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Research Article

General sum-connectivity index and general Randić index of trees with given maximum degree

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Abstract

For trees with given number of vertices n and maximum degree Δ, we present lower bounds on the general sum-connectivity index χ_a if $a > 0$ and $3 \le \Delta \le n-1$, and an upper bound on the general Randić index R_a if $-0.283 \le a < 0$ and $3 \le \Delta \le \lfloor \frac{n-1}{2} \rfloor$. All the extremal trees for our bounds are given.

Keywords: general sum-connectivity index; general Randić index; tree; maximum degree.

2020 Mathematics Subject Classification: 05C09, 05C07.

1. Introduction

For a graph G, let $V(G)$ and $E(G)$ be the set of vertices and edges, respectively. The order of G is the number of vertices of G. The degree $d_G(v)$ of a vertex $v \in V(G)$ is the number of edges incident with v. The maximum degree Δ of G is the degree of a vertex which has the largest degree in G. A pendant path of G is a path whose one end vertex has degree 1 in G, the other end vertex has degree at least 3 in G and all the internal vertices have degree 2 in G. A tree is a connected graph which does not contain cycles. A leaf is a vertex having degree one.

Indices of graphs are studied because of their wide applications, especially in chemistry. The general sum-connectivity index of a graph G was introduced by Zhou and Trinajstić [12]. For $a \in \mathbb{R}$, it is defined as

$$\chi_a(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)]^a.$$

For $a \in \mathbb{R}$, the general Randić index

$$R_a(G) = \sum_{uv \in E(G)} [d_G(u)\, d_G(v)]^a$$

of a graph G was first investigated by Bollobás and Erdős [4] in 1998. Extremal results on χ_a and R_a can be found in survey papers [3] and [9], respectively. General indices were investigated also in [2], [5] and [10]. We study trees with given order n and maximum degree Δ. We introduce families of trees which have extremal χ_a and R_a among trees with prescribed n and Δ.

For $3 \le \Delta \le n-1$, let $X_{n,\Delta}$ be a set of trees such that every tree in $X_{n,\Delta}$ has order n and contains exactly one vertex of degree greater than 2 which is an end vertex of Δ pendant paths. Note that the sum of the lengths of those Δ pendant paths is $n-1$, since every tree of order n has $n-1$ edges. Trees in $X'_{n,\Delta}$ satisfy one additional condition that if all the Δ pendant paths of a tree T from $X_{n,\Delta}$ have length at least 2, then T belongs to the set $X'_{n,\Delta}$. So $X'_{n,\Delta} \subseteq X_{n,\Delta}$.

We denote a tree in $X_{n,\Delta}$ whose $\Delta - 1$ pendant paths have length 1 (and the last pendant path has length $n - \Delta + 1$) by $B_{n,\Delta}$; see Figure 1.

Let $\lceil \frac{n-1}{2} \rceil \le \Delta \le n-1$ where $\Delta \ge 3$. We denote a tree in $X_{n,\Delta}$ which contains $2\Delta - n + 1$ pendant paths of length 1 and $n - \Delta - 1$ pendant paths of length 2 by $S^{\star}_{n,\Delta}$; see Figure 2.

For $\lceil \frac{n}{2} \rceil \le \Delta \le n-2$, the double star $S_{\Delta,n-\Delta}$ is a tree with $n-2$ leaves and two other vertices u and v, where $uv \in E(S_{\Delta,n-\Delta})$, u is adjacent to $\Delta - 1$ leaves and v is adjacent to $n - \Delta - 1$ leaves; see Figure 3.

Let us present extremal results on χ_a for trees with given order n and maximum degree Δ. Raza et al. [8] showed that for $\lceil \frac{n}{2} \rceil \le \Delta \le n-2$, the tree $S_{\Delta,n-\Delta}$ has the smallest χ_a if $a < 0$, the tree $S_{\Delta,n-\Delta}$ also has the largest χ_a if $a > 1$, the tree $B_{n,\Delta}$ has the smallest χ_a if $a > 1$, and $S^{\star}_{n,\Delta}$ has the largest χ_a if $a < 0$. The extremal tree $S^{\star}_{n,\Delta}$ was found also by Jamil and

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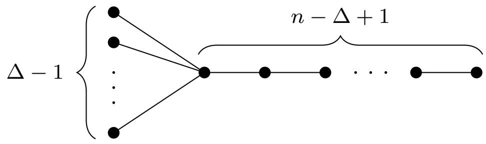

Figure 1: Tree $B_{n,\Delta}$.

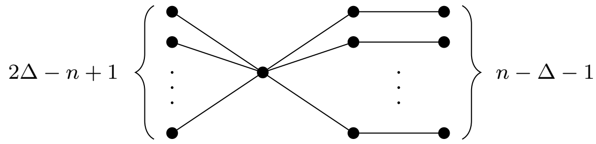

Figure 2: Tree $S^{\star}_{n,\Delta}$.

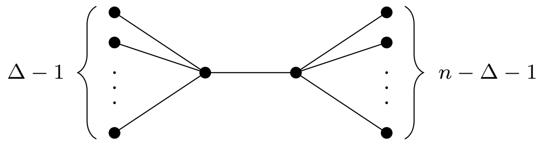

Figure 3: Tree $S_{\Delta,n-\Delta}$.

Tomescu [6] who showed that for $-1.703 \le a < 0$, the tree $S^{\star}_{n,\Delta}$ has the largest χ_a if $\frac{n}{2} \le \Delta \le n-1$ and trees in $X'_{n,\Delta}$ have the largest χ_a if $2 \le \Delta \le \frac{n-1}{2}$. The same results for $-1 \le a < 0$ were given in [1].

We show that for $3 \le \Delta \le n-1$, the tree $B_{n,\Delta}$ has the smallest χ_a if $a > 1$, and every tree in $X_{n,\Delta}$ has the smallest χ_a if $a = 1$. We also prove that for $0 < a < 1$, the tree $S^{\star}_{n,\Delta}$ has the smallest χ_a if $\lceil \frac{n-1}{2} \rceil \le \Delta \le n-1$, and every tree in the set $X'_{n,\Delta}$ has the smallest χ_a if $3 \le \Delta \le \lfloor \frac{n-1}{2} \rfloor$.

Liu, Yan and Yan [7] showed that for $\lceil \frac{n}{2} \rceil \le \Delta \le n-2$, the tree $S^{\star}_{n,\Delta}$ has the largest R_a if $a < 0$, the tree $S_{\Delta,n-\Delta}$ has the largest R_a if $a \ge 1$, and $S_{\Delta,n-\Delta}$ also has the smallest R_a if $a < 0$. Moreover, $B_{n,\Delta}$ has the smallest R_a for $a > 0$ and $3 \le \Delta \le n-1$.

We prove that every tree in the set $X'_{n,\Delta}$ has the largest R_a for $-0.283 \le a < 0$ and $3 \le \Delta \le \lfloor \frac{n-1}{2} \rfloor$. Our results and all the known trees with given n and Δ having the smallest and largest χ_a and R_a are presented in tables in Section 3.

2. Results

First, we present a few lemmas.

Lemma 2.1. *Let $c, p, r, x \in \mathbb{R}$ where $c, p, r > 0$ and $\{p, r\} \ne \{1\}$. Then the function $g_{c,p,r}(x) = c\,p^x + r^x$ is strictly convex.*

Proof. The second derivative $g''_{c,p,r}(x) = (ln\ p)^2 c\,p^x + (ln\ r)^2 r^x > 0$, thus $g_{c,p,r}(x)$ is strictly convex. $\square$

Lemma 2.2. *We have*

(i) $2(5^x) + 3^x - 3(4^x) > 0$ *for* $x > 0$,

(ii) $6^x + 3^x - 2(4^x) > 0$ *for* $x > 0$,

(iii) $2(6^x) + 2^x - 3(4^x) < 0$ *for* $-0.283 \le x < 0$,

(iv) $3(8^x) + 2(2^x) - 5(4^x) < 0$ *for* $-0.584 \le x < 0$,

(v) $10^x + 2^x - 2(4^x) < 0$ *for* $-0.349 \le x < 0$,

(vi) $4(10^x) + 3(2^x) - 7(4^x) < 0$ *for* $-0.349 \le x < 0$.

Proof. By Lemma 2.1, the functions

$$g_{2,\frac{5}{4},\frac{3}{4}}(x) = 2\left(\frac{5}{4}\right)^x + \left(\frac{3}{4}\right)^x,\ g_{1,\frac{3}{2},\frac{3}{4}}(x) = \left(\frac{3}{2}\right)^x + \left(\frac{3}{4}\right)^x,\ g_{2,\frac{3}{2},\frac{1}{2}}(x) = 2\left(\frac{3}{2}\right)^x + \left(\frac{1}{2}\right)^x,$$

$$g_{\frac{3}{2},2,\frac{1}{2}}(x) = \frac{3}{2}\,(2^x) + \left(\frac{1}{2}\right)^x \text{ and } g_{1,\frac{5}{2},\frac{1}{2}}(x) = \left(\frac{5}{2}\right)^x + \left(\frac{1}{2}\right)^x$$

are strictly convex for $x \in \mathbb{R}$.

(i) We have $g_{2,\frac{5}{4},\frac{3}{4}}(-1) = \frac{44}{15} < 3$ and $g_{2,\frac{5}{4},\frac{3}{4}}(0) = 3$. Since $g_{2,\frac{5}{4},\frac{3}{4}}(x)$ is strictly convex, we get $g_{2,\frac{5}{4},\frac{3}{4}}(x) > 3$ for $x > 0$. So $2\left(\frac{5}{4}\right)^x + \left(\frac{3}{4}\right)^x > 3$, which means that $2(5^x) + 3^x > 3(4^x)$ for $x > 0$.

(ii) We have $g_{1,\frac{3}{2},\frac{3}{4}}(-1) = g_{1,\frac{3}{2},\frac{3}{4}}(0) = 2$. Since $g_{1,\frac{3}{2},\frac{3}{4}}(x)$ is strictly convex, we get $g_{1,\frac{3}{2},\frac{3}{4}}(x) > 2$ for $x > 0$. So $\left(\frac{3}{2}\right)^x + \left(\frac{3}{4}\right)^x > 2$, which means that $6^x + 3^x > 2(4^x)$ for $x > 0$.

(iii) We have $g_{2,\frac{3}{2},\frac{1}{2}}(-0.283) < 3$ and $g_{2,\frac{3}{2},\frac{1}{2}}(0) = 3$. Since $g_{2,\frac{3}{2},\frac{1}{2}}(x)$ is strictly convex, we get $g_{2,\frac{3}{2},\frac{1}{2}}(x) < 3$ for $-0.283 \le x < 0$. So $2\left(\frac{3}{2}\right)^x + \left(\frac{1}{2}\right)^x < 3$, which means that $2(3^x) + 1^x < 3(2^x)$, and consequently $2(6^x) + 2^x - 3(4^x) < 0$ for $-0.283 \le x < 0$.

(iv) We have $g_{\frac{3}{2},2,\frac{1}{2}}(-0.584) < \frac{5}{2}$ and $g_{\frac{3}{2},2,\frac{1}{2}}(0) = \frac{5}{2}$. Thus $g_{\frac{3}{2},2,\frac{1}{2}}(x) < \frac{5}{2}$ for $-0.584 \le x < 0$. So $\frac{3}{2}(2^x) + \left(\frac{1}{2}\right)^x < \frac{5}{2}$, which means that $3(2^x) + 2\left(\frac{1}{2}\right)^x - 5 < 0$, and consequently $3(8^x) + 2(2^x) - 5(4^x) < 0$ for $-0.584 \le x < 0$.

(v) We get $g_{1,\frac{5}{2},\frac{1}{2}}(-0.349) < 2$ and $g_{1,\frac{5}{2},\frac{1}{2}}(0) = 2$, thus $g_{1,\frac{5}{2},\frac{1}{2}}(x) < 2$ for $-0.349 \le x < 0$. So $\left(\frac{5}{2}\right)^x + \left(\frac{1}{2}\right)^x < 2$, which means that $10^x + 2^x < 2(4^x)$ for $-0.349 \le x < 0$.

(vi) For $-0.349 \le x < 0$, we obtain $4(10^x) + 3(2^x) - 7(4^x) = 10^x - 4^x + 3[10^x + 2^x - 2(4^x)] < 0$ since $10^x - 4^x < 0$ and by (v), we have $10^x + 2^x - 2(4^x) < 0$. ☐

Lemma 2.3 was presented in [11] and it is used in the proofs of Lemma 2.4, and Theorems 2.1 and 2.2.

Lemma 2.3. *Let $1 \le x < y$ and $c > 0$. Then for $a > 1$ and $a < 0$,*

$$(x+c)^a - x^a < (y+c)^a - y^a.$$

For $0 < a < 1$, we have

$$(x+c)^a - x^a > (y+c)^a - y^a.$$

We prove that some extremal trees have only one vertex of degree greater than 2.

Lemma 2.4. *Among trees of order n and maximum degree Δ, where $3 \le \Delta \le n-1$, let T' be a tree having the smallest χ_a for $a > 0$ (the largest R_a for $-0.283 \le a < 0$). Then T' contains only one vertex of degree greater than 2.*

Proof. Let T' be a tree having the smallest χ_a for $a > 0$ (the largest R_a for $-0.283 \le a < 0$). We prove Lemma 2.4 by contradiction. Assume that T' contains at least two vertices of degree greater than 2. Let w be a vertex of degree Δ in T'. Among vertices of T' having degree at least 3, let v be a vertex furthest from w. So $d_{T'}(v) = x \ge 3$ where $v \ne w$. We can denote the vertices adjacent to v in T' by $v_1, v_2, \dots, v_x$ where v_x is the vertex on the path connecting w and v (possibly $v_x = w$). Note that v is an end vertex of $x-1$ pendant paths. It follows that $1 \le d_{T'}(v_i) \le 2$ for $i = 1, 2, \dots, x-1$. We consider three cases.

Case 1: v is adjacent to $x-1$ leaves.

So $d_{T'}(v_1) = d_{T'}(v_2) = \dots = d_{T'}(v_{x-1}) = 1$. We define T_1 with $V(T_1) = V(T')$ and

$$E(T_1) = \{v_1v_2, v_2v_3, \dots, v_{x-2}v_{x-1}\} \cup E(T') \setminus \{vv_2, vv_3, \dots, vv_{x-1}\}.$$

Clearly, T_1 is a tree of order n and maximum degree Δ. For χ_a, we have

$$\begin{aligned}
\chi_a(T_1) - \chi_a(T') &= [d_{T_1}(v) + d_{T_1}(v_x)]^a - [d_{T'}(v) + d_{T'}(v_x)]^a + [d_{T_1}(v) + d_{T_1}(v_1)]^a \\
&\quad + \sum_{i=1}^{x-2} [d_{T_1}(v_i) + d_{T_1}(v_{i+1})]^a - \sum_{i=1}^{x-1} (d_{T'}(v) + d_{T'}(v_i))^a \\
&= [2 + d_{T_1}(v_x)]^a - [x + d_{T'}(v_x)]^a + (2+2)^a + [(x-3)(2+2)^a + (2+1)^a] - (x-1)(x+1)^a \\
&= [2 + d_{T'}(v_x)]^a - [x + d_{T'}(v_x)]^a + 3^a - (x+1)^a + (x-2)[4^a - (x+1)^a].
\end{aligned}$$

For $x \ge 3$ and $a > 0$, we get

$$[2 + d_{T'}(v_x)]^a < [x + d_{T'}(v_x)]^a, \; 3^a < (x+1)^a \text{ and } 4^a \le (x+1)^a,$$

thus $\chi_a(T_1) - \chi_a(T') < 0$ which means that $\chi_a(T_1) < \chi_a(T')$, so T' does not have the smallest χ_a, a contradiction.

For R_a, we have

$$\begin{aligned}
R_a(T_1) - R_a(T') &= [d_{T_1}(v)d_{T_1}(v_x)]^a - [d_{T'}(v)d_{T'}(v_x)]^a + [d_{T_1}(v)d_{T_1}(v_1)]^a + \sum_{i=1}^{x-2} [d_{T_1}(v_i)d_{T_1}(v_{i+1})]^a - \sum_{i=1}^{x-1} (d_{T'}(v)d_{T'}(v_i))^a \\
&= [2 \cdot d_{T'}(v_x)]^a - [x \cdot d_{T'}(v_x)]^a + (2 \cdot 2)^a + [(x-3)(2 \cdot 2)^a + (2 \cdot 1)^a] - (x-1)(x \cdot 1)^a \\
&> 2^a - x^a + (x-2)(4^a - x^a).
\end{aligned}$$

For $x \geq 4$ and $a < 0$, we get $2^a > x^a$ and $4^a \geq x^a$, thus $R_a(T_1) - R_a(T') > 0$. For $x = 3$ and $a < 0$, we have

$$R_a(T_1) - R_a(T') > 2^a - 3^a + 4^a - 3^a > 0,$$

since by Lemma 2.3, we obtain $4^a - 3^a > 3^a - 2^a$. Hence $R_a(T_1) > R_a(T')$, a contradiction

Case 2: v is adjacent to at least one leaf and at most $x - 2$ leaves.

Without the loss of generality, we can assume that $d_{T'}(v_1) = 1$ and $d_{T'}(v_2) = 2$. Let u be the leaf of T' which is on the pendant path that contains v_2. Let z be the vertex adjacent to u in T' (possibly $z = v_2$). We define T_2 with $V(T_2) = V(T')$ and $E(T_2) = \{uv_1\} \cup E(T') \setminus \{vv_1\}$. Clearly, T_2 is a tree of order n and maximum degree Δ. For χ_a, we obtain

$$\begin{aligned}
\chi_a(T_2) - \chi_a(T') &= [d_{T_2}(v_1) + d_{T_2}(u)]^a - [d_{T'}(v_1) + d_{T'}(v)]^a + [d_{T_2}(u) + d_{T_2}(z)]^a - [d_{T'}(u) + d_{T'}(z)]^a \\
&\quad + \sum_{i=2}^{x}([d_{T_2}(v) + d_{T_2}(v_i)]^a - [d_{T'}(v) + d_{T'}(v_i)]^a) \\
&= (1+2)^a - (1+x)^a + (2+2)^a - (1+2)^a + \sum_{i=2}^{x}([(x-1) + d_{T'}(v_i)]^a - [x + d_{T'}(v_i)]^a) \\
&= 4^a - (1+x)^a + \sum_{i=2}^{x}([x - 1 + d_{T'}(v_i)]^a - [x + d_{T'}(v_i)]^a).
\end{aligned}$$

For $x \geq 3$ and $a > 0$, we get $4^a \leq (1+x)^a$ and $[x - 1 + d_{T'}(v_i)]^a < [x + d_{T'}(v_i)]^a$ for each $i = 2, 3, \ldots, x$, thus $\chi_a(T_2) < \chi_a(T')$, a contradiction.

For R_a, we obtain

$$\begin{aligned}
R_a(T_2) - R_a(T') &= [d_{T_2}(v_1) d_{T_2}(u)]^a - [d_{T'}(v_1) d_{T'}(v)]^a + [d_{T_2}(u) d_{T_2}(z)]^a - [d_{T'}(u) d_{T'}(z)]^a \\
&\quad + \sum_{i=2}^{x}([d_{T_2}(v) d_{T_2}(v_i)]^a - [d_{T'}(v) d_{T'}(v_i)]^a) \\
&= (1 \cdot 2)^a - (1 \cdot x)^a + (2 \cdot 2)^a - (1 \cdot 2)^a + \sum_{i=2}^{x}([(x-1) d_{T'}(v_i)]^a - [x \cdot d_{T'}(v_i)]^a) \\
&= 4^a - x^a + \sum_{i=2}^{x}([(x-1) d_{T'}(v_i)]^a - [x\, d_{T'}(v_i)]^a).
\end{aligned}$$

For $x \geq 4$ and $a < 0$, we get $4^a \geq x^a$ and $[(x-1) d_{T'}(v_i)]^a > [x\, d_{T'}(v_i)]^a$ for each $i = 2, 3, \ldots, x$, thus $R_a(T_2) - R_a(T') > 0$.

For $x = 3$ and $-0.283 \leq a < 0$, we obtain

$$\begin{aligned}
R_a(T_2) - R_a(T') &= 4^a - 3^a + [2\, d_{T'}(v_2)]^a - [3\, d_{T'}(v_2)]^a + [2\, d_{T'}(v_3)]^a - [3\, d_{T'}(v_3)]^a \\
&= 4^a - 3^a + (2 \cdot 2)^a - (3 \cdot 2)^a + [2 d_{T'}(v_3)]^a - [3 d_{T'}(v_3)]^a \\
&> 2(4^a) - 3^a - 6^a.
\end{aligned}$$

We have

$$2(4^a) - 3^a - 6^a = [3(4^a) - 2^a - 2(6^a)] + (2^a - 3^a)(1 - 2^a) > 0,$$

since $2^a - 3^a > 0$, $1 - 2^a > 0$ and by Lemma 2.2 (iii), $3(4^a) - 2^a - 2(6^a) > 0$. Hence $R_a(T_2) > R_a(T')$, a contradiction.

Case 3: v is not adjacent to a leaf.

So $d_{T'}(v_1) = d_{T'}(v_2) = \cdots = d_{T'}(v_{x-1}) = 2$. Let S be the sum of lengths of the $x - 1$ pendant paths with an end vertex v. We replace those $x - 1$ pendant paths by one path of length S to obtain a new tree T_3 from T'. So $d_{T_3}(v) = 2$. Clearly, T_3 is a tree of order n and maximum degree Δ. For χ_a, we obtain

$$\begin{aligned}
\chi_a(T') - \chi_a(T_3) &= [x + d_{T'}(v_x)]^a - [2 + d_{T_3}(v_x)]^a + (x-1)(x+2)^a + (x-2)(2+1)^a - (2x-3)(2+2)^a \\
&> (x-1)(x+2)^a + (x-2)3^a - (2x-3)4^a,
\end{aligned}$$

since $x \geq 3$ and $d_{T'}(v_x) = d_{T_3}(v_x)$.

For $x = 3$ and $a > 0$, by Lemma 2.2 (i), we obtain

$$\chi_a(T') - \chi_a(T_3) > 2(5^a) + 3^a - 3(4^a) > 0.$$

For $x \geq 4$ and $a > 0$, we have

$$\begin{aligned}\chi_a(T') - \chi_a(T_3) &> (x-1)(x+2)^a + (x-2)3^a - (2x-3)4^a \\ &= (x-1)[(x+2)^a + 3^a - 2(4^a)] + 4^a - 3^a \\ &> (x-1)[6^a + 3^a - 2(4^a)],\end{aligned}$$

since $4^a > 3^a$ and $(x+2)^a \geq 6^a$. By Lemma 2.2 (ii), we have

$$\chi_a(T') - \chi_a(T_3) > (x-1)[2(4^a) - 6^a - 3^a] > 0,$$

hence $\chi_a(T') > \chi_a(T_3)$, a contradiction

For R_a, we obtain

$$\begin{aligned}R_a(T') - R_a(T_3) &= [x \cdot d_{T'}(v_x)]^a - [2 \cdot d_{T_3}(v_x)]^a + (x-1)(2\cdot x)^a + (x-2)(2\cdot 1)^a - (2x-3)(2\cdot 2)^a \\ &< (x-1)(2x)^a + (x-2)2^a - (2x-3)4^a,\end{aligned}$$

since $x \geq 3$ and $d_{T'}(v_x) = d_{T_3}(v_x)$.

For $x = 3$ and $-0.283 \leq a < 0$, by Lemma 2.2 (iii), we obtain

$$R_a(T') - R_a(T_3) < 2(6^a) + 2^a - 3(4^a) < 0.$$

For $x = 4$, by Lemma 2.2 (iv), we obtain

$$R_a(T') - R_a(T_3) < 3(8^a) + 2(2^a) - 5(4^a) < 0.$$

For $x = 5$, by Lemma 2.2 (vi), we obtain

$$R_a(T') - R_a(T_3) < 4(10^a) + 3(2^a) - 7(4^a) < 0.$$

Let us consider the function

$$f(x) = (x-1)(2x)^a + (x-2)2^a - (2x-3)4^a$$

for $x \geq 5$. Note that $f(5) < 0$. We have

$$\begin{aligned}f'(x) &= (2x)^a + (x-1)(2)^a a x^{a-1} + 2^a - 2(4^a) \\ &< (2x)^a + 2^a - 2(4^a) \\ &\leq 10^a + 2^a - 2(4^a)\end{aligned}$$

which is less than 0 by Lemma 2.2 (v). Since $f'(x) < 0$ for $x \geq 5$, the function $f(x)$ is strictly decreasing which means that $f(x) < f(5)$ for $x \geq 6$. So $R_a(T') - R_a(T_3) < f(x) < f(5) < 0$ for $x \geq 6$. Hence $R_a(T') < R_a(T_3)$ for every $x \geq 3$, which means that T' does not have the largest R_a, a contradiction. □

We use Lemma 2.5 in the proof of Theorem 2.1 (iii).

Lemma 2.5. *Let $x \geq 1$ and $a < 0$. Then the function $f(x) = (2x)^a - x^a$ is strictly increasing.*

Proof. We get $f'(x) = (2^a - 1)ax^{a-1}$. For $a < 0$, we have $2^a - 1 < 0$ and $x^{a-1} > 0$. So $f'(x) > 0$. Thus $f(x)$ is strictly increasing. □

In Theorem 2.1, we present the main results of this paper.

Theorem 2.1. *Let T be any tree of order n and maximum degree $\Delta \geq 3$. Then*

(i) $\chi_a(T) \geq (n-\Delta-1)[(\Delta+2)^a + 3^a] + (2\Delta - n + 1)(\Delta+1)^a$ *if* $\lceil \frac{n-1}{2} \rceil \leq \Delta \leq n-1$ *and* $0 < a < 1$,

(ii) $\chi_a(T) \geq \Delta[(\Delta+2)^a + 3^a] + (n - 2\Delta - 1)4^a$ *if* $3 \leq \Delta \leq \lfloor \frac{n-1}{2} \rfloor$ *and* $0 < a < 1$,

(iii) $R_a(T) \leq \Delta[(2\Delta)^a + 2^a] + (n-2\Delta-1)4^a$ *if* $3 \leq \Delta \leq \lfloor \frac{n-1}{2} \rfloor$ *and* $-0.283 \leq a < 0$.

The equality in (i) holds if and only if T is $S^\star_{n,\Delta}$. The equalities in (ii) and (iii) hold if and only if T is in the set $X'_{n,\Delta}$.

Proof. Among trees of order n and maximum degree Δ, let T' be a tree having the smallest χ_a for $0 < a < 1$ and $3 \le \Delta \le n-1$ (the largest R_a for $-0.283 \le a < 0$ and $3 \le \Delta \le \frac{n-1}{2}$). Let w be a vertex of degree Δ in T'. By Lemma 2.4, every vertex different from w has degree at most 2 in T'. So, T' is in $X_{n,\Delta}$.

Claim 1. All pendant paths of T' either have length at least 2 or they have length at most 2.

Assume to the contrary that T' contains a pendant path of length 1 and a pendant path of length $p \ge 3$. We replace those two pendant paths by pendant paths of lengths 2 and $p-1$ to obtain a new tree T_1 from T'. For χ_a, we obtain

$$\chi_a(T_1) - \chi_a(T') = (\Delta+2)^a - (\Delta+1)^a + 3^a - 4^a < 0,$$

since for $0 < a < 1$, by Lemma 2.3, $(\Delta+2)^a - (\Delta+1)^a < 4^a - 3^a$. So $\chi_a(T_1) < \chi_a(T')$, a contradiction.

For R_a, we obtain

$$R_a(T_1) - R_a(T') = (2\Delta)^a - \Delta^a + 2^a - 4^a > 0,$$

since for $-0.283 \le a < 0$, by Lemma 2.5, we have $(2\Delta)^a - \Delta^a > 4^a - 2^a$. Thus $R_a(T_1) > R_a(T')$, so T' does not have the largest R_a, which is a contradiction. The proof of Claim 1 is complete.

(i) Let $\lceil \frac{n-1}{2} \rceil \le \Delta \le n-1$. Then, clearly also $\frac{n-1}{2} \le \Delta$ holds, which means that $n \le 2\Delta+1$. Then no pendant path of T' has length greater than 2 (otherwise if T' contains a pendant path of length at least 3, then by Claim 1, all the other $\Delta-1$ pendant paths have length at least 2, and then T' would have at least $2\Delta+2$ vertices which contradicts the fact that $n \le 2\Delta+1$). So, each of the Δ pendant paths has length 1 or 2.

Let k be the number of vertices of degree 2 adjacent to w. Then w is adjacent to $\Delta-k$ leaves which implies that $n = 1+2k+(\Delta-k) = 1+k+\Delta$ and consequently $k = n-\Delta-1$. So T' is $S^\star_{n,\Delta}$ and

$$\begin{aligned}\chi_a(S^\star_{n,\Delta}) &= k(\Delta+2)^a + k(2+1)^a + (\Delta-k)(\Delta+1)^a \\ &= (n-\Delta-1)[(\Delta+2)^a + 3^a] + (2\Delta-n+1)(\Delta+1)^a.\end{aligned}$$

(ii) and (iii) Let $3 \le \Delta \le \lfloor \frac{n-1}{2} \rfloor$. Then also $\Delta \le \frac{n-1}{2}$ holds, which means that $n \ge 2\Delta+1$. Then no pendant path of T' has length 1 (otherwise if T' contains a pendant path of length 1, then by Claim 1, all the other $\Delta-1$ pendant paths have length 1 or 2, and then T' would have at most 2Δ vertices which contradicts the fact that $n \ge 2\Delta+1$). So, each of the Δ pendant paths has length at least 2 which means that T' is in the set $X'_{n,\Delta}$. Note that w is adjacent to Δ vertices of degree 2, T' has Δ leaves and $n-1-2\Delta$ edges with both end vertices of degree 2. Thus

$$\chi_a(T') = \Delta[(\Delta+2)^a + 3^a] + (n-2\Delta-1)4^a$$

and

$$R_a(T') = \Delta[(2\Delta)^a + 2^a] + (n-2\Delta-1)4^a.$$

□

In Section 1, we mentioned that it was shown in [8] that $B_{n,\Delta}$ has the smallest χ_a for $a > 1$ and $\lceil \frac{n}{2} \rceil \le \Delta \le n-2$. We extend that result also for $\Delta < \lceil \frac{n}{2} \rceil$.

Theorem 2.2. *Let T be any tree of order n and maximum degree Δ, where $3 \le \Delta \le n-1$. Then for $a > 1$,*

$$\chi_a(T) \ge (\Delta-1)(\Delta+1)^a + (\Delta+2)^a + (n-\Delta-2)4^a + 3^a$$

with equality if and only if T is $B_{n,\Delta}$.

Proof. Among trees of order n and maximum degree Δ, where $3 \le \Delta \le n-1$, let T' be a tree having the smallest χ_a for $a > 1$. Let w be a vertex of degree Δ in T'. By Lemma 2.4, every vertex different from w has degree at most 2 in T'. So, T' is in $X_{n,\Delta}$. We prove that T' is $B_{n,\Delta}$.

Assume to the contrary that T' is not $B_{n,\Delta}$. It follows that T' contains (at least) two pendant paths of lengths $n_1 \ge 2$ and $n_2 \ge 2$, respectively. We replace those two pendant paths by pendant paths of lengths 1 and n_1+n_2-1 to obtain a new tree T_1 from T'. We obtain

$$\chi_a(T_1) - \chi_a(T') = (\Delta+1)^a - (\Delta+2)^a + 4^a - 3^a < 0,$$

since for $a > 1$, by Lemma 2.3, we have $4^a - 3^a < (\Delta+2)^a - (\Delta+1)^a$. So $\chi_a(T_1) < \chi_a(T')$. Thus T' does not have the smallest χ_a, a contradiction. Hence T' is $B_{n,\Delta}$ and

$$\chi_a(B_{n,\Delta}) = (\Delta-1)(\Delta+1)^a + (\Delta+2)^a + (n-\Delta-2)4^a + 3^a.$$

□

3. Conclusion

In Theorems 2.1 and 2.2, we presented lower bounds on χ_a for $0 < a < 1$ and $a > 1$, respectively. It is easy to find extremal trees for $a = 1$. By Lemma 2.4, a tree T' of order n and maximum degree Δ (where $3 \le \Delta \le n-1$) with the smallest χ_a contains only one vertex of degree greater than 2. So T' is in the set $X_{n,\Delta}$. Every tree in $X_{n,\Delta}$ has the degree sequence $(\Delta, \underbrace{2,\dots,2}_{n-\Delta-1}, \underbrace{1,\dots,1}_{\Delta})$. Thus

$$\chi_1(T') = \sum_{uv \in E(T')} [d_{T'}(u) + d_{T'}(v)]^1 = \sum_{v \in V(T')} [d_{T'}(v)]^2 = \Delta^2 + (n-\Delta-1)2^2 + \Delta \cdot 1^2 = 4n + \Delta^2 - 3\Delta - 4.$$

So, all the trees in $X_{n,\Delta}$ have the same χ_1, therefore each of them is the extremal tree with the smallest χ_1.

Let us present trees with the largest χ_1. Since $\chi_1(T) = \sum_{v \in V(T)} [d_T(v)]^2$, having two vertices with degrees x and y for $x \le y$ yields a smaller χ_1 than having two vertices with degrees $x-1$ and $y+1$ in a tree T. Therefore, among trees with given n and Δ for $\lceil \frac{n}{2} \rceil \le \Delta \le n-2$, a tree with the degree sequence

$$(\Delta, n-\Delta, \underbrace{1,\dots,1}_{n-2})$$

has the largest χ_1. The only tree with such a degree sequence is $S_{\Delta,n-\Delta}$.

For every tree of order $n \ge 3$ and maximum degree Δ, we have $2 \le \Delta \le n-1$. The only tree having maximum degree 2 is the path P_n and the only tree having maximum degree $n-1$ is the star S_n, therefore we are interested in the case $3 \le \Delta \le n-2$. Known trees with the smallest and largest χ_a and R_a are presented in Tables 1 and 2. A bold text is used for our new results. When a result holds for say $3 \le \Delta \le \lfloor \frac{n-1}{2} \rfloor$, we do not mention the lower bound on Δ in our tables, because that bound is obvious. Similarly, if an upper bound on Δ is $n-2$ or $n-1$, we again do not mention it in the tables.

a	trees with the smallest χ_a	trees with the largest χ_a
$(-\infty, 0)$	tree $S_{\Delta,n-\Delta}$ if $\lceil \frac{n}{2} \rceil \le \Delta$	set $X'_{n,\Delta}$ if $-1.703 \le a < 0$ and $\Delta \le \lfloor \frac{n-1}{2} \rfloor$ tree $S^\star_{n,\Delta}$ if $\lceil \frac{n}{2} \rceil \le \Delta$
$(0, 1)$	**set $\boldsymbol{X'_{n,\Delta}}$ if $\boldsymbol{\Delta \le \lfloor \frac{n-1}{2} \rfloor}$** **tree $\boldsymbol{S^\star_{n,\Delta}}$ if $\boldsymbol{\lceil \frac{n-1}{2} \rceil \le \Delta}$**	
$\{1\}$	**set $\boldsymbol{X_{n,\Delta}}$**	**tree $\boldsymbol{S_{\Delta,n-\Delta}}$ if $\boldsymbol{\lceil \frac{n}{2} \rceil \le \Delta}$**
$(1, \infty)$	**tree $\boldsymbol{B_{n,\Delta}}$**	tree $S_{\Delta,n-\Delta}$ if $\lceil \frac{n}{2} \rceil \le \Delta$

Table 1: Trees having the smallest and largest χ_a among trees of order n and maximum degree Δ for different intervals.

a	trees with the smallest R_a	trees with the largest R_a
$(-\infty, 0)$	tree $S_{\Delta,n-\Delta}$ if $\lceil \frac{n}{2} \rceil \le \Delta$	**set $\boldsymbol{X'_{n,\Delta}}$ if $\boldsymbol{-0.283 \le a < 0}$ and $\boldsymbol{\Delta \le \lfloor \frac{n-1}{2} \rfloor}$** tree $S^\star_{n,\Delta}$ if $\lceil \frac{n-1}{2} \rceil \le \Delta$
$(0, 1)$	tree $B_{n,\Delta}$	
$[1, \infty)$	tree $B_{n,\Delta}$	tree $S_{\Delta,n-\Delta}$ if $\lceil \frac{n}{2} \rceil \le \Delta$

Table 2: Trees having the smallest and largest R_a among trees of order n and maximum degree Δ for different intervals.

It is interesting that in some cases there is only one tree having the extremal index, and in some cases there is a set of trees having the extremal index. To make this clearer, we included the words "tree" and "set" in the tables. Another interesting observation is that $B_{n,\Delta}$ has the smallest R_a for every $a > 0$. On the other hand, our results on χ_a show that there are several different trees having the smallest R_a in that interval $(0, \infty)$.

In Table 1, we can see that any tree in $X'_{n,\Delta}$ has the smallest χ_a if $\Delta \le \lfloor \frac{n-1}{2} \rfloor$, and $S^\star_{n,\Delta}$ has the smallest χ_a if $\lceil \frac{n-1}{2} \rceil \le \Delta$. So, both results hold for $\Delta = \frac{n-1}{2}$. It follows that if n is odd, then the only tree in $X'_{n,\frac{n-1}{2}}$ is $S^\star_{n,\frac{n-1}{2}}$.

Let us note that the value $a = 0$ is not included in Tables 1 and 2, because trivially for every tree T, we have

$$\chi_0(T) = \sum_{uv \in E(T)} [d_T(u) + d_T(v)]^0 = \sum_{uv \in E(T)} 1 = |E(T)| = n - 1$$

and

$$R_0(T) = \sum_{uv \in E(T)} [d_T(u)\, d_T(v)]^0 = n - 1.$$

So, it remains to solve the cases included in Problems 3.1 and 3.2.

Problem 3.1. *Among trees of order n and maximum degree Δ, find trees having the smallest χ_a for*

- $a < 0$ *and* $\Delta \leq \lfloor \frac{n-1}{2} \rfloor$,

and trees having the largest χ_a for

- $a < -1.703$ *and* $\Delta \leq \lfloor \frac{n-1}{2} \rfloor$,
- $0 < a < 1$,
- $a \geq 1$ *and* $\Delta \leq \lfloor \frac{n-1}{2} \rfloor$.

Problem 3.2. *Among trees of order n and maximum degree Δ, find trees having the smallest R_a for*

- $a < 0$ *and* $\Delta \leq \lfloor \frac{n-1}{2} \rfloor$,

and trees having the largest R_a for

- $a < -0.283$ *and* $\Delta \leq \lfloor \frac{n-1}{2} \rfloor$,
- $0 < a < 1$,
- $a \geq 1$ *and* $\Delta \leq \lfloor \frac{n-1}{2} \rfloor$.

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