uu_1 \dots u_k$ and $uv_1 \dots v_r$.

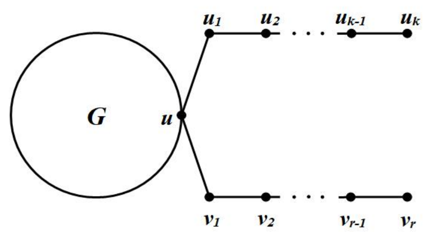

Fig. 2: Graph $G_u(k,r)$.

Theorem 3.1. *Let G be a connected nontrivial graph with $u_0 \in V(G)$. Let k and r be positive integers. Then $\varrho(G_{u_0}(k+r,0)) < \varrho(G_{u_0}(k,r))$.*

Proof. Let $H = G_{u_0}(k,r)$. Let $P := u_0u_1 \dots u_k$ and $Q := u_0v_1 \dots v_r$ be the two pendant paths at u_0 in H. Let $H' = G - \{u_0w : w \in N_G(u_0)\} + \{u_kw : w \in N_G(u_0)\}$. It is evident that $H' \cong G_{u_0}(k+r,0)$.

Let $\mathbf{x}$ be the closeness Perron vector of H'. Let $\Lambda = \sum_{i=0}^{k}(2^{-i} - 2^{-(k-i)})x_{u_i}$. Let $d = d_G(u_0,w)$ for $w \in V(G)$. It is easy to see that as we pass from H to H', the distance between any two vertices in $V(G) \setminus \{u_0\}$ and in $V(P) \cup V(Q)$ remains unchanged. By considering the changes of the entries of the closeness matrix as H is changed into H' and using Rayleigh's principle, we have

$$
\begin{aligned}
&\frac{1}{2}(\varrho(H') - \varrho(H)) \\
&\le \frac{1}{2}\mathbf{x}^\top (C(H') - C(H))\mathbf{x} \\
&= \sum_{w \in V(G)\setminus\{u_0\}} x_w \left[\sum_{i=0}^{k} \left(2^{-(d+k-i)} - 2^{-(d+i)}\right) x_{u_i} + \sum_{i=1}^{r} \left(2^{-(d+k+i)} - 2^{-(d+i)}\right) x_{v_i} \right] \\
&= \sum_{w \in V(G)\setminus\{u_0\}} 2^{-d} x_w \left[\sum_{i=0}^{k} (2^{-(k-i)} - 2^{-i}) x_{u_i} + \sum_{i=1}^{r} (2^{-(k+i)} - 2^{-i}) x_{v_i} \right],
\end{aligned}
$$

so

$$\begin{aligned}&\frac{1}{2}(\varrho(H')-\varrho(H))\\&\leq\sum_{w\in V(G)\setminus\{u_0\}}2^{-d}x_w(-\Lambda)+\sum_{w\in V(G)\setminus\{u_0\}}2^{-d}x_w\sum_{i=1}^{r}(2^{-(k+i)}-2^{-i})x_{v_i}.\end{aligned}\tag{3.1}$$

Now define a new vector $\mathbf{y}$ by setting $y_{u_i}=x_{u_{k-i}}$ if $0\leq i\leq k$, and $y_w=x_w$ if $w\in V(H')\setminus\{u_0,\ldots,u_k\}$. It is evident that $\|\mathbf{y}\|=\|\mathbf{x}\|=1$. Then, we have

$$\begin{aligned}&\frac{1}{2}(\varrho(H')-\varrho(H))\\&\leq\frac{1}{2}(\mathbf{x}^\top C(H')\mathbf{x}-\mathbf{y}^\top C(H)\mathbf{y})\\&=\sum_{w\in V(G)\setminus\{u_0\}}x_w\left(\sum_{i=0}^{k}2^{-(d+k-i)}x_{u_i}+\sum_{i=1}^{r}2^{-(d+k+i)}x_{v_i}\right)+\sum_{i=1}^{r}x_{v_i}\sum_{j=0}^{k}2^{-(i+j)}x_{u_j}\\&\quad-\sum_{w\in V(G)\setminus\{u_0\}}y_w\left(\sum_{i=0}^{k}2^{-(d+i)}y_{u_i}+\sum_{i=1}^{r}2^{-(d+i)}y_{v_i}\right)-\sum_{i=1}^{r}x_{v_i}\sum_{j=0}^{k}2^{-(i+j)}y_{u_j}\\&=\sum_{w\in V(G)\setminus\{u_0\}}2^{-d}x_w\left(\sum_{i=0}^{k}2^{-(k-i)}x_{u_i}+\sum_{i=1}^{r}2^{-(k+i)}x_{v_i}\right.\\&\quad\left.-\sum_{i=0}^{k}2^{-i}x_{u_{k-i}}-\sum_{i=1}^{r}2^{-i}x_{v_i}\right)+\sum_{i=1}^{r}2^{-i}x_{v_i}\sum_{j=0}^{k}2^{-j}(x_{u_j}-x_{u_{k-j}})\\&=\sum_{w\in V(G)\setminus\{u_0\}}2^{-d}x_w\sum_{i=1}^{r}\left(2^{-(k+i)}-2^{-i}\right)x_{v_i}+\sum_{i=1}^{r}2^{-i}x_{v_i}\sum_{j=0}^{k}\left(2^{-j}-2^{-(k-j)}\right)x_{u_j},\end{aligned}$$

so

$$\frac{1}{2}(\varrho(H')-\varrho(H))\leq\sum_{w\in V(G)\setminus\{u_0\}}2^{-d}x_w\sum_{i=1}^{r}(2^{-(k+i)}-2^{-i})x_{v_i}+\sum_{i=1}^{r}2^{-i}x_{v_i}\Lambda.\tag{3.2}$$

If $\Lambda\geq 0$, then, as $(2^{-(k+i)}-2^{-i})x_{v_i}<0$ for $1\leq i\leq r$, we have $\varrho(H')<\varrho(H)$ from (3.1). Otherwise, as $(2^{-(k+i)}-2^{-i})x_{v_i}<0$ for $1\leq i\leq r$, we have $\varrho(H')<\varrho(H)$ from (3.2). □

Theorem 3.2. *Let G be a connected graph with a cut edge uv that is not a pendant edge. Let*

$$G_{uv}=G-\{vw:w\in N_G(v)\setminus\{u\}\}+\{uw:w\in N_G(v)\setminus\{u\}\}.$$

Then $\varrho(G_{uv})>\varrho(G)$.

Proof. Let $\mathbf{x}$ be the closeness Perron vector of G.

Let G_1 and G_2 be the components of $G-uv$ containing u and v, respectively, see Fig. 3. As we pass from G to G_{uv}, the distance between any vertex in $V(G_2)\setminus\{v\}$

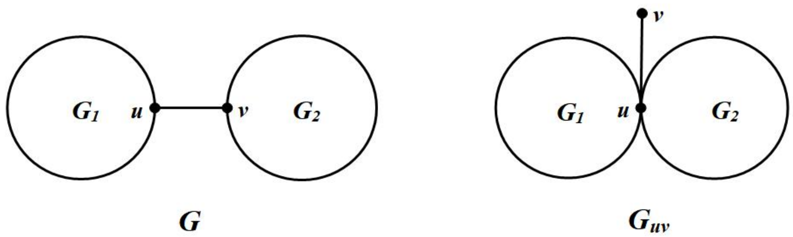

Fig. 3: Graphs G and G_{uv} in proof of Theorem 3.2.

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

$$\begin{aligned}
&\frac{1}{2}(\varrho(G_{uv})-\varrho(G))\\
&\geq \frac{1}{2}\mathbf{x}^\top(C(G_{uv})-C(G))\mathbf{x}\\
&=\sum_{w\in V(G_2)\setminus\{v\}} x_w \left[\sum_{z\in V(G_1)} \left(2^{-(d_G(w,z)-1)}-2^{d_G(w,z)}\right)x_z\right.\\
&\qquad \left. +\left(2^{-(d_G(w,v)+1)}-2^{-d_G(w,v)}\right)x_v\right]\\
&=\sum_{w\in V(G_2)\setminus\{v\}} x_w \left(\sum_{z\in V(G_1)\setminus\{u\}} 2^{-d_G(w,z)}x_z+2^{-d_G(w,u)}x_u-2^{-(d_G(w,v)+1)}x_v\right)\\
&=\sum_{w\in V(G_2)\setminus\{v\}} x_w \left[\sum_{z\in V(G_1)\setminus\{u\}} 2^{-d_G(w,z)}x_z+2^{-d_G(w,u)}(x_u-x_v)\right].
\end{aligned}$$

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

$$\begin{aligned}
&\frac{1}{2}(\varrho(G_{vu})-\varrho(G))\\
&\geq \frac{1}{2}\mathbf{x}^\top(C(G_{vu})-C(G))\mathbf{x}\\
&=\sum_{w\in V(G_1)\setminus\{u\}} x_w \left[\sum_{z\in V(G_2)\setminus\{v\}} 2^{-d_G(w,z)}x_z+2^{-d_G(w,v)}(x_v-x_u)\right].
\end{aligned}$$

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

Theorem 3.3. *Let G be a connected graph. Let H be an induced subgraph of G of order p and $H \cong K_p$. Suppose that $G - E(H)$ consists of p components. Suppose that G_u and G_v are two nontrivial components of $G - E(H)$ containing $u, v \in V(H)$, respectively. Let*

$$H_1 = G - \{uw : w \in N_{G_u}(u)\} + \{vw : w \in N_{G_u}(u)\}$$

and

$$H_2 = G - \{vw : w \in N_{G_v}(v)\} + \{uw : w \in N_{G_v}(v)\},$$

see Fig. 4. Then $\varrho(H_1) > \varrho(G)$ or $\varrho(H_2) > \varrho(G)$.

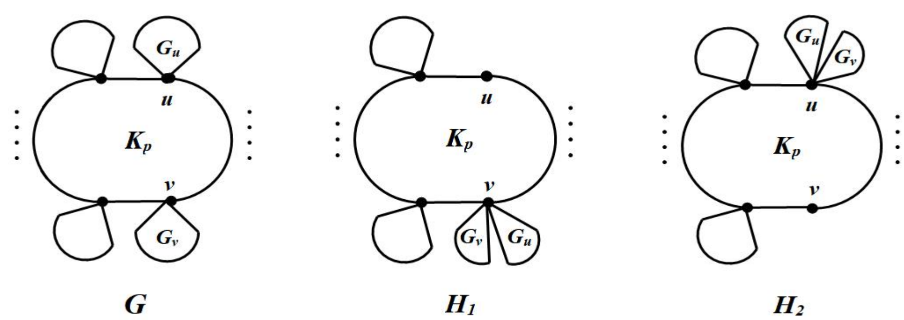

Fig. 4: Graphs G, H_1 and H_2 in Theorem 3.3.

Proof. Let $\mathbf{x}$ be the closeness Perron vector of G.

Note that as we pass from G to H_1, the distance between a vertex $w \in V(G_u)\backslash\{u\}$ and u is increased by 1, the distance between a vertex $w \in V(G_u) \setminus \{u\}$ and any vertex in $V(G_v)$ is decreased by 1, and the distance between any other vertex pair remains unchanged. So we have by Rayleigh's principle that

$$\begin{aligned}
&\frac{1}{2}(\varrho(H_1) - \varrho(G)) \\
\geq &\frac{1}{2}(\mathbf{x}^\top (C(H_1) - C(G))\mathbf{x}) \\
= &\sum_{w \in V(G_u)\backslash\{u\}} x_w \Bigg[\left(2^{-(d_G(w,u)+1)} - 2^{-d_G(w,u)}\right) x_u \\
&+ \left(2^{-d_G(w,u)} - 2^{-(d_G(w,u)+1)}\right) x_v \\
&+ \sum_{z \in V(G_v)\backslash\{v\}} \left(2^{-(d_G(w,u)+d_G(v,z))} - 2^{-(d_G(w,u)+1+d_G(v,z))}\right) x_z \Bigg] \\
= &\sum_{w \in V(G_u)\backslash\{u\}} 2^{-(d_G(w,u)+1)} x_w \left(x_v - x_u + \sum_{z \in V(G_v)\backslash\{v\}} 2^{-d_G(v,z)} x_z \right).
\end{aligned}$$

If $x_v \geq x_u$, then, as $\sum_{z\in V(G_v)\setminus\{v\}} 2^{-d_G(v,z)}x_z > 0$, we have $\frac{1}{2}(\varrho(H_1) - \varrho(G)) > 0$, so $\varrho(H_1) > \varrho(G)$. Suppose that $x_v < x_u$. Similarly as above, we have

$$\begin{aligned}
&\frac{1}{2}(\varrho(H_2) - \varrho(G)) \\
&\geq \frac{1}{2}(\mathbf{x}^\top(C(H_2) - C(G))\mathbf{x}) \\
&= \sum_{w\in V(G_v)\setminus\{v\}} x_w \Bigg[\left(2^{-d_G(w,v)} - 2^{-(d_G(w,v)+1)}\right) x_u \\
&\quad + \left(2^{-(d_G(w,v)+1)} - 2^{-d_G(w,v)}\right) x_v \\
&\quad + \sum_{z\in V(G_u)\setminus\{u\}} \left(2^{-(d_G(w,v)+d_G(u,z))} - 2^{-(d_G(w,v)+1+d_G(u,z))}\right) x_z \Bigg] \\
&= \sum_{w\in V(G_v)\setminus\{v\}} 2^{-(d_G(w,v)+1)} x_w \left(x_u - x_v + \sum_{z\in V(G_u)\setminus\{u\}} 2^{-d_G(u,z)} x_z \right) \\
&> 0,
\end{aligned}$$

so $\varrho(H_2) > \varrho(G)$. □

Theorem 3.4. *Let G be a connected graph with a cycle $C_g := v_1 \ldots v_g v_1$ such that $G - E(C_g)$ consists of g components $G_1, \ldots, G_g$, where $v_i \in V(G_i)$ for $i = 1, \ldots, g$ and $g \geq 4$. Let $\mathbf{x}$ be the closeness Perron vector of G. Let $x_{v_1} = \max\{x_{v_i} : i = 1, \ldots, g\}$. Let*

$$\begin{aligned}
H_1 = G &- v_2v_3 - v_{g-1}v_g + v_1v_3 + v_1v_{g-1} - \{v_2w : w \in N_{G_2}(v_2)\} \\
&- \{v_gw : w \in N_{G_g}(v_g) + \{v_1w : w \in N_{G_2}(v_2) \cup N_{G_g}(v_g)\}
\end{aligned}$$

if g is odd, and

$$H_2 = G - v_2v_3 + v_1v_3 - \{v_2w : w \in N_{G_2}(v_2)\} + \{v_1w : w \in N_{G_2}(v_2)\}$$

if g is even, see Fig. 5. Then $\varrho(H_1) > \varrho(G)$ if g is odd, $\varrho(H_2) > \varrho(G)$ if g is even.

Proof. Let $V_i = V(G_i)$ for $3, \ldots, g-1$, $V_i = V(G_i) \setminus \{v_i\}$ for $i = 2, g$.

Suppose first that g is odd. As we pass from G to H_1, the distance between v_2 and any vertex in $\cup_{i=2}^{(g+1)/2} V_i$ is increased by 1, the distance between v_g and any vertex in $\cup_{i=(g+3)/2}^{g} V_i$ is increased by 1, the distance between v_1 and any vertex in $\cup_{i=2}^{g} V_i$ is decreased by 1, and the distance between each other pair of vertices remains unchanged or is decreased. Thus

$$\begin{aligned}
\frac{1}{2}(\varrho(H_1) - \varrho(G)) &\geq \frac{1}{2}(\mathbf{x}^\top(C(H_1) - C(G))\mathbf{x}) \\
&\geq x_{v_2} \sum_{i=2}^{(g+1)/2} \sum_{w\in V_i} \left(2^{-(d_G(v_2,w)+1)} - 2^{-d_G(v_2,w)}\right) x_w
\end{aligned}$$

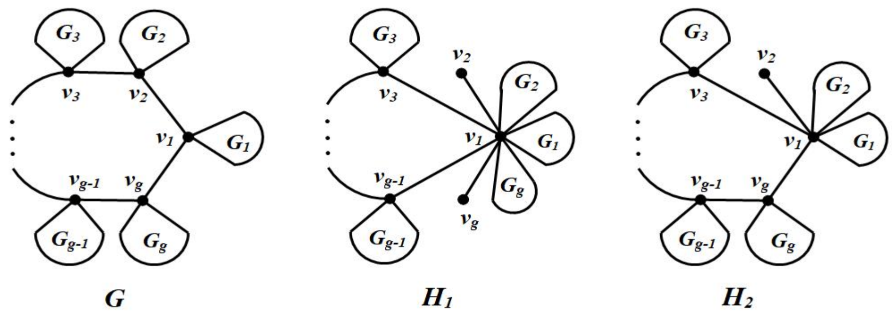

Fig. 5: Graphs G, H_1 and H_2 in Theorem 3.4.

$$
\begin{aligned}
&+ x_{v_g} \sum_{i=(g+3)/2}^{g} \sum_{w \in V_i} \left(2^{-(d_G(v_g,w)+1)} - 2^{-d_G(v_g,w)}\right) x_w \\
&+ x_{v_1} \sum_{i=2}^{g} \sum_{w \in V_i} \left(2^{-(d_G(v_1,w)-1)} - 2^{-d_G(v_1,w)}\right) x_w \\
= &-x_{v_2} \sum_{i=2}^{(g+1)/2} \sum_{w \in V_i} 2^{-d_G(v_2,w)-1} x_w \\
&- x_{v_g} \sum_{i=(g+3)/2}^{g} \sum_{w \in V_i} 2^{-d_G(v_g,w)-1} x_w \\
&+ x_{v_1} \sum_{i=2}^{g} \sum_{w \in V_i} 2^{-d_G(v_1,w)} x_w \\
= &\sum_{i=2}^{(g+1)/2} \sum_{w \in V_i} 2^{-d_G(v_1,w)} x_w \left(x_{v_1} - x_{v_2}\right) \\
&+ \sum_{i=(g+3)/2}^{g} \sum_{w \in V_i} 2^{-d_G(v_1,w)} x_w \left(x_{v_1} - x_{v_g}\right) \\
\geq &\ 0,
\end{aligned}
$$

which implies that $\varrho(H_1) \geq \varrho(G)$ as $x_{v_1} = \max\{x_{v_i} : i = 1, \dots, g\}$.

Suppose that $\varrho(H_1) = \varrho(G)$. Then, all the above inequalities are equalities. In particular, $\mathbf{x}$ is the closeness Perron vector of H_1, and $x_{v_1} = x_{v_2}$. By the closeness equations of H_1 at v_1, v_2, we have

$$\varrho(H_1)x_{v_1} = \sum_{w \in V(H_1)\setminus\{v_1,v_2\}} 2^{-d_{H_1}(w,v_1)} x_w + 2^{-d_{H_1}(v_2,v_1)} x_{v_2}$$

and

$$\varrho(H_1)x_{v_2} = \sum_{w \in V(H_1)\setminus\{v_1,v_2\}} 2^{-d_{H_1}(w,v_2)} x_w + 2^{-d_{H_1}(v_1,v_2)} x_{v_1}.$$

So

$$\left(\varrho(H_1)+2^{-d_{H_1}(v_1,v_2)}\right)(x_{v_1}-x_{v_2}) = \sum_{w\in V(H_1)\setminus\{v_1,v_2\}}\left(2^{-d_{H_1}(w,v_1)}-2^{-d_{H_1}(w,v_2)}\right)x_w.$$

As $d_{H_1}(v_1,w) < d_{H_1}(v_2,w)$ for $w \in V(H_1)\setminus\{v_1,v_2\}$, we have

$$\sum_{w\in V(H_1)\setminus\{v_1,v_2\}}\left(2^{-d_{H_1}(w,v_1)}-2^{-d_{H_1}(w,v_2)}\right)x_w > 0,$$

so $x_{v_1} > x_{v_2}$, which is a contradiction. It thus follows that $\varrho(H_1) > \varrho(G)$.

Suppose next that g is even. As we pass from G to H_2, the distance between v_2 and any vertex in $\cup_{i=2}^{g/2+1}V_i$ is increased by 1, the distance between v_1 and any vertex in $\cup_{i=2}^{g/2+1}V_i$ is decreased by 1, and the distance between each other pair of vertices remains unchanged or is decreased. Thus

$$\begin{aligned}
\frac{1}{2}(\varrho(H_2)-\varrho(G)) &\geq \frac{1}{2}(\mathbf{x}^\top(C(H_2)-C(G))\mathbf{x})\\
&\geq x_{v_2}\sum_{i=2}^{g/2+1}\sum_{w\in V_i}\left(2^{-d_G(v_2,w)-1}-2^{-d_G(v_2,w)}\right)x_w\\
&\quad + x_{v_1}\sum_{i=2}^{g/2+1}\sum_{w\in V_i}\left(2^{-d_G(v_1,w)+1}-2^{-d_G(v_1,w)}\right)x_w \qquad (3.3)\\
&= \sum_{i=2}^{g/2+1}\sum_{w\in V_i}2^{-d_G(v_1,w)}x_w(x_{v_1}-x_{v_2})\\
&\geq 0,
\end{aligned}$$

implying that $\varrho(H_2) \geq \varrho(G)$.

Suppose that $\varrho(H_2) = \varrho(G)$. Then all inequalities in (3.3) are equalities, and thus $\mathbf{x}$ is the closeness Perron vector of H_2 and $x_{v_1} = x_{v_2}$. By the closeness equations of H_2 at v_1, v_2, we have

$$\varrho(H_2)x_{v_1} = \sum_{w\in V(H_2)\setminus\{v_1,v_2\}}2^{-d_{H_2}(w,v_1)}x_w + 2^{-d_{H_2}(v_2,v_1)}x_{v_2}$$

and

$$\varrho(H_2)x_{v_2} = \sum_{w\in V(H_2)\setminus\{v_1,v_2\}}2^{-d_{H_2}(w,v_2)}x_w + 2^{-d_{H_2}(v_1,v_2)}x_{v_1}.$$

Note that $d_{H_2}(v_1,w) < d_{H_2}(v_2,w)$ for $w \in V(H_2)\setminus\{v_1,v_2\}$. By similar argument as above, we have $x_{v_1} > x_{v_2}$, a contradiction. Hence, $\varrho(H_2) > \varrho(G)$. □

4 Graphs minimizing or maximizing the spectral closeness

Rupnik Poklukar and Žerovnik [19] determined the graphs that minimize and maximize the closeness among several classes of graphs including trees and cacti. In this section, we find those graphs that uniquely minimize or maximize the spectral closeness in some classes of graphs.

Theorem 4.1. *Let G be a graph on n vertices. Then*

$$0 \leq \varrho(G) \leq \frac{n-1}{2}$$

with left equality if and only if G is the empty graph and with right equality if and only if G is the complete graph.

Proof. If there is an edge uv in G, then $C(G)$ has a principal submatrix

$$\begin{pmatrix} 0 & \frac{1}{2} \\ \frac{1}{2} & 0 \end{pmatrix}$$

whose spectral radius is $\frac{1}{2}$, so by Interlacing Theorem, we have $\varrho(G) \geq \frac{1}{2} > 0$. Therefore, $\varrho(G) \geq 0$ with equality if and only if G is the empty graph.

On the other hand, we have $C(K_n) - C(G)$ is nonnegative and $C(K_n)$ is irreducible. Note that $\varrho(K_n) = \frac{n-1}{2}$ by Lemma 2.3. So, by Lemma 2.2, $\varrho(G) \leq \frac{n-1}{2}$ with equality and only if G is the complete graph K_n. $\square$

Theorem 4.2. *Let G be a bipartite graph on $n \geq 2$ vertices. Then*

$$\varrho(G) \leq \begin{cases} \frac{3n-2}{8} & \text{if } n \text{ is even} \\ \frac{n-2+\sqrt{4n^2-3}}{8} & \text{if } n \text{ is odd} \end{cases}$$

with equality if and only if $G \cong K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$.

Proof. By Lemma 2.2, $\varrho(G) \leq \varrho(K_{r,s})$ for some r and s with $1 \leq r \leq s$ and $r+s = n$. Let $\mathbf{x}$ be the closeness Perron vector of $\varrho = \varrho(K_{r,s})$. By Lemma 2.1, we denote by x (y, respectively) the entry of $\mathbf{x}$ at a vertex of degree s and (r, respectively). Then

$$\varrho x = \frac{r-1}{4}x + \frac{s}{2}y$$

and

$$\varrho y = \frac{r}{2}x + \frac{s-1}{4}y.$$

So

$$\det \begin{pmatrix} \varrho - \frac{r-1}{4} & -\frac{s}{2} \\ -\frac{r}{2} & \varrho - \frac{s-1}{4} \end{pmatrix} = 0,$$

i.e., $\varrho^2 - \frac{n-2}{4}\varrho - \frac{3rs+n-1}{16} = 0$, i,e., $\varrho = \frac{n-2+\sqrt{n^2+12rs}}{8}$, which is maximized if and only if $r = \lfloor \frac{n}{2} \rfloor$ and $s = \lceil \frac{n}{2} \rceil$. $\square$

Theorem 4.3. *Let G be a connected graph of order n. Then $\varrho(G) \geq \varrho(P_n)$ with equality if and only if $G \cong P_n$.*

Proof. Let G be a connected graph of order n that minimizes the spectral closeness. By Lemma 2.2, G is a tree.

We show that $G \cong P_n$. Otherwise, there is a vertex u in G of degree at least 3. If u is not the only vertex of degree at least three in G, then we may choose a vertex v of degree at least three such that $d_G(u,v)$ is as large as possible. In this case, there are at least two pendant paths, say P and Q, at v in G. Then $G \cong H_v(p,q)$, where H is the graph obtained from G by deleting the vertices of P and Q except v, p is the length of P and q is the length of Q. By Theorem 3.1, $\varrho(H_v(p+q,0)) < \varrho(H_v(p,q)) = \varrho(G)$, a contradiction. Thus, u is the only vertex of degree at least three. Let L and S be two pendant paths at u in G with lengths ℓ and s, respectively. Then $G \cong H'_u(\ell,s)$, where H' is the graph obtained from G by deleting the vertices of L and S except u. By Theorem 3.1 again, $\varrho(H'_u(\ell+s,0)) < \varrho(H'_u(\ell,s)) = \varrho(G)$, also a contradiction. □

Theorem 4.4. *Let G be an n-vertex tree. Then*

$$\varrho(G) \leq \frac{n-2+\sqrt{n^2+12n-12}}{8}$$

with equality if and only if $G \cong S_n$.

Proof. If G is not the star, then there is an edge uv that is not a pendant edge, and as uv is a cut edge, we have by Theorem 3.2 that $\varrho(G_{uv}) > \varrho(G)$. So the star S_n is the unique n-vertex tree that maximizes the spectral closeness. By direct calculation, we have $\det(tI_n - C(S_n)) = (t+\frac{1}{4})^{n-2}(t^2 - \frac{n-2}{4}t - \frac{n-1}{4})$. Then $\varrho(S_n) = \frac{n-2+\sqrt{n^2+12n-12}}{8}$. □

Lemma 4.1. *For integers ℓ and n with $2 \leq \ell \leq \lfloor \frac{n-2}{2} \rfloor$, we have $\varrho(D_{n,\ell}) < \varrho(D_{n,\ell-1})$.*

Proof. Denote by u and v be the centers of $D_{n,\ell}$ with degree $\ell+1$ and $n-\ell-1$ respectively. Let $\mathbf{x}$ be the closeness Perron vector of G. By Lemma 2.1, the entries of $\mathbf{x}$ at all pendant neighbors of u (v, respectively) have the same value, which we denote by α (β, respectively). Let $\varrho = \varrho(D_{n,\ell})$.

By the closeness equations of $D_{n,\ell}$ at u and v, we have

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

and

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

Then

$$\left(\varrho + \frac{1}{2}\right)(x_v - x_u) = -\frac{1}{4}\ell\alpha + \frac{1}{4}(n-\ell-2)\beta. \tag{4.1}$$

By the closeness equations of $D_{n,\ell}$ at pendant vertices that are adjacent to u and v, we have

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

and

$$\varrho\beta = \frac{1}{4}x_u + \frac{1}{2}x_v + \frac{1}{8}(\ell-1)\alpha + \frac{1}{4}(n-\ell-3)\beta + \frac{1}{8}\alpha,$$

Then

$$\left(\varrho+\frac{1}{8}\right)(\beta-\alpha)=\frac{1}{4}(x_v-x_u)-\frac{1}{8}(\ell-1)\alpha+\frac{1}{8}(n-\ell-3)\beta. \tag{4.2}$$

From (4.1) and (4.2), we have

$$(4\varrho+1)(\beta-\alpha)=2(\varrho+1)(x_v-x_u). \tag{4.3}$$

Note that $n-\ell-2\geq\ell$. From (4.1) and (4.3), we have

$$\left(\varrho+\frac{1}{2}\right)(x_v-x_u)\geq\frac{\ell}{4}(\beta-\alpha)=\frac{\ell}{4}\cdot\frac{2(\varrho+1)}{4\varrho+1}(x_v-x_u),$$

i.e.,

$$\left(\varrho+\frac{1}{2}-\frac{\ell}{4}\cdot\frac{2(\varrho+1)}{4\varrho+1}\right)(x_v-x_u)\geq 0. \tag{4.4}$$

By Lemma 2.3 and the fact that $n\geq 2\ell+2$, one has

$$\varrho\geq\min\left\{\frac{n+\ell+2}{8},\frac{n+\ell}{4},\frac{2n-\ell}{8},\frac{2n-\ell-2}{4}\right\}=\frac{n+\ell+2}{8}>\frac{\ell}{4}.$$

So

$$\varrho+\frac{1}{2}-\frac{\ell}{4}\cdot\frac{2(\varrho+1)}{4\varrho+1}>0.$$

Now (4.4) implies that $\beta-\alpha\geq 0$. So, by Rayleigh's principle and (4.1), we have

$$\begin{aligned}\frac{1}{2}(\varrho(D_{n,\ell-1})-\varrho(D_{n,\ell}))&\geq\frac{1}{2}(\mathbf{x}^\top C(D_{n,\ell-1})\mathbf{x}-\mathbf{x}^\top C(D_{n,\ell})\mathbf{x})\\&=\alpha\left[\frac{1}{8}(n-\ell-2)\beta-\frac{1}{8}(\ell-1)\alpha+\frac{1}{4}x_v-\frac{1}{4}x_u\right]\\&>\alpha\left[\frac{1}{8}(n-\ell-2)\beta-\frac{1}{8}\ell\alpha+\frac{1}{4}x_v-\frac{1}{4}x_u\right]\\&=\frac{1}{2}\alpha\left(\varrho+1\right)(x_v-x_u)\\&\geq 0.\end{aligned}$$

Hence, $\varrho(D_{n,\ell})<\varrho(D_{n,\ell-1})$. □

Theorem 4.5. *If G is an n-vertex tree that is not isomorphic to S_n, then $\varrho(G)\leq\varrho(D_{n,1})$ with equality if and only if $G\cong D_{n,1}$.*

Proof. Suppose that G is an n-vertex tree not isomorphic to S_n that maximizes the spectral closeness. Let d be the diameter of G. As G is not isomorphic to S_n, we have $d\geq 3$. Suppose that $d\geq 4$. Then, for any edge uv that is not a pendant edge, G_{uv} is an n-vertex tree that is not isomorphic to S_n as its diameter is at least $d-1\geq 3$. However, we have by Theorem 3.2 that $\varrho(G_{uv})>\varrho(G)$, a contradiction. Therefore $d=3$. That is, $G\cong D_{n,\ell}$ for some ℓ with $1\leq\ell\leq\lfloor\frac{n-2}{2}\rfloor$. By Lemma 4.1, we have $G\cong D_{n,1}$. □

Recall that a graph G is unicyclic if it is connected and $|E(G)| = |V(G)|$.

Theorem 4.6. *For an n-vertex unicyclic graph G, we have $\varrho(G) \leq \varrho(S_n^+)$ with equality if and only if $G \cong S_n^+$, where $\varrho(S_n^+)$ is the largest root of $t^3 - \frac{n-2}{4}t^2 - \frac{2n-1}{8}t - \frac{1}{8} = 0$.*

Proof. Let G be an n-vertex unicyclic graph that maximizes the spectral closeness. By Theorems 3.2 and 3.4, G consists of a triangle and $n-3$ pendant edges. Then by Theorem 3.3, $G \cong S_n^+$.

In the following we compute $\varrho = \varrho(S_n^+)$. Let $\mathbf{x}$ be the closeness Perron vector of S_n^+. By Lemma 2.1, we denote by x_0 (x_1, x_2, respectively) the entry $\mathbf{x}$ at the vertex of degree $n-1$ (a vertex of degree 1, a vertex of degree 2, respectively). Then

$$\varrho x_0 = \frac{n-3}{2}x_1 + x_2,$$

$$\varrho x_1 = \frac{1}{2}x_0 + \frac{n-4}{4}x_1 + \frac{1}{2}x_2$$

and

$$\varrho x_2 = \frac{1}{2}x_0 + \frac{n-3}{4}x_1 + \frac{1}{2}x_2.$$

As $(x_0, x_1, x_2)^\top$ is nonzero, we have

$$\det \begin{pmatrix} \varrho & -\frac{n-3}{2} & -1 \\ -\frac{1}{2} & \varrho - \frac{n-4}{4} & -\frac{1}{2} \\ -\frac{1}{2} & -\frac{n-3}{4} & \varrho - \frac{1}{2} \end{pmatrix} = 0,$$

i.e., $f(\rho) = 0$ with

$$f(t) = t^3 - \frac{n-2}{4}t^2 - \frac{2n-1}{8}t - \frac{1}{8} = 0.$$

It follows that ρ is the largest root of $f(t) = 0$. $\square$

Let G be an n-vertex graph with p pendant vertices, where $0 \leq p \leq n-1$ and $n \geq 3$. If $p = 0$, then $\varrho(G) \leq \frac{n-1}{2}$ with equality if and only if $G \cong K_n$. If $p = n-1$, then $G \cong S_n$. If $p = n-2$ with $n \geq 4$, then G is a tree, so by Theorem 4.5, $\varrho(G) \leq (D_{n,1})$ with equality if and only $G \cong D_{n,1}$.

Theorem 4.7. *For an n-vertex connected graph with p pendant vertices, where $1 \leq p \leq n-3$, we have $\varrho(G) \leq \varrho(K_1 \vee (K_{n-p-1} \cup \overline{K_p}))$ with equality if and only if $G \cong K_1 \vee (K_{n-p-1} \cup \overline{K_p})$, where $\varrho(K_1 \vee (K_{n-p-1} \cup \overline{K_p}))$ is the largest root of $t^3 + \frac{p-2n+5}{4}t^2 - \frac{p^2-(n-1)p+6n-8}{16}t - \frac{p^2-(n-2)p+n-1}{16} = 0$.*

Proof. Let G be an n-vertex connected graph with p pendant vertices that maximizes the spectral closeness. By Lemma 2.2, the graph obtained from G by deleting all pendant vertices is a complete graph. Then, by Theorem 3.3, $G \cong K_1 \vee (K_{n-p-1} \cup \overline{K_p})$.

In the following we compute $\varrho = \varrho(K_1 \vee (K_{n-p-1} \cup \overline{K_p}))$.

Let $\mathbf{x}$ be the closeness Perron vector of $K_1 \vee (K_{n-p-1} \cup \overline{K}_p)$ for $1 \le p \le n-3$. Denote by x_0 the entry of $\mathbf{x}$ at the vertex of degree $n-1$. By Lemma 2.1, $\mathbf{x}$ has equal entries for any two vertices with degree larger than one and less than $n-1$ (degree one, respectively), which we denote by x_1 (x_2, respectively). Then

$$\varrho x_0 = \frac{n-p-1}{2}x_1 + \frac{p}{2}x_2,$$

$$\varrho x_1 = \frac{1}{2}x_0 + \frac{n-p-2}{2}x_1 + \frac{p}{4}x_2,$$

and

$$\varrho x_2 = \frac{1}{2}x_0 + \frac{n-p-1}{4}x_1 + \frac{p-1}{4}x_2.$$

As $(x_0, x_1, x_2)^\top$ is nonzero, we have

$$\det\begin{pmatrix} \varrho & -\frac{n-p-1}{2} & -\frac{p}{2} \\ -\frac{1}{2} & \varrho - \frac{n-p-2}{2} & -\frac{p}{4} \\ -\frac{1}{2} & -\frac{n-p-1}{4} & \varrho - \frac{p-1}{4} \end{pmatrix} = 0.$$

i.e., $f(\varrho) = 0$ with

$$f(t) = t^3 + \frac{p-2n+5}{4}t^2 - \frac{p^2-(n-1)p+6n-8}{16}t - \frac{p^2-(n-2)p+n-1}{16}.$$

It follows that ϱ is the largest root of $f(t) = 0$. □

The *connectivity* of a graph G is the minimum number of vertices whose removal results in a disconnected or trivial graph. For an n-vertex connected graph G with connectivity s, we have $1 \le s \le n-1$, and $s = n-1$ if and only if G is complete.

Theorem 4.8. *Let G be an n-vertex connected graph with connectivity s, where $1 \le s \le n-2$. Then $\varrho(G) \le \varrho(K_s \vee (K_1 \cup K_{n-s-1}))$ with equality if and only if $G \cong K_s \vee (K_1 \cup K_{n-s-1})$, where $\varrho(K_s \vee (K_1 \cup K_{n-s-1}))$ is the largest root of $t^3 - \frac{n-3}{2}t^2 - \frac{5n+3s-9}{16}t - \frac{s^2-(n-4)s+n-1}{32} = 0$.*

Proof. Let G be an n-vertex connected graph with connectivity s that maximizes the spectral closeness. Then $G-S$ is disconnected for some $S \subset V(G)$ with $|S| = s$. By Lemma 2.2, we have $G[S] = K_s$, there exist positive integers n_1 and n_2 with $s + n_1 + n_2 = n$ such that $G - S = K_{n_1} \cup K_{n_2}$, and $G \cong K_s \vee (K_{n_1} \cup K_{n_2})$. Assume that $n_2 \ge n_1$. Let $\mathbf{x}$ be the closeness Perron vector of G. By Lemma 2.1, $\mathbf{x}$ has the same entry for any corresponding vertex of G in S ($V(K_{n_1})$, $V(K_{n_2})$, respectively), which we denote by x_0 (x_1, x_2, respectively). Suppose that $n_1 > 1$. For $u \in V(K_{n_1})$, let $H = G - \{uw : w \in V(K_{n_1})\} + \{uz : z \in V(K_{n_2})\}$. By considering the distance changes as we pass from G to H and using Rayleigh's principle, we have

$$\begin{aligned}
&\frac{1}{2}(\varrho(H) - \varrho(G)) \\
&\ge x_u \left[\sum_{w \in V(K_{n_1}) \setminus \{u\}} (2^{-2} - 2^{-1})x_w + \sum_{z \in V(K_{n_2})} (2^{-1} - 2^{-2})x_z\right] \qquad (4.5) \\
&= \frac{1}{4}x_1(n_2x_2 - n_1x_1 + x_1)
\end{aligned}$$

By the closeness equations of G at any vertex in $V(K_{n_1})$ and in $V(K_{n_2})$, we have

$$\left(\varrho(G)+\frac{1}{2}\right)(x_2-x_1)=\frac{1}{4}(n_2x_2-n_1x_1)\geq\frac{1}{4}n_1(x_2-x_1),$$

i.e.,

$$\left(\varrho(G)+\frac{1}{2}-\frac{1}{4}n_1\right)(x_2-x_1)\geq 0.$$

As K_{n_1} is an induced subgraph of G, we have by Lemma 2.3 that $\varrho(G)>\frac{n_1}{4}$. So $x_2\geq x_1$. Therefore, (4.5) implies that $\varrho(H)>\varrho(G)$, a contradiction. It follows that $n_1=1$. That is, $G\cong K_s\vee(K_1\cup K_{n-s-1})$.

In the following we compute $\varrho=\varrho(K_s\vee(K_1\cup K_{n-s-1}))$. Let $\mathbf{x}$ be the closeness Perron vector of $K_s\vee(K_1\cup K_{n-s-1})$. By Lemma 2.1, we denote by x_0 the entry of $\mathbf{x}$ at a vertex of degree $n-1$, x_1 the entry of $\mathbf{x}$ at a vertex of degree s, and x_3 the entry of $\mathbf{x}$ at a vertex of degree $n-2$. Then

$$\varrho x_0=\frac{s-1}{2}x_0+\frac{1}{2}x_1+\frac{n-s-1}{2}x_2,$$

$$\varrho x_1=\frac{s}{2}x_0+\frac{n-s-1}{4}x_2$$

and

$$\varrho x_2=\frac{s}{2}x_0+\frac{1}{4}x_1+\frac{n-s-2}{2}x_2.$$

So

$$\det\begin{pmatrix}\varrho-\frac{s-1}{2} & -\frac{1}{2} & -\frac{n-s-1}{2}\\ -\frac{s}{2} & \varrho & -\frac{n-s-1}{4}\\ -\frac{s}{2} & -\frac{1}{4} & \varrho-\frac{n-s-2}{2}\end{pmatrix}=0.$$

It follows that ϱ is the largest root of $f(t)=0$, where

$$f(t)=t^3-\frac{n-3}{2}t^2-\frac{5n+3s-9}{16}t-\frac{s^2-(n-4)s+n-1}{32}.$$ □

5 Residual spectral closeness

Recall that there have been lots of results on the computational aspect [2–4,11,12,18] and on the extremal aspect [8,22,24]. The residual spectral closeness may be used as a spectral measure of graph or network structures. In this section, we give some extremal results on the residual spectral closeness.

If G is a tree of order $n\geq 2$, it is easy to see that $\varrho^R(G)\geq 0$ with equality if and only if $G\cong S_n$.

Theorem 5.1. *Let G be a graph on $n\geq 2$ vertices. Then*

$$0\leq\varrho^R(G)\leq\frac{n-2}{2}$$

with left equality if and only if G is a spanning subgraph of S_n and with right equality if and only if $G\cong K_n$.

Proof. It is trivial if $n = 2$. Suppose that $n \geq 3$. Assume that $\varrho^R(G) = \varrho(G - v)$. By Lemma 4.2,

$$0 \leq \varrho(G - v) \leq \frac{n-2}{2},$$

where left equality holds if and only if $G - v$ is the empty graph, i.e., v is an end vertex of any edge, i.e., G is a spanning subgraph of S_n, and right equality holds if and only if $G - v$ is the complete graph, or equivalently, $G \cong K_n$, as, if the degree of v is smaller than $n - 1$, then for any vertex w that is not a neighbor of v, $G - w$ is not complete, so $\varrho^R(G) \leq \varrho(G - w) < \frac{n-2}{2}$, which is a contradiction. □

Theorem 5.2. *Let G be a bipartite graph on $n \geq 4$ vertices. Then*

$$\varrho^R(G) \leq \begin{cases} \frac{3n-5}{8} & \text{if } n \text{ is odd} \\ \frac{n-3+\sqrt{4(n-1)^2-3}}{8} & \text{if } n \text{ is even} \end{cases}$$

with equality if and only if $G \cong K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$.

Proof. Assume that $\varrho^R(G) = \varrho(G - v)$. By Theorem 4.2,

$$\varrho^R(G) = \varrho(G - v) \leq \begin{cases} \frac{3n-5}{8} & \text{if } n-1 \text{ is even} \\ \frac{n-3+\sqrt{4(n-1)^2-3}}{8} & \text{if } n-1 \text{ is odd} \end{cases}$$

with equality if and only if $G - v \cong K_{\lfloor (n-1)/2 \rfloor, \lceil (n-1)/2 \rceil}$.

Suppose that the upper for $\varrho^R(G)$ is attained. Then $G - v \cong K_{\lfloor (n-1)/2 \rfloor, \lceil (n-1)/2 \rceil}$. Let X and Y be the partite sets of G. Suppose first that n is odd. Then $G \cong K_{(n-1)/2,(n+1)/2}$. Otherwise, assume that $v \in X$. Then v is not adjacent to each vertex in Y, so for any vertex w in X, $G - w$ is not a complete bipartite graph and then by Theorem 4.2, $\varrho^R(G) \leq \varrho(G - w) < \frac{3n-5}{8}$, a contradiction. Suppose next that n is even. Then $|X| = \frac{n}{2}$ or $\frac{n}{2} + 1$. If $|X| = \frac{n}{2} + 1$, then $|Y| = \frac{n}{2} - 1$ and $v \in X$, so for any $w \in Y$, we have by Lemma 4.2 that $\varrho^R(G) \leq \varrho(G - w) < \frac{n-3+\sqrt{4(n-1)^2-3}}{8}$, a contradiction. So $|X| = \frac{n}{2}$. Assume that $v \in X$. Then $G \cong K_{n/2,n/2}$. Otherwise, v is not adjacent to each vertex in Y, so for any vertex w in X, $G - w$ is not a complete bipartite graph and then by Theorem 4.2, $\varrho^R(G) \leq \varrho(G - w) < \frac{n-3+\sqrt{4(n-1)^2-3}}{8}$, a contradiction. □

Theorem 5.3. *Let G be a graph in which two vertices u and v are not adjacent. Then $\varrho^R(G) \leq \varrho^R(G + uv)$.*

Proof. Let $H = G + uv$. Assume that $\varrho^R(H) = \varrho(H - w)$ with $w \in V(H)$. If $w \neq u, v$, then $H - w = G - w + uv$, so, by Lemma 2.2, we have $\varrho^R(G) \leq \varrho(G - w) \leq \varrho(H - w) = \varrho^R(H)$. If $w = u$ or v, say $w = u$, then, as $H - u = G - u$, we have $\varrho^R(G) \leq \varrho(G - u) = \varrho(H - u) = \varrho^R(H)$. □

Note that, for a connected graph G in which two vertices u and v are not adjacent, we have $\varrho(G) < \varrho(G + uv)$ by Perron-Frobenius theorem and $\varrho^R(G) \leq \varrho^R(G + uv)$ by Theorem 5.3. So, to characterize completely the graphs in some classes that minimize (maximize, respectively) the residual spectral closeness is generally harder than to characterize completely the graphs in some classes that minimize (maximize, respectively) the spectral closeness. So, we leave more extremal problems to determine the graphs that minimize (maximize, respectively) the residual spectral closeness in some classes of graphs in the future.

Besides extremal problems on the residual spectral closeness, in the following steps, one may study the relation between the residual spectral closeness, the spectral closeness, closeness and residual closeness.

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