# Trees with extremal spectral radius of weighted adjacency matrices among trees weighted by degree-based indices[1]

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**Abstract**

For a graph $G = (V, E)$ and $i, j \in V$, denote by $d_i$, $d_j$ the degrees of vertices $i$, $j$ in $G$. Let $f(d_i, d_j) > 0$ be a function symmetric in $i$ and $j$. Define a matrix $A_f(G)$, called the weighted adjacency matrix of $G$, with the $ij$-entry $A_f(G)(i, j) = f(d_i, d_j)$ if $i \sim j$ and $A_f(G)(i, j) = 0$ otherwise. In this paper, we find the extremal trees with the largest radius of $A_f$ when $f(x, y)$ is increasing and convex in variable $x$. We also find the extremal tree with the smallest radius of $A_f$ when $f(x, y)$ has a form $P(x, y)$ or $\sqrt{P(x, y)}$, where $P(x, y)$ is a symmetric polynomial with nonnegative coefficients and zero constant term. This paper tries to unify the spectral study of weighted adjacency matrices of graphs weighted by some topological indices.

**Keyword:** weighted adjacency matrix, trees weighted by degree-based indices, spectral radius, extremal tree.

**AMS subject classification 2020:** 05C50, 05C09, 05C92, 15A18, 15A42.

## 1 Introduction

Throughout the paper, we denote a simple graph by $G = (V, E)$ with order $|V(G)| = n$. The adjacency matrix of $G$ is denoted by $A(G)$. If $e \in E$ is an edge with two ends $i$ and $j$, we say that $e = ij \in E$ or simply $i \sim j$. We use $d_i$ to represent the degree of a vertex $i$ in $G$. $N(i)$ is the set of neighbors of vertex $i$ in $G$, and $N[i] = N(i) \cup \{i\}$.

In molecular graph theory, topological indices in chemistry are used to represent structural properties of molecular graphs. The general form of these indices is

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$\sum_{i\sim j} f(d_i, d_j)$, where $f$ is a symmetric real function. Gutman [12] collected some important and well-studied indices. We list them below, as well as some recently introduced so-called "exponential" indices, see [3, 4, 5, 21, 23].

Table 1: Some chemical indices

| $f(x,y)$ | name |
|---|---|
| $x+y$ | 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 |
| $\sqrt{(x+y-2)/(xy)}$ | 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 index |
| $(x+y)/2\sqrt{xy}$ | Arithmetic-geometric 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 |
| $\sqrt{x^2+y^2}$ | Somber index |
| $e^{x+y}$ | Exponential first Zagreb index |
| $e^{xy}$ | Exponential second Zagreb index |
| $e^{\frac{1}{\sqrt{xy}}}$ | Exponential Randić index |
| $e^{\sqrt{\frac{x+y-2}{xy}}}$ | Exponential ABC index |
| $e^{2\frac{\sqrt{xy}}{x+y}}$ | Exponential Geometric-arithmetic index |

Each index maps a molecular graph into a single number, obtained by summing up the weights of all pairs of adjacent vertices in a molecular graph. If we use a matrix to represent the structure of a molecular graph with weights separately on its pairs of adjacent vertices, it will completely keep the structural information of the graph, i.e., a matrix keeps much more structural information than an index. So, further study on the algebraic properties of these structural matrices should be made in the future. This idea was first proposed by one of the authors Li in [16]. Several special examples were ever studied, such as the Zagreb matrix [13], Randić matrix, ABC matrix [2, 9], Harmonic matrix [14] and AG matrix [10, 11, 24], which are essentially the adjacency matrix weighted by a symmetric function $f(d_i, d_j)$ defined in the degrees of vertices $i$ and $j$. On the basis of these examples, the authors in [8] gave the following definition of the *weighted adjacency matrix* of a graph weighted by its degrees as a generalization.

**Definition 1.1.** *Let $G = (V, E)$ be a graph. Denote by $d_i$ the degree of a vertex $i$ in $G$. Let $f(d_i, d_j)$ be a function symmetric in $i$ and $j$. The weighted adjacency matrix $A_f(G)$ of $G$ is defined as follows: the $ij$-entry of $A_f(G)$*

$$A_f(G)(i, j) = \begin{cases} f(d_i, d_j), & i \sim j, \\ 0, & \textit{otherwise.} \end{cases}$$

Now, for any topological index we can define the corresponding weighted adjacency matrix of a graph weighted by this index. Let $\lambda_i(A)$ $(i = 1, 2, \cdots, n)$ be the eigenvalues of a matrix $A$. Remember that the *spectral radius* of $A$ is $\rho(A) = \max_i |\lambda_i(A)|$. We are interested in the extremal trees with the largest and smallest spectral radii of $A_f(G)$ for a fixed index $f(d_i, d_j)$. In order to study the properties of these various matrices, we need to classify the indices and try to find unified methods suitable for as many indices as possible, as we have done in [17, 18, 19], where we managed to get the asymptotic values of energy and four Laplacian-type energies of random graphs in $\mathcal{G}_{n,p}$, under the assumption that $f((1+o(1))np, (1+o(1))np) = (1+o(1))f(np, np)$, which covers almost all the topological indices proposed so far. The idea of unification was also adopted by some mathematicians in the study of extremal values for chemical indices of graphs, see [3, 4, 5, 6, 7], but on the whole, the spectral properties of weighted adjacency matrices have been hardly studied except for very few examples, and they have been treated one by one for different topological indices, without using unified approaches. We will list the former results below as far as we know, including the case of classical adjacency matrix. We use $P_n$ and $S_n$ to represent a path and star on $n$ vertices, and $S_{d,n-d}$ to represent a double star on $n$ vertices with the degrees of two centers equal to $d$ and $n - d$.

**Theorem 1.2.** *(Lovas and Pelikan, see [22]) Let $T$ be a tree of order $n \geq 3$, and $A(T)$ is the adjacency matrix of $T$. Then*

$$\rho(A(P_n)) \leq \rho(A(T)) \leq \rho(A(S_n)).$$

*The equalities hold if and only if $T \cong P_n$ or $S_n$, respectively.*

**Theorem 1.3.** *([20]) Let $f(x, y)$ be the weight function for Randić index. If $G$ is a non-empty graph, then $\rho(A_f(G)) = 1$.*

**Theorem 1.4.** *([2]) Let $f(x, y)$ be the weight function for ABC index. Then*

$$\rho(A_f(P_n)) \leq \rho(A(T)) \leq \rho(A_f(S_n)).$$

*The equalities hold if and only if $T \cong P_n$ or $S_n$, respectively.*

The question is that can we give a unified approach to solve the spectral extremal problem like we did in [17, 18, 19] for the asymptotic values of energies for random graphs weighted by chemical indices. This time we are not that lucky for all kinds of chemical indices, but fortunately we can get some substantial progress for some classes of chemical indices. See the following.

**Theorem 1.5.** *Assume that $f(x, y) > 0$ is a symmetric real function, increasing and convex in variable $x$. Then the tree on $n$ vertices with the largest spectral radius of $A_f(T)$ is $S_n$ or a double star $S_{d,n-d}$ for some $d \in \{2, \ldots, n-2\}$.*

**Theorem 1.6.** *Assume that $f(x, y)$ has a 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 $n$ ($n \geq 9$) vertices with the smallest spectral radius of $A_f(T)$ is uniquely $P_n$.*

In the next two sections, we shall present the proofs of the two theorems, separately. We will need some important results in linear algebra from [1] as follows.

**Lemma 1.7.** *Let $A$ be an $n \times n$ real symmetric matrix. Then the largest eigenvalue $\lambda_1(A) = \max\limits_{x \in \mathbb{R}^n, \|x\|=1} x^\top Ax$.*

**Lemma 1.8.** *Let $A$, $B$ be nonnegative matrices and $A \leq B$. Then $\rho(A) \leq \rho(B)$.*

**Lemma 1.9.** *Let $A \geq 0$ be an irreducible matrix. For $t \in \mathbb{R}$, if there exists a nonzero vector $x \geq 0$ such that $Ax \geq tx$ ($Ax \leq tx$), then $\rho(A) \geq t$ ($\rho(A) \leq t$).*

**Lemma 1.10.** *Let $A \geq 0$ be an irreducible matrix. $\rho(A)$ equals the largest eigenvalue with multiplicity 1, and the principal eigenvector $x > 0$. If $u \geq 0$ satisfies $Au \geq \rho(A)u$, then $u$ is an eigenvector of $\rho(A)$.*

**Lemma 1.11.** *Let $A \geq 0$ be an irreducible matrix. Then $\overline{R} \leq \rho(A) \leq R_{max}$, where $\overline{R}$ is the average value of row sums of $A$ and $R_{max}$ is the value of the largest row sum. Either equality holds if and only if the row sums are equal.*

Suppose that $A$ is a symmetric real matrix whose rows and columns are indexed by $X = \{1, \ldots, n\}$. Let $\{X_1, \ldots, X_m\}$ be a partition of $X$, and rewrite $A$ according to $\{X_1, \ldots, X_m\}$ as follows:

$$A = \begin{bmatrix} A_{1,1} & \ldots & A_{1,m} \\ \vdots & & \vdots \\ A_{m,1} & \ldots & A_{m,m} \end{bmatrix}$$

wherein $A_{i,j}$ denotes the blocks 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*. If the row sum of each block $A_{i,j}$ is constant, then the partition is called an *equitable partition*.

**Lemma 1.12.** *Let $A \geq 0$ be an irreducible matrix, $B$ be the quotient matrix of an equitable partition of $A$. Then $\rho(A) = \rho(B)$.*

## 2 Proof of Theorem 1.5

As well-known [15], Kelmans once used a simple local modification of a graph $G$ to describe the relationship between edge moving and spectral radius. He showed that the spectral radius increases after the operation. Fortunately enough, it also behaves well under our assumption that $f(x, y)$ is increasing and convex in $x$ (in $y$ too, of course). Now we give a description of it below:

**The Kelmans operation:** Given a graph $G$ and two specified vertices $u$ and $v$, replace the edge $uw$ by a new edge $vw$ for all vertices $w$ such that $u \sim w \nsim v$.

**Lemma 2.1.** *Let $T$ be a tree and $T'$ be the tree after a Kelmans operation on $T$. If $T \ncong T'$, then $\rho(A_f(T)) < \rho(A_f(T'))$.*

*Proof.* Suppose the two involved vertices are $u$ and $v$. For convenience, we introduce some new notations: $N_1 := N(u) - N(v)$, $N_2 := N(u) \cap N(v)$, $N_3 := N(v) - N(u)$, $n_1 = |N_1|$, and the principal eigenvector of $A_f(T)$ is $x$. We assume that $N_1 \neq \emptyset$ and $N_3 \neq \emptyset$ or it makes no sense. Notice that the two graphs obtained from moving edges from $N_1$ to $N_3$ and from $N_3$ to $N_1$ are essentially the same, and so we can suppose $x_u \leq x_v$. Then,

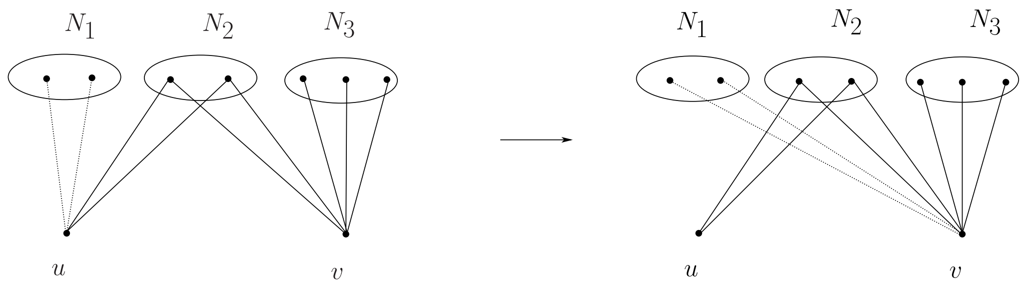


Figure 1: The Kelmans operation

$$x^\top A_f(T')x - x^\top A_f(T)x = 2\sum_{w\in N_1}(f(d_v+n_1, d_w)x_vx_w - f(d_u, d_w)x_ux_w)+$$
$$2\sum_{w\in N_2}[(f(d_u-n_1, d_w) - f(d_u, d_w))x_ux_w + (f(d_v+n_1, d_w) - f(d_v, d_w))x_vx_w]+$$
$$2\sum_{w\in N_3}(f(d_v+n_1, d_w) - f(d_v, d_w))x_vx_w.$$

Since $f(x, y)$ is convex in $x$, we have that for every $w \in N_2$, $f(d_v+n_1, d_w) - f(d_v, d_w) \geq f(d_u, d_w) - f(d_u - n_1, d_w)$, and thus $\rho(A_f(T')) \geq \rho(A_f(T))$. If the equality holds, $x$

is also the principal eigenvector of $A_f(T')$. It can be deduced from

$$\begin{cases} \rho(A_f(T))x_u = \sum\limits_{w\in N_1} f(d_u,d_w)x_w + \sum\limits_{w\in N_2} f(d_u,d_w)x_w, \\ A_f(T')x_u = \sum\limits_{w\in N_2} f(d_u-n_1,d_w)x_w \end{cases}$$

that $\sum\limits_{w\in N_1} f(d_u,d_w)x_w = 0$, a contradiction. ∎

For any tree $T$ rooted at a vertex $r$, if there exists a vertex $r' \in N(r)$ such that $r'$ is not a pendent vertex, apply the Kelmans operation to $r'$ and other non-pendent vertices in $N(r)$ by removing edges to $r'$, until all vertices except $r'$ in $N(r)$ are pendent. Now we obtain a new tree with more leaves, denoted by $T'$. Replace $T$ by the smaller tree induced by $V(T')-N[r]+\{r'\}$ and replace $r$ by $r'$, and repeat the process above recursively. The whole process ends up with a caterpillar tree. According to Lemma 2.1, the spectral radius of any tree is not larger than the spectral radius of some caterpillar tree, and thus the extremal tree lies in the family of caterpillar trees.

For a caterpillar tree, suppose its backbone is $P_\ell$. Label the vertices of $P_\ell$ by $w_1, w_2, \ldots, w_\ell$ successively. When $\ell \geq 3$, apply the Kelmans operation to $w_1$ and $w_3$ and obtain a new caterpillar tree with the length of backbone reduced by 1. The process ends up with a double star. Now we can say that the extremal tree is a double star or a star.

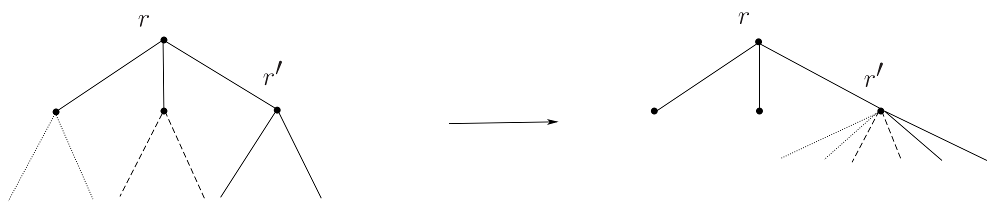


Figure 2: The concentration of edges

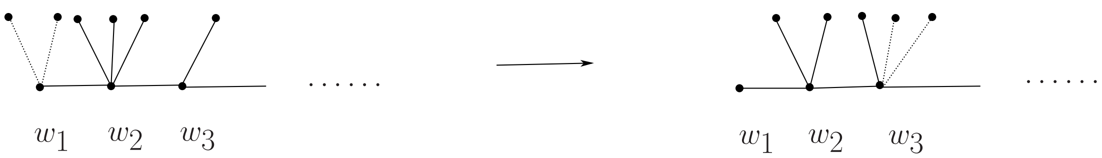


Figure 3: Reducing the length of backbone

Actually we can calculate the spectral radius of any star and double star weighted by $f(x,y)$ directly. It is easy to check that $\rho(A(S_n)) = \sqrt{n-1}$, and so $\rho(A_f(S_n)) = f(1,n-1)\sqrt{n-1}$. As for double stars, assume that the two centers are $u$ and $v$, with degrees $d$ and $n-d$ $(2 \leq d \leq \lfloor \frac{n}{2} \rfloor)$. The quotient matrix of the equitable partition

$\{N(u)-v, \{u\}, \{v\}, N(v)-u\}$ is

$$\begin{bmatrix} 0 & \alpha & 0 & 0 \\ (d-1)\alpha & 0 & \beta & 0 \\ 0 & \beta & 0 & (n-1-d)\gamma \\ 0 & 0 & \gamma & 0 \end{bmatrix},$$

where $\alpha = f(1, d)$, $\beta = f(d, n-d)$, $\gamma = f(1, n-d)$.

The characteristic polynomial is

$$\phi(\lambda) = \lambda^4 - [(n-1-d)\gamma^2 + (d-1)\alpha^2 + \beta^2]\lambda^2 + (d-1)(n-1-d)\alpha^2\gamma^2,$$

and the spectral radius is $\sqrt{\frac{(n-1-d)\gamma^2+(d-1)\alpha^2+\beta^2+\sqrt{[(n-1-d)\gamma^2+(d-1)\alpha^2+\beta^2]^2-4(d-1)(n-1-d)\alpha^2\gamma^2}}{2}}$.

Denote this formula by $DS(n, d)$. The extremal tree is a star or a double star depending on the size relationship between $f(1, n-1)\sqrt{n-1}$ and $\max_{2\le d\le\lfloor\frac{n}{2}\rfloor} DS(n, d)$.

**Remark 2.2.** *An important special case is when $f(x, y) = g(x) + g(y)$ for some function $g$, and $g$ is increasing and convex. For any edge $e = ij \in E(T)$, assume $1 \le d_i \le \lfloor\frac{n}{2}\rfloor$, $f(d_i, d_j) = g(d_i)+g(d_j) \le g(d_i)+g(n-d_i) \le g(1)+g(n-1) = f(1, n-1)$. Combining Lemma 1.8 and Theorem 1.2, $S_n$ is the unique extremal tree with the maximum spectral radius. Thus, the extremal trees with weight functions as the two Zagreb indices, first hyper-Zagreb index, reciprocal sum-connectivity index, forgotten index and Somber index are determined. But in general, the precise structure and uniqueness of the extremal trees are hard to tell since the formula $DS(n, d)$ is too complicated to deal with. With the aid of MATLAB, we have computed the extremal trees with weight functions as some indices, as well as some new weight functions we invented as guinea pigs, but the data did not show much sign of regularity. For example, take $f(x, y) = x^3y + xy^3$.*

# 3 Proof of Theorem 1.6

Based on the example indices listed in Table 1, we construct two classes of weight functions. Let $P(x, y)$ be a symmetric polynomial with nonnegative coefficients and zero constant term, and $f(x, y) = P(x, y)$ or $\sqrt{P(x, y)}$. We find that $P_n$ is the only extremal tree with the smallest spectral radius of $A_f(T)$. The theorem covers about half of the indices listed in Table 1, including the two (hyper-)Zagreb indices, reciprocal Randić index, reciprocal sum-connectivity index, forgotten index, somber index, the two (hyper-)Gourava indices, and product-connectivity Gourava index.

We will show this fact by a series of siftings. It is easy to check that $\rho(A_f(P_n)) = 2f(2, 2)+O(\frac{1}{n})$ by Lemma 1.11, so it is reasonable that we regard $2f(2, 2)$ as $\rho(A_f(P_n))$. From now on, we use $a$, $b$, $c$ and $d$ to represent $f(1, 2)$, $f(2, 2)$, $f(1, 3)$ and $f(2, 3)$, respectively. The four values are indispensable in our proof.

Denote by $T^*$ the smallest extremal tree.

**Claim 3.1.**

$$\Delta(T^*) \leq 3.$$

*Proof.* Otherwise, $\rho(A_f(T^*)) \geq 2f(1,4) \geq 2f(2,2) > \rho(P_n)$, a contradiction. ∎

**Claim 3.2.** *Every 3-degree vertex in $T^*$ has a pendent vertex as a neighbor.*

*Proof.* Otherwise, according to Lemma 1.8, $\rho(A_f(T^*))$ is larger than that of the graph shown in Figure 4. Then it has an obvious equitable partition of three parts and the

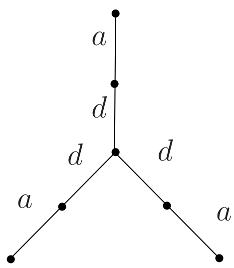


Figure 4: The figure for Claim 3.2.

quotient matrix is $\begin{bmatrix} 0 & a & 0 \\ a & 0 & d \\ 0 & 3d & 0 \end{bmatrix}$, whose characteristic polynomial is $\phi(\lambda) = \lambda(\lambda^2 - 3d^2 - a^2)$. Because $f^2(x, y)$ is a convex function, we have $d^2 - b^2 \geq b^2 - a^2$, and so $3d^2 + a^2 \geq 4b^2$, i.e., $\rho(A_f(T^*)) \geq 2b > \rho(P_n)$, a contradiction. ∎

**Claim 3.3.** *Every 3-degree vertex in $T^*$ has at most one neighbor with degree $> 1$.*

*Proof.* Otherwise, according to Lemma 1.8, $\rho(A_f(T^*))$ is larger than that of the graph shown in Figure 5. Then it also has an equitable partition of four parts and the

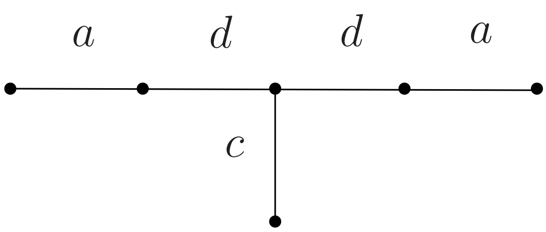


Figure 5: The figure for Claim 3.3.

quotient matrix is

$$\begin{bmatrix} 0 & a & 0 & 0 \\ a & 0 & d & 0 \\ 0 & 2d & 0 & c \\ 0 & 0 & c & 0 \end{bmatrix},$$

whose characteristic polynomial is $\phi(\lambda) = \lambda^4 - (a^2 + c^2 + 2d^2)\lambda^2 + a^2c^2$.

We will show that the spectral radius of this weighted graph is larger than $2b$ by showing that $\phi(4b^2) \leq 0$ as follows:

$\phi(4b^2) = 16b^4 - 4(a^2+c^2+2d^2)b^2 + a^2c^2 \leq \phi(4b^2) = 16b^4 - 4(a^2+c^2+2d^2)b^2+b^2c^2$, the inequality

$$\phi(4b^2) = 16b^4 - 4(a^2 + c^2 + 2d^2)b^2 + b^2c^2 \leq 0$$

is equivalent to

$$\frac{4a^2 + 3c^2 + 8d^2}{b^2} \geq 16. \tag{*}$$

Every monomial term of a symmetric polynomial $P(x, y)$ has the following three different types: (i) $x^\alpha + y^\alpha$ ($\alpha \geq 1$); (ii) $(xy)^\alpha$ ($\alpha \geq 1$); (iii) $(xy)^\alpha(x^\beta + y^\beta)$ ($\alpha, \beta \geq 1$). We use $M(x, y)$ to denote the monomial term. The inequality $(*)$ holds if and only if the inequality

$$\frac{4M(1, 2) + 3M(1, 3) + 8M(2, 3)}{M(2, 2)} \geq 16$$

holds for the three kinds of monomials, respectively. We will proceed the proof by distinguishing three cases.

**Case 1.** $M(x, y) = x^\alpha + y^\alpha$.

$$\frac{4M(1, 2) + 3M(1, 3) + 8M(2, 3)}{M(2, 2)} = \frac{7}{2} \cdot \frac{1}{2^\alpha} + \frac{11}{2} \cdot (\frac{3}{2})^\alpha + 6,$$

this is an increasing function in $\alpha$, achieving the minimum value 16 when $\alpha = 1$.

**Case 2.** $M(x, y) = (xy)^\alpha$.

$$\frac{4M(1, 2) + 3M(1, 3) + 8M(2, 3)}{M(2, 2)} = 8(\frac{3}{2})^\alpha + 3(\frac{3}{4})^\alpha + 4(\frac{1}{2})^\alpha,$$

this is an increasing function in $\alpha$, achieving the minimum value $16 + \frac{1}{4}$ when $\alpha = 1$.

**Case 3.** $M(x, y) = (xy)^\alpha(x^\beta + y^\beta)$.

$$\frac{4M(1, 2) + 3M(1, 3) + 8M(2, 3)}{M(2, 2)} = 2(\frac{1}{2})^\alpha(1+\frac{1}{2^\beta})+\frac{3}{2}(\frac{3}{4})^\alpha((\frac{3}{2})^\beta+\frac{1}{2^\beta})+4(\frac{3}{2})^\alpha(1+(\frac{3}{2})^\beta).$$

For any fixed $\alpha \geq 1$, this is an increasing function in $\beta$. So by taking $\beta = 1$, the formula becomes

$$10(\frac{3}{2})^\alpha + 3(\frac{1}{2})^\alpha + 3(\frac{3}{4})^\alpha.$$

One can check that it is an increasing function in $\alpha$ by derivation. So, the minimum value is $10 \cdot \frac{3}{2} + \frac{3}{2} + 3 \cdot \frac{3}{4} = 18 + \frac{3}{4} > 16$. ∎

From the three claims above, one can see that $T^*$ has three possible forms: (1) $P_n$; (2) $D_n$; (3) $\hat{D}_n$; see Figure 6. We will compare their weighted spectral radius by more accurate discussion.

**Claim 3.4.** *When $n \geq 9$, $A_f(P_n) < A_f(D_n) < A_f(\hat{D}_n)$.*


Figure 6: The trees $D$ and $\hat{D}_n$.

*Proof.* Let us show the former inequality first. We use two different methods for the cases $f(x,y) = P(x,y)$ or $\sqrt{P(x,y)}$.

If $f(x,y) = P(x,y)$, cut off one pendent vertex of $P_n$ and link it to the neighbor of the other pendent vertex, and the new graph obtained is just $D_n$. We use a figure labeled by the components of the principal eigenvector $Y$ of $A_f(P_n)$; see Figure 7. The components of symmetric vertices are equal, of course. Then, $Y^\top A_f(D_n)Y -$

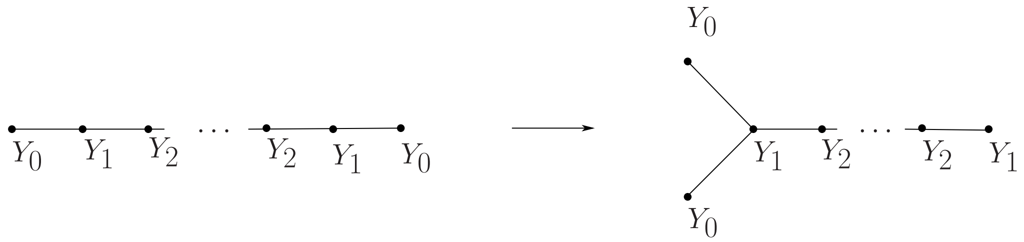


Figure 7: The figure for $f(x,y) = P(x,y)$.

$Y^\top A_f(P_n)Y = 2[(2c-2a)Y_0Y_1 + (a+d-2b)Y_1Y_2]$. Since $f(x,y)$ is increasing and convex in $x$, we have $a+d-2b \geq 0$, and $\rho(A_f(D_n)) \geq \rho(A_f(P_n))$.

If the inequality holds, $Y$ is also the principal eigenvector of $A_f(D_n)$. It can be deduced from

$$\begin{cases} \rho(A_f(P_n))Y_1 = aY_0 + bY_2, \\ \rho(A_f(D_n))Y_1 = aY_2 \end{cases}$$

that $Y_0 = 0$, a contradiction.

If $f(x,y) = \sqrt{P(x,y)}$, we wish to find a nonnegative vector $X \geq 0$ so that $AX \geq 2bX$, by means of Lemma 1.9. Relabel the graph $D_n$ using the components of $X$ as shown in Figure 8. Then, write $AX \geq 2bX$ open in the following form of linear equation system:

$$\begin{cases} X_1 = X_2 \\ cX_3 \geq 2bX_1 \\ \underline{cX_1 + cX_2 + dX_4 \geq 2bX_3} \\ dX_3 + bX_5 \geq 2bX_4 \end{cases} \quad \textit{and} \quad \begin{cases} aX_{n-1} \geq 2bX_n \\ aX_n + bX_{n-2} \geq 2bX_{n-1} \\ b(X_{n-1} + X_{n-3}) \geq 2bX_{n-2} \\ \qquad \vdots \\ b(X_4 + X_6) \geq 2bX_5 \end{cases}$$

Let all the equalities hold except the underlined one, and let $X_n = a$. The latter part of the linear equations produces a formula of $X_i$: $X_i = 2(n-i)b - (n-1-i)\frac{a^2}{b}$ for

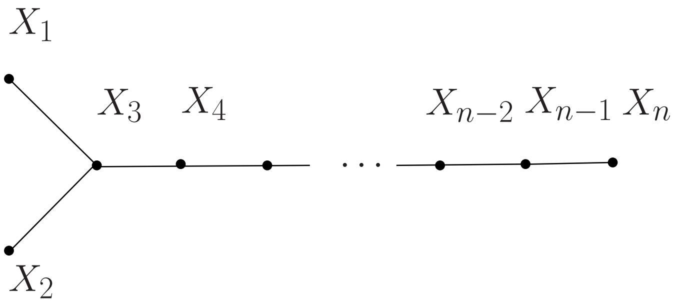


Figure 8: The figure for $f(x,y)=\sqrt{P(x,y)}$.

$i=4,\ldots,n-1$. As for the former part, compute $X_1$, $X_2$, $X_3$ and $X_5$ in the form of an expression about $X_4$, we get

$$X_1=X_2=\frac{c(bX_4+2b^2-a^2)}{2bd},\quad X_3=\frac{bX_4+2b^2-a^2}{d},\quad X_5=X_4-2b+\frac{a^2}{b}.$$

The only thing we need to do is to check the correctness of the underlined inequality. Since $X_4=2(n-4)b-(n-5)\frac{a^2}{b}$, the inequality is equivalent to

$$(c^2+d^2-2b^2)(2(n-4)b^2-(n-5)a^2)\geq(2b^2-c^2)(2b^2-a^2).$$

It is true if

$$(n-4)(c^2+d^2-2b^2)\geq 2b^2-c^2\quad\Leftrightarrow\quad\frac{(n-3)c^2+(n-4)d^2}{b^2}\geq 2(n-3).$$

The method is the same as that in the proof of Claim 3.3. We prove $\frac{(n-3)M(1,3)+(n-4)M(2,3)}{M(2,2)}\geq 2(n-3)$ for any symmetric monomial $M(x,y)$.

**Case 1.** $M(x,y)=x^\alpha+y^\alpha$ $(\alpha\geq 1)$.

$$\frac{(n-3)M(1,3)+(n-4)M(2,3)}{M(2,2)}=\frac{n-3}{2}(\frac{1}{2^\alpha}+(\frac{3}{2})^\alpha)+\frac{n-4}{2}(1+(\frac{3}{2})^\alpha),$$

this is an increasing function in $\alpha$, achieving the minimum value $\frac{9}{4}n-8$ when $\alpha=1$, and $\frac{9}{4}n-8\geq 2(n-3)$ $(n\geq 8)$.

**Case 2.** $M(x,y)=(xy)^\alpha$ $(\alpha\geq 1)$.

$$\frac{(n-3)M(1,3)+(n-4)M(2,3)}{M(2,2)}=(n-4)(\frac{3}{2})^\alpha+(n-3)(\frac{3}{4})^\alpha,$$

this is an increasing function in $\alpha$, achieving the minimum value $\frac{9n-33}{4}$ when $\alpha=1$, and $\frac{9n-33}{4}\geq 2(n-3)$ $(n\geq 9)$.

**Case 3.** $M(x,y)=(xy)^\alpha(x^\beta+y^\beta)$ $(\alpha,\beta\geq 1)$.

$$\frac{(n-3)M(1,3)+(n-4)M(2,3)}{M(2,2)}=\frac{1}{2}[(n-3)(\frac{3}{4})^\alpha(\frac{1}{2^\beta}+(\frac{3}{2})^\beta)+(n-4)(\frac{3}{2})^\alpha(1+(\frac{3}{2})^\beta)],$$

this is an increasing function in $\beta$, By taking $\beta = 1$, one can check that $(n-3)(\frac{3}{4})^\alpha + \frac{5(n-4)}{4}(\frac{3}{2})^\alpha$ is increasing in $\alpha$ by derivation. The minimum value is $\frac{21n-78}{8} \geq 2(n-3)$ $(n \geq 6)$.

Now the proof of the first inequality of Claim 3.4 is complete. We turn to proving the second one. Assume that $\rho(A_f(D_n)) = r$, the principal eigenvector of $A_f(D_n)$ is $Z$, and label the vertices of $D_n$ by the components of $Z$. Then $\hat{D}_n$ can be obtained from $D_n$ in a similar way as we used to transform $P_n$ into $D_n$; see Figure 9. Then

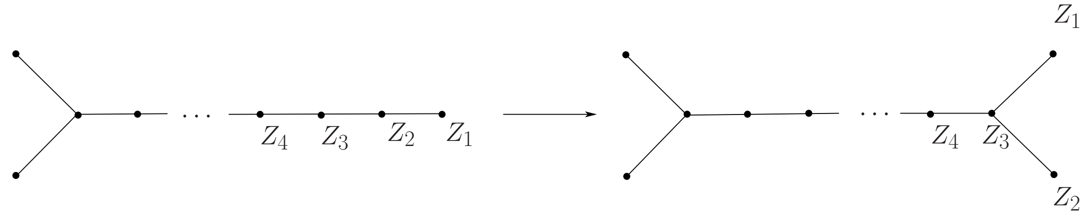


Figure 9: $\hat{D}_n$ is obtained from $D_n$.

from

$$\begin{cases} rZ_1 = aZ_2 \\ rZ_2 = aZ_1 + bZ_3 \\ rZ_3 = bZ_2 + bZ_4, \end{cases}$$

one can get that

$$\begin{cases} Z_2 = \frac{r}{a}Z_1 \\ Z_3 = \frac{r^2-a^2}{ab}Z_1 \\ Z_4 = \frac{r(r^2-a^2-b^2)}{ab^2}. \end{cases}$$

Because $r > 2b > \frac{b+\sqrt{b^2+4a^2}}{2}$, $r^2 - br - a^2 > 0$, $Z_2 < Z_3$, and $\frac{r(r^2-a^2-b^2)}{ab^2} > \frac{2(r^2-a^2-b^2)}{ab} > \frac{r^2-a^2}{ab}$, we have $Z_3 < Z_4$.

From $Z^\top A_f(\hat{D}_n)Z - Z^\top A_f(D_n)Z = 2[cZ_1Z_3 - aZ_1Z_2 + (c-b)Z_2Z_3 + (d-b)Z_3Z_4]$, we will show that $Z^\top A_f(\hat{D}_n)Z - Z^\top A_f(D_n)Z > 0$ by showing $|d-b| \geq |b-c|$. After taking square for both sides and doing some simplification, it is equivalent to $d + c \geq 2b$, which is obvious when $f(x,y) = P(x,y)$. If $f(x,y) = \sqrt{P(x,y)}$, take squares again, and it is sufficient if we can show $cd \geq b^2$. The monomial method remains suitable, but with a little difference. Denote the three types of monomials by $M_1$, $M_2$, $M_3$, in the order of that in the previous proofs. We need to show that for $i$, $j \in \{1,2,3\}$, $M_i(1,3)M_j(2,3) + M_j(1,3)M_i(2,3) > 2M_i(2,2)M_j(2,2)$. The case $i = j$ is easy to check and we omit the routine. Assume $i \neq j$.

**Case 1.** $\{i,j\} = \{1,2\}$.

Prove $\frac{3^\alpha(2^\beta+3^\beta)+6^\alpha(1+3^\beta)}{4^\alpha(2^\beta+2^\beta)} > 2$ when $\alpha$, $\beta \geq 1$. The function

$$\frac{1}{2}[(\frac{3}{4})^\alpha(1+(\frac{3}{2})^\beta) + (\frac{3}{2})^\alpha(\frac{1}{2^\beta}+(\frac{3}{2})^\beta)]$$

is increasing in $\beta$. Taking $\beta = 1$, the function $\frac{5}{4}(\frac{3}{4})^\alpha + (\frac{3}{2})^\alpha$ is increasing in $\alpha$, and so the minimum value is $\frac{39}{16} > 2$.

**Case 2.** $\{i, j\} = \{1, 3\}$.

Prove $\frac{(1+3^\alpha)\cdot 6^\gamma(2^\beta+3^\beta)+(2^\alpha+3^\alpha)\cdot 3^\gamma(1+3^\beta)}{(2^\alpha+2^\alpha)\cdot 4^\gamma(2^\beta+2^\beta)} > 2$ when $\alpha$, $\beta$, $\gamma \geq 1$. The function

$$\frac{1}{4}[(\frac{1}{2^\alpha} + (\frac{3}{2})^\alpha)(\frac{3}{2})^\gamma(1 + (\frac{3}{2})^\beta) + (1 + (\frac{3}{2})^\alpha)(\frac{3}{4})^\gamma(\frac{1}{2^\beta} + (\frac{3}{2})^\beta)]$$

is increasing in $\alpha$ and $\beta$. Taking $\alpha = \beta = 1$, the function $\frac{5}{4}[(\frac{3}{2})^\gamma + (\frac{3}{4})^\gamma]$ is increasing in $\gamma$, and so the minimum value is $\frac{45}{16} > 2$.

**Case 3.** $\{i, j\} = \{2, 3\}$.

Prove $\frac{3^\alpha\cdot 6^\gamma(2^\beta+3^\beta)+6^\alpha\cdot 3^\gamma(1+3^\beta)}{4^{\alpha+\gamma}(2^\beta+2^\beta)} > 2$. The function

$$\frac{1}{2}[(\frac{3}{4})^\alpha(\frac{3}{2})^\gamma(1 + (\frac{3}{2})^\beta) + (\frac{3}{2})^\alpha(\frac{3}{4})^\gamma(\frac{1}{2^\beta} + (\frac{3}{2})^\beta)]$$

is increasing in $\beta$. Taking $\beta = 1$, $\frac{5}{4}(\frac{3}{4})^\alpha(\frac{3}{2})^\gamma + (\frac{3}{2})^\alpha(\frac{3}{4})^\gamma \geq \sqrt{5}(\frac{9}{8})^{\frac{\alpha+\gamma}{2}} > 2$. Combining all the cases, the second inequality has thus been proved. ∎

# 4 Concluding remarks

In this paper we try to unify the solution for spectral extremal trees weighted by some topological indices. In this way we do not need to deal with the weighted adjacency matrix of graphs with weight functions as topological indices one by one separately. However, at the moment we only solve the case when the indices are defined by a symmetric function $f(x, y)$ such that $f(x, y)$ has some nice properties. For those functions $f(x, y)$ with complicated forms, further study is needed, by dividing them into several suitable classes. We hope that in the near future more results can be worked out for much wider classes of topological indices.

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