Extremal results on the spectral radius of function-weighted adjacency matrices

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Abstract

For a graph $G = (V, E)$ and $v_i \in V$, denote by d_i the degree of vertex v_i. Let $f(x, y) > 0$ be a C^2-function in $(\mathbb{R}^+)^2$ and be symmetric in x and y. If for every $\bar{x}$ such that $\{\bar{x}\} \times \mathbb{R}^+ \neq \varnothing$, then $f'_x(\bar{x}, y) \geq 0$ (resp. $f''_x(\bar{x}, y) \geq 0$) for all $(\bar{x}, y) \in (\mathbb{R}^+)^2$, we say $f(x, y)$ is increasing (resp. convex) in variable x. The function-weighted adjacency matrix $A_f(G)$ of a graph G is a square matrix, where the (i, j)-entry is equal to $f(d_i, d_j)$ if the vertices v_i and v_j are adjacent and 0 otherwise.

In this paper, we consider the unimodality of the principal eigenvector of the path P_n and characterize the tree on n vertices with the smallest A_f-spectral radius of G under the condition that $f(x, y) > 0$ is increasing and convex in variable x. We also obtain the unicyclic graph on n vertices with the largest A_f-spectral radius of G under the same condition.

Keywords: Spectral radius, Function-weighted adjacency matrix, Tree, Unicyclic graph
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1. Introduction

Let $G = (V(G), E(G))$ be a finite, undirected, simple and connected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. An edge $e \in E(G)$ with end vertices v_i and v_j is usually denoted by v_iv_j. For

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$i = 1, 2, \ldots, n$, we denote by d_i the degree of the vertex v_i in G, $\Delta(G)$ the maximum degree of G, $N(v_i)$ the set of neighbours of vertex v_i in G and $N[v_i] = N(v_i) \cup \{v_i\}$. A vertex of degree 1 is called a pendent vertex. As usual, let P_n, S_n and C_n be the path, star and cycle of order $n \geq 3$, $S_{d,n-d}$ be the double star of order $n \geq 4$ with two centers v_1, v_2 such that $d_1 = d$ and $d_2 = n - d$ where $2 \leq d \leq \lfloor \frac{n}{2} \rfloor$, $S_n + e$ be the unicyclic graph with $n \geq 4$ obtained from S_n by adding an edge as shown in Fig. 1.

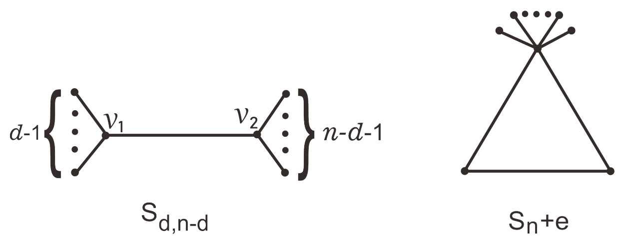

Figure 1: The double star $S_{d,n-d}$ and $S_n + e$ of order $n \geq 4$.

Let $\lambda_i(M)(i = 1, 2, \ldots, n)$ be the eigenvalues of a complex matrix M. Then the spectral radius of M is $\rho(M) = \max\{|\lambda_i(M)| \mid 1 \leqslant i \leqslant n\}$. By Perron-Frobenius theorem, if M is an $n \times n$ nonnegative and irreducible matrix, then its spectral radius $\rho(M)$ is a simple eigenvalue of M.

In molecular graph theory, the topological indices of molecular graphs are used to reflect chemical properties of chemical molecules. There are many topological indices and among them there is a family of degree-based indices. The degree-based index $TI_f(G)$ of G with positive symmetric function $f(x, y)$ is defined as

$$TI_f(G) = \sum_{v_i v_j \in E(G)} f(d_i, d_j).$$

Gutman [10] collected many important and well-studied chemical or topological indices; see them in Table 1. In order to study the discrimination property, Rada [30] introduced the exponentials of the best known degree-based chemical or topological indices; see them in Table 2.

Each index maps a molecular graph into a single number. One of the authors [20] proposed that if we use a matrix to represent the structure of a molecular graph with weights separately on its pairs of adjacent vertices, it will keep more structural information of the graph. For example, the Randić matrix [28, 29], the Atom-Bond-Connectivity matrix [8],

Function f(x,y)	The corresponding index
$x+y$	first Zagreb index
xy	second Zagreb index
$(x+y)^2$	first hyper-Zagreb index
$(xy)^2$	second hyper-Zagreb index
$x^{-3}+y^{-3}$	modified first Zagreb index
$\|x-y\|$	Albertson index
$(x/y+y/x)/2$	extended index
$(x-y)^2$	sigma index
$1/\sqrt{xy}$	Randić index
$\sqrt{xy}$	reciprocal Randić index
$1/\sqrt{x+y}$	sum-connectivity index
$\sqrt{x+y}$	reciprocal sum-connectivity index
$2/(x+y)$	harmonic index
$\sqrt{(x+y-2)/(xy)}$	atom-bond-connectivity (ABC) index
$(xy/(x+y-2))^3$	augmented Zagreb index
x^2+y^2	forgotten index
$x^{-2}+y^{-2}$	inverse degree
$2\sqrt{xy}/(x+y)$	geometric-arithmetic (GA) index
$(x+y)/(2\sqrt{xy})$	arithmetic-geometric (AG) index
$xy/(x+y)$	inverse sum index
$x+y+xy$	first Gourava index
$(x+y)xy$	second Gourava index
$(x+y+xy)^2$	first hyper-Gourava index
$((x+y)xy)^2$	second hyper-Gourava index
$1/\sqrt{x+y+xy}$	sum-connectivity Gourava index
$\sqrt{(x+y)xy}$	product-connectivity Gourava index
$\sqrt{x^2+y^2}$	Sombor index

Table 1: Some well-studied chemical or topological indices

Function f(x,y)	**The corresponding index**
e^{x+y}	exponential first Zagreb index
e^{xy}	exponential second Zagreb index
$e^{1/\sqrt{xy}}$	exponential Randić index
$e^{\sqrt{(x+y-2)/(xy)}}$	exponential ABC index
$e^{2\sqrt{xy}/(x+y)}$	exponential GA index
$e^{2/(x+y)}$	exponential harmonic index
$e^{1/\sqrt{x+y}}$	exponential sum-connectivity index
$e^{(xy/(x+y-2))^3}$	exponential augmented Zagreb index

Table 2: Some well-known exponential chemical or topological indices

the Arithmetic-Geometric matrix [32] and the Sombor matrix [19] were considered separately. Based on these examples, the function-weighted adjacency matrix $A_f(G)$ first appeared in Das et al. [7], and it is defined as

$$A_f(G)(i,j) = \begin{cases} f(d_i, d_j), & v_iv_j \in E(G); \\ 0, & otherwise. \end{cases}$$

Since G is a connected graph, the weighted adjacency matrix $A_f(G)$ is an $n \times n$ nonnegative and irreducible symmetric matrix. Thus $\rho(A_f(G))$ is exactly the largest eigenvalue of $A_f(G)$ and it has a positive eigenvector $\mathbf{x} = (x_1, x_2, \ldots, x_n)^\intercal$. Throughout this paper, we choose $\mathbf{x}$ such that $\|\mathbf{x}\|_2 = 1$ and x_i corresponds to vertex v_i, and we call the unique unit positive vector $\mathbf{x}$ the principal eigenvector of G.

As one can see that from each index in the above two tables, one can get a weighted matrix defined by that index. There have been a lot of publications studying these matrices one by one separately. However, the methods used in these publications are the same or similar. So in recent years, there is a trend to develop unified methods to deal with extremal problems for such degree-based indices and function-weighted adjacency matrices, see [6, 13, 16, 17, 21, 22, 23, 26, 27] and the survey [24]. The first author et al. were the first to seek unified methods to study the spectral radius of function-weighted adjacency matrices of graphs with edge-weighted by topological function-indices (see [27]). They obtained the trees with the largest A_f-spectral radius of G is S_n or double star $S_{d,n-d}$, when $f(x,y)$ is increasing and convex in variable x. Moreover, if $f(x,y)$ has the form $P(x,y)$ or $\sqrt{P(x,y)}$, where $P(x,y)$ is a symmetric polynomial with nonnegative coefficients and zero constant term, then the tree on $n \geq 9$ vertices with the smallest A_f-spectral radius of G is uniquely P_n. In [33], the second author et al. showed that among all trees of order n, P_n $(S_n + e)$ is the unique tree (unicyclic graph) with the smallest (largest) A_f-spectral radius of G if $f(x,y) > 0$ is increasing and convex in variable x and satisfies that $f(x_1, y_1) \geq f(x_2, y_2)$ when $\mid x_1 - y_1 \mid > \mid x_2 - y_2 \mid$ and $x_1 + y_1 = x_2 + y_2$.

Spectral radius and energy are two notable invariants in the study of spectral graph theory. They are closely related to the graph operations. It is a hot topic to explore the influence of graph operations on the spectral radius and energy of graphs, see [2, 3, 4, 5, 31]. In [11, 12, 25], the authors used unified methods to study the effect on the spectral radius of function-weighted adjacency matrices of graphs by graph operations.

In this paper, we first consider the unimodality of principal eigenvector of the path P_n and use this property and graph operations to get the following results.

Theorem 1.1. *Let $f(x,y) > 0$ be a symmetric real function, increasing and convex in variable x. Then the tree on n vertices with the smallest A_f-spectral radius of G is P_n or S_n.*

The result is obtained only under the conditions that $f(x,y) > 0$ is increasing and convex in variable x. Moreover, if $f(x,y)$ such that $f(2,2) \leq f(1,4)$, we then get that P_n is the unique extremal tree with the minimum A_f-spectral radius of G for $n \geq 5$. It works for the weighted adjacency matrices defined by almost half of the indices listed in Tables 1 and 2.

For the unicyclic graphs of order n, the second author et al. [33] obtained that C_n has the smallest A_f-spectral radius of G if $f(x,y)$ is increasing in variable x and showed that $S_n + e$ is the unique unicyclic graph with the largest A_f-spectral radius of G when $f(x,y) > 0$ is increasing and convex in variable x and satisfies that $f(x_1, y_1) \geq f(x_2, y_2)$ when $\mid x_1 - y_1 \mid > \mid x_2 - y_2 \mid$ and $x_1 + y_1 = x_2 + y_2$. Now we reconsider the unicyclic graph with the largest A_f-spectral radius of G only under the conditions that $f(x,y)>0$ is increasing and convex in variable x, and as a result, we obtain the following theorem.

Theorem 1.2. *Let $f(x,y)>0$ be a symmetric real function, increasing and convex in variable x. Then the unicyclic graphs on n vertices with the largest A_f-spectral radius of G are unicyclic graphs with $n-3$ pendent vertices.*

2. Some preliminary results

In this section, we provide some matrix-theoretical background on nonnegative matrices and recall how the Kelmans operation affects the spectral radius of weighted adjacency matrices.

Theorem 2.1. *[15] Let A and B be both $n\times n$ nonnegative symmetric matrices. Then $\rho(A+B)\geq\rho(A)$. Furthermore, if A is irreducible and B is not null, then $\rho(A+B)>\rho(A)$.*

Theorem 2.2. *[1] Let A be an $n\times n$ real symmetric matrix and B be the principal submatrix of A. Then $\rho(A)\geq\rho(B)$.*

Let $A=[a_{ij}]$ and $B=[b_{ij}]$ be $m\times n$ matrices. If A and B have real entries, we write

$$A\geq 0 \text{ if all } a_{ij}\geq 0, \text{ and } A>0 \text{ if all } a_{ij}>0$$
$$A\geq B \text{ if } A-B\geq 0, \text{ and } A>B \text{ if } A-B>0.$$

Theorem 2.3. *[15] Let A be an $n\times n$ nonnegative matrix and $\boldsymbol{x}=(x_1,x_2,\ldots,x_n)^\intercal$ be a positive vector. If $\alpha,\beta\geq 0$ such that $\alpha\boldsymbol{x}\leq A\boldsymbol{x}\leq\beta\boldsymbol{x}$, then $\alpha\leq\lambda_1(A)\leq\beta$. If $\alpha\boldsymbol{x}<A\boldsymbol{x}$, then $\alpha<\lambda_1(A)$; if $A\boldsymbol{x}<\beta\boldsymbol{x}$, then $\lambda_1(A)<\beta$.*

Theorem 2.4. *[1] Let A be an $n\times n$ nonnegative and symmetric matrix. Then $\rho(A)\geq\boldsymbol{x}^\top A\boldsymbol{x}$ for any unit vector $\boldsymbol{x}$, and the equality holds if and only if $A\boldsymbol{x}=\rho(A)\boldsymbol{x}$.*

Definition 2.1. Let A be an $n\times n$ real matrix whose rows and columns are indexed by $X=\{1,2,...,n\}$. We partition X into $\{X_1,X_2,...,X_k\}$ in order and rewrite A according to $\{X_1,X_2,...,X_k\}$ as follows:

$$A=\begin{pmatrix} A_{1,1} & \ldots & A_{1,k}\\ \vdots & \ddots & \vdots\\ A_{k,1} & \ldots & A_{k,k}\end{pmatrix},$$

where $A_{i,j}$ is the block of A formed by rows in X_i and the columns in X_j. Let $b_{i,j}$ denote the average row sum of $A_{i,j}$. Then the matrix $B = [b_{i,j}]$ is called the **quotient matrix** of the partition of A. In particular, the partition is called an **equitable partition** when the row sum of each block $A_{i,j}$ is constant.

Theorem 2.5. *[9] Let $A \geq 0$ be an irreducible matrix, B be the quotient matrix of an equitable partition of A. Then $\rho(A) = \rho(B)$.*

Kelmans [18] introduced the following operation on a graph to describe the relation between the edge-moving and the spectral radius, and obtained that the spectral radius increases after the operation.
The Kelmans operation: Let v_1, v_2 be two vertices of a graph G. We denote $N_1 = N(v_1) \setminus N[v_2]$. We use the Kelmans operation on G as follows: Replace the edge v_1v_w by a new edge v_2v_w for all vertices $v_w \in N_1$ (as shown in Fig. 2). In general, we will denote the obtained graph by G'.

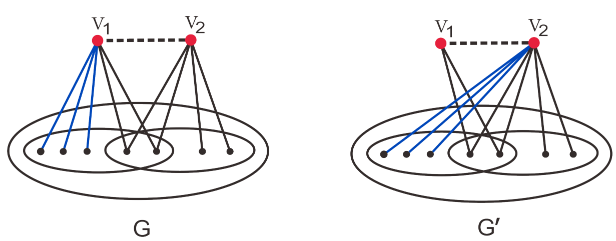

Figure 2: The Kelmans operation.

In [27], the first author et al. considered the relation between the Kelmans operation on a graph and the spectral radius of a function-weighted adjacency matrix, and they obtained the following theorem.

Theorem 2.6. *[27] Let $f(x, y) > 0$ be a symmetric real function, increasing and convex in variable x, and G be a connected graph. Assume that G' is obtained by using the Kelmans operation on nonadjacent vertices v_1 and v_2 of G. If $G \ncong G'$, then $\rho(A_f(G)) < \rho(A_f(G'))$.*

3. Proof of Theorem 1.1

Our aim is to show that P_n or S_n is the tree with the smallest A_f-spectral radius of G among all trees of order n if $f(x, y) > 0$ is a symmetric real function, increasing and convex in variable x. Firstly, we give the following two lemmas.

Lemma 3.1. *Let $f(x,y) > 0$ be a symmetric real function, increasing and convex in variable x, and T_1 be the tree shown in Fig. 3. Then we have $\rho(A_f(T_1)) \geq 2f(2,2) > \rho(A_f(P_n))$.*

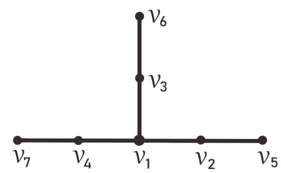

Figure 3: The tree T_1.

Proof. As is well-known, the spectral radius of the adjacency matrix of P_n is $2\cos\dfrac{\pi}{n+1}$. Because $f(x,y) > 0$ is increasing in variable x, by Theorem 2.1, we have $\rho(A_f(P_n)) \leq 2f(2,2)\cos\dfrac{\pi}{n+1} < 2f(2,2)$.

It is easy to see that the quotient matrix of the equitable partition $\{\{v_1\},\{v_2,v_3,v_4\},\{v_5,v_6,v_7\}\}$ of $A_f(T_1)$ is

$$Q = \begin{pmatrix} 0 & 3f(2,3) & 0 \\ f(2,3) & 0 & f(1,2) \\ 0 & f(1,2) & 0 \end{pmatrix}.$$

Let $P(x,T_1)$ be the characteristic polynomial of the quotient matrix Q. By calculation, we get

$$P(x,T_1) = x\big(x^2 - 3f^2(2,3) - f^2(1,2)\big).$$

Since $f(x,y) > 0$ is increasing and convex in variable x, $f^2(x,y)$ is convex in variable x and we obtain

$$\sqrt{3f^2(2,3) + f^2(1,2)} \geq 2f(2,2).$$

It follows from Theorem 2.5 that

$$\rho(A_f(T_1)) \geq 2f(2,2).$$

Consequently, we obtain that

$$\rho(A_f(T_1)) \geq 2f(2,2) > \rho(A_f(P_n)).$$

$\square$

Lemma 3.2. *Let $f(x,y) > 0$ be a symmetric real function, increasing and convex in variable x. Assume that $P_n = v_1v_2\dots v_n$ is the path of order $n \geq 3$ and $\boldsymbol{x} = (x_1, x_2, \dots, x_n)^\intercal$ is the principal eigenvector of P_n. Then we have*

$$x_1 < x_2 < \cdots < x_{\lfloor \frac{n+1}{2} \rfloor} = x_{\lceil \frac{n+1}{2} \rceil} > \cdots > x_{n-1} > x_n$$

and $x_i = x_{n+1-i}$.

Proof. By the symmetry of P_n, it is clearly that $x_i = x_{n+1-i}$. Next, we show that

$$x_1 < x_2 < \cdots < x_{\lfloor \frac{n+1}{2} \rfloor}.$$

Claim 1. $x_1 < x_2$.

We show $x_1 < x_2$ by negation. Suppose that $x_1 \geq x_2$. Then

$$\rho(A_f(P_n))x_1 = f(1,2)x_2 \geq \rho(A_f(P_n))x_2 \geq f(1,2)x_1 + f(1,2)x_3.$$

We obtain $x_3 \leq 0$, this contradicts $\mathbf{x} > 0$. Hence $x_1 < x_2$.

Claim 1 directly implies cases $n = 3$ and $n = 4$. Then we consider the case $n \geq 5$.

Claim 2. For $3 \leq i \leq \lfloor \frac{n+1}{2} \rfloor$, we have $x_i > \min\{x_{i-1}, x_{i+1}\}$.

From

$$\rho(A_f(P_n)) \leq 2f(2,2)\cos\tfrac{\pi}{n+1} < 2f(2,2),$$

it follows that

$$\rho(A_f(P_n))x_i = f(2,2)x_{i-1} + f(2,2)x_{i+1} < 2f(2,2)x_i$$

for $3 \leq i \leq \lfloor \frac{n+1}{2} \rfloor$ and $n \geq 5$. Thus $x_i > \min\{x_{i-1}, x_{i+1}\}$.

Next, we show $x_{i-1} < x_i$ for $3 \leq i \leq \lfloor \frac{n+1}{2} \rfloor$.

If there exists h such that $x_{h-1} \geqslant x_h$ for $3 \leqslant h \leqslant \lfloor \frac{n+1}{2} \rfloor$, by Claim 2 it follows that

$$x_h > x_{h+1} > \cdots > x_{\lfloor \frac{n+1}{2} \rfloor}.$$

Yet, by the symmetry of P_n, we would have $x_{\lfloor \frac{n+1}{2} \rfloor} \leqslant \min\left\{x_{\lfloor \frac{n+1}{2} \rfloor -1}, x_{\lfloor \frac{n+1}{2} \rfloor +1}\right\}$ which is against Claim 2.

Thus we have

$$x_{i-1} < x_i$$

for $3 \leq i \leq \lfloor \frac{n+1}{2} \rfloor$. Combining Claim 1, we deduce that

$$x_1 < x_2 < \cdots < x_{\lfloor \frac{n+1}{2} \rfloor}.$$

The proof is thus complete. □

Proof of Theorem 1.1. It suffices to prove that for any tree T with order $n \geq 5$ such that $T \ncong P_n$ and S_n, the inequality $\rho(A_f(T)) > \rho(A_f(P_n))$ holds. Additionally, let $N(v_i)$ be the set of neighbours of vertex v_i in T in this proof. Since $T \ncong P_n$, we get $\Delta(T) \geq 3$. We consider the following two cases.

Case 1. There is a vertex $v_i \in V(T)$ with $d_i \geq 3$, and at least three vertices belong to $N(v_i)$ with degrees at least 2.

It is obvious that T contains T_1 as its subgraph. By Theorems 2.1 and 2.2 and Lemma 3.1, we obtain that

$$\rho(A_f(T)) \geq \rho(A_f(T_1)) \geq 2f(2,2) > \rho(A_f(P_n)).$$

Case 2. For every vertex $v_i \in V(T)$ with $d_i \geqslant 3$, the set $N(v_i)$ contains at most two non-pendent vertices.

The tree T is a caterpillar by [[14], Theorem 1].

Subcase 2.1. T is not a double star.

We assume the diameter of T is $k+1$, where $3 \leq k \leq n-3$. For simplicity, we denote the vertices on the path achieving the diameter of T as $v_1, v_{i+1}, \ldots, v_{i+k}, v_n$ and the remaining pendent vertices as v_2, $\ldots, v_i, v_{i+k+1}, \ldots, v_{n-1}$ from left to right in order. Without loss of generality, we assume that $0 \leq n-2i-k \leq 1$ and $2 \leq d_{i+1} \leq d_{i+k}$. For example, the tree T is shown in Fig. 4. We distinguish the following two subcases.

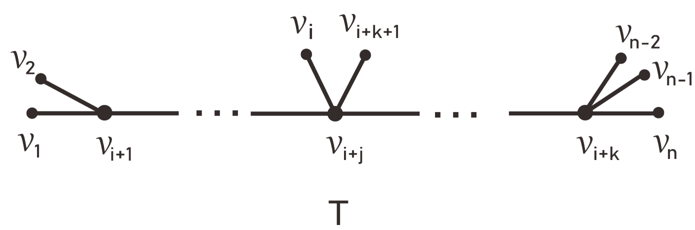

Figure 4: The tree T.

Subcase 2.1.1. There exist two adjacent vertices with degrees at least 3.

Since T is a caterpillar tree. The two vertices must lie on the path $v_1v_{i+1}\dots v_{i+k}v_n$. We suppose these two vertices are v_{i+j} and v_{i+j+1}.

If $1 \leq j \leq k-j$, then we can obtain T from T_2 by using the Kelmans operation on the vertices v_p and v_{i+j} as shown in Fig. 5. Since $1 \leq j \leq k-j$, we get that T_1 is a subgraph of T_2.

Otherwise, we can also obtain T from another tree T_2' by using the Kelmans operation on the vertices v_t and v_{i+j+1}, where v_t is adjacent to the vertex v_{i+j} in T_2'. Similarly, T_2' has T_1 as its subgraph. Thus according to Theorem 2.6 and Case 1, we can get that

$$\rho(A_f(T)) > \rho(A_f(T_2))(\text{or } \rho(A_f(T_2'))) > \rho(A_f(P_n)).$$

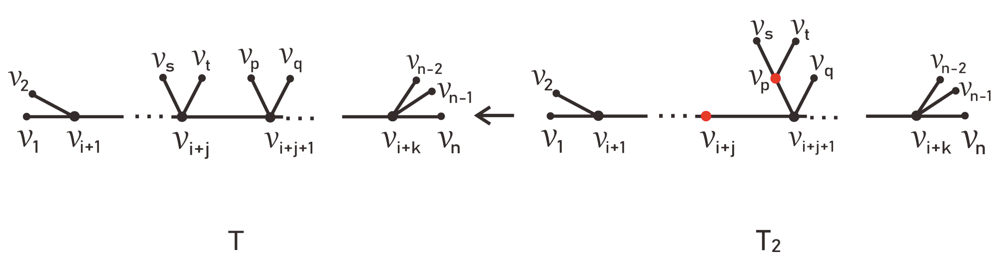

Figure 5: The Kelmans operation for Subcase 2.1.1.

Subcase 2.1.2. There are no adjacent vertices with degrees at least 3.

Let $P_n = v_1v_2\dots v_n$ and $\mathbf{x} = (x_1, x_2, \dots, x_n)^\intercal$ be the principal eigenvector of P_n. Then we can obtain T from P_n by deleting the edges

$$v_1v_2, \dots v_{i-1}v_i, v_{i+k}v_{i+k+1}, \dots, v_{n-1}v_n$$

and adding the pendent edges

$$v_1v_{i+1},\ldots,v_{i+k}v_n$$

to the path $v_{i+1}v_{i+2}\ldots v_{i+k}$. From the assumption that $0\le n-2i-k\le 1$ and $2\le d_{i+1}\le d_{i+k}$, it follows that if $v_p\in N(v_{i+1})$ then $1\le p\le i$. We then obtain that

$$\begin{aligned}
& \frac{1}{2}\big[\mathbf{x}^\top A_f(T)\mathbf{x}-\mathbf{x}^\top A_f(P_n)\mathbf{x}\big]\\
= & \sum_{\substack{v_p\in N(v_{i+1})\\ 2\le p\le i}}\big[f(1,d_{i+1})x_{i+1}x_p-f(2,2)x_px_{p+1}\big]\\
+ & \big[f(1,d_{i+1})x_{i+1}x_1-f(1,2)x_1x_2\big]+\big[f(d_{i+2},d_{i+1})-f(2,2)\big]x_{i+1}x_{i+2}\\
+ & \sum_{\substack{v_p\in N(v_{i+k})\\ 2\le p\le i}}\big[f(1,d_{i+k})x_{i+k}x_p-f(2,2)x_px_{p+1}\big]\\
+ & \sum_{\substack{v_p\in N(v_{i+k})\\ i+k+1\le p\le n-1}}\big[f(1,d_{i+k})x_{i+k}x_p-f(2,2)x_px_{p-1}\big]\\
+ & \big[f(2,d_{i+k})-f(2,2)\big]x_{i+k-1}x_{i+k}+\big[f(1,d_{i+k})x_{i+k}x_n-f(1,2)x_{n-1}x_n\big]\\
+ & \sum_{\substack{2\le j\le k-1\\ d_{i+j}\ge 3}}\Big\{\sum_{\substack{v_p\in N(v_{i+j})\\ 2\le p\le i}}\big[f(1,d_{i+j})x_{i+j}x_p-f(2,2)x_px_{p+1}\big]\\
+ & \sum_{\substack{v_p\in N(v_{i+j})\\ i+k+1\le p\le n-1}}\big[f(1,d_{i+j})x_{i+j}x_p-f(2,2)x_px_{p-1}\big]\\
+ & \big[f(2,d_{i+j})-f(2,2)\big]x_{i+j-1}x_{i+j}+\big[f(2,d_{i+j})-f(2,2)\big]x_{i+j}x_{i+j+1}\Big\}.
\end{aligned}$$

For the vertex v_{i+1}, since $0\le n-2i-k\le 1$ and T is not a double star, we get

$$i+1\le \lfloor\frac{n+1}{2}\rfloor-1.$$

Then by Lemma 3.2, we have

$$x_p<x_{p+1}\le x_{i+1}<x_{i+2}$$

for $2\le p\le i$. Because $f(x,y)>0$ is increasing and convex in variable

x, we obtain

$$\begin{aligned}
& \sum_{\substack{v_p\in N(v_{i+1})\\ 2\leq p\leq i}} \big[f(1,d_{i+1})x_{i+1}x_p - f(2,2)x_px_{p+1}\big] \\
+ & \ \big[f(1,d_{i+1})x_{i+1}x_1 - f(1,2)x_1x_2\big] + \big[f(d_{i+2},d_{i+1}) - f(2,2)\big]x_{i+1}x_{i+2} \\
\geq & \sum_{\substack{v_p\in N(v_{i+1})\\ 2\leq p\leq i}} \big[f(1,2)x_{p+1}x_p - f(2,2)x_px_{p+1}\big] \\
+ & \ \big[f(1,2)x_{i+1}x_1 - f(1,2)x_1x_2\big] + (d_{i+1}-2)\big[f(2,3) - f(2,2)\big]x_{i+1}x_{i+2} \\
\geq & \ (d_{i+1}-2)\big[f(1,2) - f(2,2)\big]x_{i+1}x_{i+2} + f(1,2)\big[x_{i+1}x_1 - x_1x_2\big] \\
+ & \ (d_{i+1}-2)\big[f(2,3) - f(2,2)\big]x_{i+1}x_{i+2} \\
\geq & \ (d_{i+1}-2)\big[f(1,2) - f(2,2) + f(2,3) - f(2,2)\big]x_{i+1}x_{i+2} \geq 0.
\end{aligned}$$

Similarly, for the vertex v_{i+k}, we get

$$i+k \geq \lfloor \frac{n+1}{2} \rfloor + 1.$$

By Lemma 3.2 and $0 \leq n-2i-k \leq 1$, we have

$$x_p < x_{p+1} \leq x_{i+k} < x_{i+k-1}$$

for $2 \leq p \leq i$, and

$$x_p < x_{p-1} \leq x_{i+k} < x_{i+k-1}$$

for $i+k+1 \leq p \leq n-1$.

Furthermore, because $T \ncong P_n$ and $0 \leq n-2i-k \leq 1$, we have $i+k \leq n-2$. Since T is not a double star, we get $2 < i+k$. Thus we obtain $x_{i+k} > x_{n-1}$. Then

$$\begin{aligned}
& \sum_{\substack{v_p\in N(v_{i+k})\\ 2\leq p\leq i}} \big[f(1,d_{i+k})x_{i+k}x_p - f(2,2)x_px_{p+1}\big] \\
+ & \sum_{\substack{v_p\in N(v_{i+k})\\ i+k+1\leq p\leq n-1}} \big[f(1,d_{i+k})x_{i+k}x_p - f(2,2)x_px_{p-1}\big] \\
+ & \ \big[f(2,d_{i+k}) - f(2,2)\big]x_{i+k}x_{i+k-1} + \big[f(1,d_{i+k})x_{i+k}x_n - f(1,2)x_{n-1}x_n\big]
\end{aligned}$$

$$
\begin{aligned}
\geq\ & \sum_{\substack{v_p \in N(v_{i+k})\\ 2\leq p\leq i}} \big[f(1,2)x_{p+1}x_p - f(2,2)x_p x_{p+1}\big]\\
+\ & \sum_{\substack{v_p \in N(v_{i+k})\\ i+k+1\leq p\leq n-1}} \big[f(1,2)x_{p-1}x_p - f(2,2)x_p x_{p-1}\big]\\
+\ & (d_{i+k}-2)\big[f(2,3)-f(2,2)\big]x_{i+k}x_{i+k-1} + \big[f(1,2)x_{i+k}x_n - f(1,2)x_{n-1}x_n\big]\\
=\ & \sum_{\substack{v_p \in N(v_{i+k})\\ 2\leq p\leq i}} \big[f(1,2)-f(2,2)\big]x_p x_{p+1} + \sum_{\substack{v_p \in N(v_{i+k})\\ i+k+1\leq p\leq n-1}} \big[f(1,2)-f(2,2)\big]x_p x_{p-1}\\
+\ & (d_{i+k}-2)\big[f(2,3)-f(2,2)\big]x_{i+k}x_{i+k-1} + f(1,2)x_n\big[x_{i+k}-x_{n-1}\big]\\
>\ & \sum_{\substack{v_p \in N(v_{i+k})\\ 2\leq p\leq i}} \big[f(1,2)-f(2,2)\big]x_p x_{p+1} + \sum_{\substack{v_p \in N(v_{i+k})\\ i+k+1\leq p\leq n-1}} \big[f(1,2)-f(2,2)\big]x_p x_{p-1}\\
+\ & (d_{i+k}-2)\big[f(2,3)-f(2,2)\big]x_{i+k}x_{i+k-1}\\
\geq\ & \sum_{\substack{v_p \in N(v_{i+k})\\ 2\leq p\leq i}} \big[f(1,2)-f(2,2)\big]x_{i+k}x_{i+k-1}\\
+\ & \sum_{\substack{v_p \in N(v_{i+k})\\ i+k+1\leq p\leq n-1}} \big[f(1,2)-f(2,2)\big]x_{i+k}x_{i+k-1}\\
+\ & (d_{i+k}-2)\big[f(2,3)-f(2,2)\big]x_{i+k}x_{i+k-1} \geq 0.
\end{aligned}
$$

Analogously, for every vertex v_{i+j} such that $d_{i+j} \geq 3$ and $2 \leq j \leq k-1$, according to Lemma 3.2 and $0 \leq n-2i-k \leq 1$, if $2 \leq p \leq i$, then we have

$$x_p < x_{p+1} < x_{i+j} \text{ and } x_p < x_{p+1} \leq x_{i+j-1}.$$

If $i+k+1 \leq p \leq n-1$, then we get

$$x_p < x_{p-1} \leq x_{i+j} \text{ and } x_p < x_{p-1} \leq x_{i+j+1}.$$

We then obtain

$$\sum_{\substack{v_p \in N(v_{i+j})\\ 2\leq p\leq i}} \big[f(1,d_{i+j})x_{i+j}x_p - f(2,2)x_p x_{p+1}\big]$$

$$
\begin{aligned}
&+ \sum_{\substack{v_p \in N(v_{i+j}) \\ i+k+1 \le p \le n-1}} \big[f(1, d_{i+j}) x_{i+j} x_p - f(2,2) x_p x_{p-1}\big] \\
&+ \big[f(2, d_{i+j}) - f(2,2)\big] x_{i+j-1} x_{i+j} + \big[f(2, d_{i+j}) - f(2,2)\big] x_{i+j} x_{i+j+1} \\
&\ge \sum_{\substack{v_p \in N(v_{i+j}) \\ 2 \le p \le i}} \big[f(1,2) - f(2,2)\big] x_{i+j-1} x_{i+j} \\
&+ \sum_{\substack{v_p \in N(v_{i+j}) \\ i+k+1 \le p \le n-1}} \big[f(1,2) - f(2,2)\big] x_{i+j} x_{i+j+1} \\
&+ (d_{i+j} - 2)\big[f(2,3) - f(2,2)\big] x_{i+j-1} x_{i+j} \\
&+ (d_{i+j} - 2)\big[f(2,3) - f(2,2)\big] x_{i+j} x_{i+j+1} \\
&\ge (d_{i+j} - 2)\big[f(1,2) - f(2,2) + f(2,3) - f(2,2)\big] x_{i+j-1} x_{i+j} \\
&+ (d_{i+j} - 2)\big[f(1,2) - f(2,2) + f(2,3) - f(2,2)\big] x_{i+j} x_{i+j+1} \ge 0.
\end{aligned}
$$

In conclusion, we have

$$\frac{1}{2}\big[\mathbf{x}^\top A_f(T)\mathbf{x} - \mathbf{x}^\top A_f(P_n)\mathbf{x}\big] > 0.$$

From Theorem 2.4, it follows that

$$\rho(A_f(T)) > \rho(A_f(P_n)).$$

Subcase 2.2. T is a double star.

If $T \cong S_{d,n-d}$ with $d \ge 4$, then we can obtain T from T_3 by using the Kelmans operation on the vertices v_3 and v_1, v_4 and v_1 as shown in Fig. 6. It is easy to see that T_1 is a subgraph of T_3. According to Theorem 2.6 and Case 1, we get

$$\rho(A_f(T)) > \rho(A_f(T_3)) > \rho(A_f(P_n)).$$

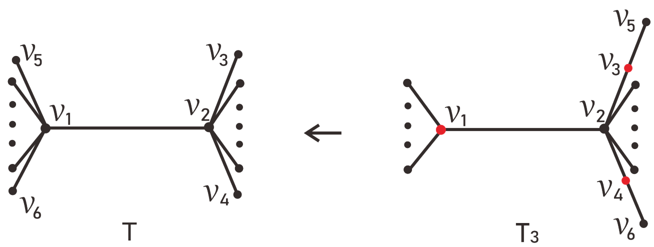

Figure 6: The Kelmans operation for $T \cong S_{d,n-d}$ with $d \geq 4$.

If $T \cong S_{3,n-3}$, then we can obtain T from T_4 by using the Kelmans operation on the vertices v_1 and v_3 as shown in Fig. 7. Because T_4 is not a double star, by Theorem 2.6 and Subcase 2.1, we get

$$\rho(A_f(T)) > \rho(A_f(T_4)) > \rho(A_f(P_n)).$$

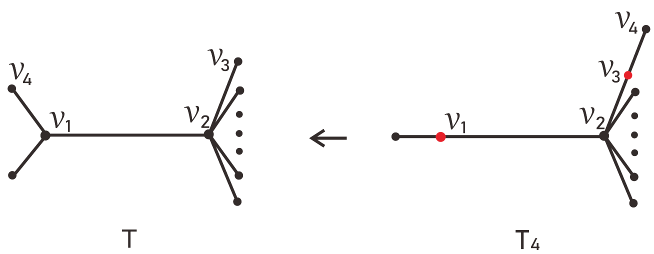

Figure 7: The Kelmans operation for $T \cong S_{3,n-3}$.

Assume that $T \cong S_{2,n-2}$. Let $P_n = v_1v_2 \dots v_n$ and $\mathbf{x} = (x_1, x_2, \dots, x_n)^\intercal$ be the principal eigenvector of P_n. Since $n \geq 5$, we have $x_{\lceil \frac{n+1}{2} \rceil} > x_{n-1}$. Similar to Subcase 2.1, we denote the two center vertices of $S_{2,n-2}$ as $v_{\lceil \frac{n+1}{2} \rceil -1}$ and $v_{\lceil \frac{n+1}{2} \rceil}$. And we can obtain $S_{2,n-2}$ from P_n by shifting edges. We then get

$$\begin{aligned} & \frac{1}{2}\big[\mathbf{x}^\top A_f(T)\mathbf{x} - \mathbf{x}^\top A_f(P_n)\mathbf{x}\big] \\ = \ & \big[f(2, n-2) - f(2,2)\big] x_{\lceil \frac{n+1}{2} \rceil} x_{\lceil \frac{n+1}{2} \rceil -1} \\ + \ & f(1,2)\big[x_1 x_{\lceil \frac{n+1}{2} \rceil -1} - x_1x_2\big] + \big[f(1, n-2) x_n x_{\lceil \frac{n+1}{2} \rceil} - f(1,2) x_{n-1}x_n\big] \end{aligned}$$

$$
\begin{aligned}
&+ \sum_{\substack{v_p \in N(v_{\lceil \frac{n+1}{2} \rceil}) \\ 2 \le p \le \lceil \frac{n+1}{2} \rceil - 2}} \big[f(1, n-2) x_{\lceil \frac{n+1}{2} \rceil} x_p - f(2,2) x_p x_{p+1} \big] \\
&+ \sum_{\substack{v_p \in N(v_{\lceil \frac{n+1}{2} \rceil}) \\ \lceil \frac{n+1}{2} \rceil + 1 \le p \le n-1}} \big[f(1, n-2) x_{\lceil \frac{n+1}{2} \rceil} x_p - f(2,2) x_p x_{p-1} \big] \\
&\ge \big[f(2, n-2) - f(2,2) \big] x_{\lceil \frac{n+1}{2} \rceil} x_{\lceil \frac{n+1}{2} \rceil - 1} \\
&+ f(1,2) \big[x_1 x_{\lceil \frac{n+1}{2} \rceil - 1} - x_1 x_2 \big] + f(1,2) \big[x_n x_{\lceil \frac{n+1}{2} \rceil} - x_{n-1} x_n \big] \\
&+ \sum_{\substack{v_p \in N(v_{\lceil \frac{n+1}{2} \rceil}) \\ 2 \le p \le \lceil \frac{n+1}{2} \rceil - 2}} \big[f(1, n-2) x_{\lceil \frac{n+1}{2} \rceil} x_p - f(2,2) x_p x_{p+1} \big] \\
&+ \sum_{\substack{v_p \in N(v_{\lceil \frac{n+1}{2} \rceil}) \\ \lceil \frac{n+1}{2} \rceil + 1 \le p \le n-1}} \big[f(1, n-2) x_{\lceil \frac{n+1}{2} \rceil} x_p - f(2,2) x_p x_{p-1} \big] \\
&> \big[f(2, n-2) - f(2,2) \big] x_{\lceil \frac{n+1}{2} \rceil} x_{\lceil \frac{n+1}{2} \rceil - 1} + f(1,2) \big[x_1 x_{\lceil \frac{n+1}{2} \rceil - 1} - x_1 x_2 \big] \\
&+ \sum_{\substack{v_p \in N(v_{\lceil \frac{n+1}{2} \rceil}) \\ 2 \le p \le \lceil \frac{n+1}{2} \rceil - 2}} \big[f(1, n-2) x_{\lceil \frac{n+1}{2} \rceil} x_p - f(2,2) x_p x_{p+1} \big] \\
&+ \sum_{\substack{v_p \in N(v_{\lceil \frac{n+1}{2} \rceil}) \\ \lceil \frac{n+1}{2} \rceil + 1 \le p \le n-1}} \big[f(1, n-2) x_{\lceil \frac{n+1}{2} \rceil} x_p - f(2,2) x_p x_{p-1} \big] \\
&\ge (n-4) \big[f(2,3) - f(2,2) + f(1,2) - f(2,2) \big] x_{\lceil \frac{n+1}{2} \rceil} x_{\lceil \frac{n+1}{2} \rceil - 1} \ge 0.
\end{aligned}
$$

Using Theorem 2.4, we get

$$\rho(A_f(T)) > \rho(A_f(P_n)).$$

The proof of the theorem is now complete. □

Remark 3.3 Clearly, $\rho(A_f(S_n)) = \sqrt{n-1} f(1, n-1)$ and $\rho(A_f(P_n)) < 2f(2,2)$. An important special case is that if $f(x,y) > 0$ is a symmetric real function, increasing and convex in variable x such that $f(2,2) \le$

$f(1,4)$, then

$$\rho(A_f(P_n)) < 2f(2,2) \leq 2f(1,4) = \rho(A_f(S_5)) \leq \rho(A_f(S_n))$$

for $n \geq 5$. We then get that P_n is the unique extremal tree with the minimum A_f-spectral radius of G. This result works for the weighted adjacency matrices defined by almost half of the indices listed in Tables 1 and 2. Such as first Zagreb index, second hyper-Zagreb index, extended index, reciprocal Randić index, forgotten index, first Gourava index, first hyper-Gourava index, Sombor index and so on. But in general, the precise structure and uniqueness of the extremal trees are hard to tell since the values of $f(2,2)$ and $f(1,4)$ are unknown. This problem still eludes us.

4. Proof of Theorem 1.2

For $n = 3$, the result is obvious. For $n = 4$, since $f(x,y) > 0$ be a symmetric real function, increasing and convex in variable x, by Theorem 2.1, we have $\rho(A_f(C_4)) = 2f(2,2) = \rho(A_f(C_3)) \leq \rho(A_f(S_4+e))$, and the result also follows.

Next, we consider the case $n \geq 5$. Let $U(n)$ be the set of unicyclic graphs of order n with $n-3$ pendent vertices. We need only to prove that if $G \notin U(n)$, then there exist a unicyclic graph $G^* \in U(n)$ such that $\rho(A_f(G^*)) > \rho(A_f(G))$. We distinguish the following two cases.

Case 1. G contains an odd cycle.

We use the Kelmans operations on the vertices in the cycle with distance 2 over and over again until we get C_3 as shown in Fig. 8.

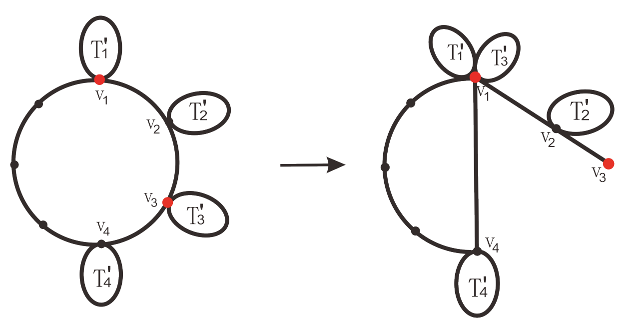

Figure 8: The Kelmans operation on the vertices v_1 and v_3.

Suppose the resulting graph is G_1 where T_i and C_3 have a unique common vertex v_i for $i = 1, 2, 3$ as shown in Fig. 9. Note that if the length of the cycle of G is greater than 5, then the graph G_1 (at least one Kelmans operation is performed) will contain at least 4 non-pendent vertices. Since $G \notin U(n)$, there exist a vertex v_4 with degree at least 2. Without loss of generality, we suppose that v_4 is adjacent to v_1 in T_1.

Analogous to the proof of Lemma 2.1 in [27], we first use similar Kelamns operations on the vertices in T_1 to obtain a double star with two centers v_1 and v_4, obtaining a new graph G_2 as shown in Fig. 9. Next, we use the Kelmans operation on the vertices v_2 and v_4 to obtain a new graph G_3. It is easy to see that all the vertices adjacent to v_1 are pendent vertices but v_2 and v_3. Subsequently, we use similar operations on the vertices in T_2 and T_3. Finally, we will get a new graph $G^* \in U(n)$. Because $G \notin U(n)$, we have $G^* \ncong G$. According to Theorem 2.6, we get $\rho(A_f(G)) < \rho(A_f(G^*))$.

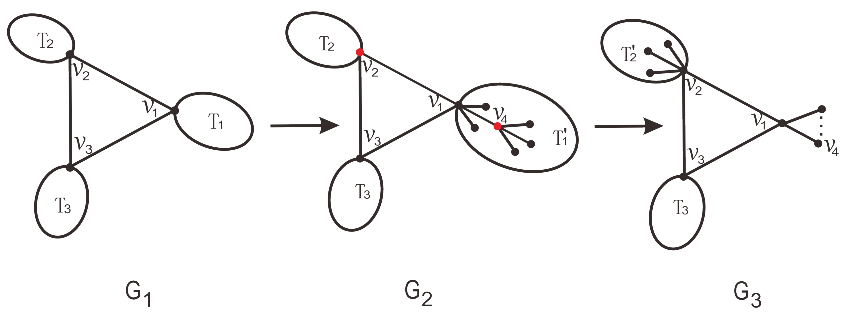

Figure 9: The unicyclic graphs G_1, G_2 and G_3.

Case 2. G contains an even cycle.

Similarly, we use the Kelmans operations on the vertices in the cycle with distance 2 over and over again until we get C_4. Suppose the resulting graph is G_4 where T_i and C_4 have a unique common vertex v_i for $i = 1, 2, 3, 4$ as shown in Fig. 10. Let $v(T_i)$ be the order of T_i. We assume that $v(T_1) = \max\{v(T_1), v(T_2), v(T_3), v(T_4)\}$. Because $n \geq 5$, we get $v(T_1) \geq 2$. Assume that $v_5 \in V(T_1)$ is adjacent to v_1. Next, we use the Kelmans operation on the vertices v_1 and v_3, v_2 and v_4, obtaining a new graph G_5. Subsequently, we delete the vertex v_4, the edges v_1v_4, v_3v_4 and add the edge v_1v_3. Denote by G_6 the resulting graph.

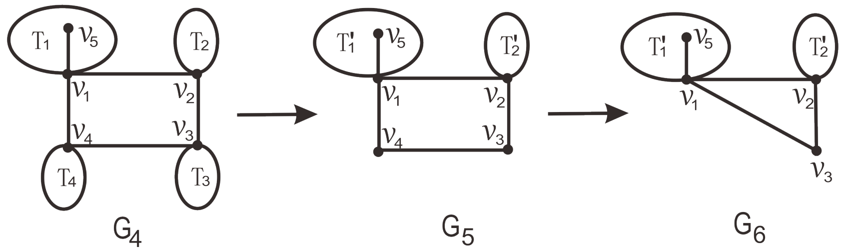

Figure 10: The unicyclic graphs G_4, G_5 and G_6.

Let $\mathbf{x} = (x_1, x_2, x_3, x_5, \ldots, x_n)^\intercal$ be the principal eigenvector of G_6 where x_i corresponds to vertex v_i. Denote by d_i the degree of vertex v_i in G_6. We show $x_1 > x_3$ by contradiction.

If $x_1 = x_3$, then

$$\begin{aligned} \rho(A_f(G_6))x_3 &= f(2, d_2)x_2 + f(2, d_1)x_1 = \rho(A_f(T))x_1 \\ &\geq f(d_1, d_2)x_2 + f(d_1, 2)x_3 + f(d_1, d_5)x_5. \end{aligned}$$

We then obtain $x_5 \leq 0$. This contradicts $\mathbf{x} > 0$.

If $x_1 < x_3$, we can get a new graph $G_7 \cong G_6$ as shown in Fig. 11.

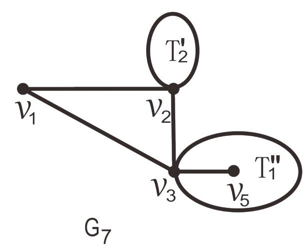

Figure 11: The unicyclic graphs G_7.

Since $f(x, y) > 0$ is a symmetric real function, increasing and convex in variable x and the principal eigenvector$\mathbf{x} > 0$, we obtain

$$\begin{aligned} & \frac{1}{2}\big[\mathbf{x}^\top A_f(G_7)\mathbf{x} - \mathbf{x}^\top A_f(G_6)\mathbf{x}\big] \\ = & \sum_{v_i \in V(T_1)\backslash v_1} \big[f(d_1, d_i)x_i x_3 - f(d_1, d_i)x_i x_1\big] \\ + & \big[f(2, d_2)x_1x_2 - f(d_1, d_2)x_1x_2\big] + \big[f(d_1, d_2)x_2x_3 - f(2, d_2)x_2x_3\big] \end{aligned}$$

$$
\begin{aligned}
= & \sum_{v_i \in V(T_1)\backslash v_1} f(d_1, d_i)x_i\big(x_3 - x_1\big) \\
+ & \big[f(d_1, d_2) - f(2, d_2)\big]\big[x_2x_3 - x_1x_2\big] > 0.
\end{aligned}
$$

This contradicts $G_7 \cong G_6$. Thus we have $x_1 > x_3$. Analogously, we get $x_2 \geq x_3$ with equality if and only if $d_2 = 2$.

Let $\mathbf{y} = (y_1, y_2, y_3, y_4, y_5, \ldots, y_n)^\intercal$, where $y_i = x_i$ for $i \neq 4$ and $y_4 = x_3$. Then we get

$$(A_f(G_5)\mathbf{y})_i = \rho(A_f(G_6))y_i$$

for $i \neq 3, 4$.

For $i = 3$,

$$
\begin{aligned}
(A_f(G_5)\mathbf{y})_3 &= f(2, d_2)y_2 + f(2, 2)y_4 = f(2, d_2)x_2 + f(2, 2)x_3 \\
&< f(2, d_2)x_2 + f(2, d_1)x_1 = \rho(A_f(G_6))x_3 = \rho(A_f(G_6))y_3.
\end{aligned}
$$

For $i = 4$,

$$
\begin{aligned}
(A_f(G_5)\mathbf{y})_4 &= f(2, d_1)y_1 + f(2, 2)y_3 = f(2, d_1)x_1 + f(2, 2)x_3 \\
&\leq f(2, d_1)x_1 + f(2, d_2)x_2 = \rho(A_f(G_6))x_3 = \rho(A_f(G_6))y_4.
\end{aligned}
$$

According to Theorem 2.3, we have

$$\rho(A_f(G_5)) < \rho(A_f(G_6))$$

where G_6 is a unicyclic graph of order $n-1$ with $n-4$ pendent vertices. Since $f(x, y) > 0$ is increasing in variable x, there exist a graph $G^* \in U(n)$ such that $\rho(A_f(G^*)) > \rho(A_f(G_6))$. Thus by Theorem 2.6, we get

$$\rho(A_f(G)) < \rho(A_f(G_6)) < \rho(A_f(G^*)).$$

The proof is thus complete.

Remark 4.1 The second author et al. [33] obtained that $S_n + e$ is the unique unicyclic graph with the largest A_f-spectral radius of G if $f(x, y) > 0$ is increasing and convex in variable x and satisfies that $f(x_1, y_1) \geq f(x_2, y_2)$ when $| x_1 - y_1 |>| x_2 - y_2 |$ and $x_1 + y_1 = x_2 + y_2$. Let $U(n, \lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor)$ be the unicyclic graph of order n with degree sequences $(\lceil \frac{n-3}{2} \rceil + 2, \lfloor \frac{n-3}{2} \rfloor + 2, 2, 1 \ldots, 1)$. With the aid of MATLAB, we compute the extremal unicyclic graphs for many functions $f(x, y) > 0$ to be increasing and convex in variable x but not to satisfy that $f(x_1, y_1) \geq f(x_2, y_2)$ when $\mid x_1 - y_1 \mid > \mid x_2 - y_2 \mid$ and $x_1 + y_1 = x_2 + y_2$. We find that the unicyclic graph on n vertices with the largest A_f-spectral radius of G is not $S_n + e$ but $U(n, \lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor)$ in many cases. For examples, take $n = 9$ and $f(x, y) = xy, (xy)^2$ or e^{xy}. Yet, the data do not show any predictable trend. Hence, for those functions $f(x, y)$ with general forms, further study is needed.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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