ROMANIAN JOURNAL OF INFORMATION SCIENCE AND TECHNOLOGY
Volume **16**, Number 4, 2013, 351–364

Ordering Trees by Sum-Connectivity Indices

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Abstract. The sum-connectivity index of graph G is defined as the sum of the weights of the edges of G, where the weight of an edge uv of G is $(d_G(u)+d_G(v))^{-\frac{1}{2}}$ with $d_G(u)$ being the degree of vertex u in G. We determine the n-vertex trees with the fourth for $n \geq 7$, the fifth for $n \geq 10$, the sixth, and the seventh for $n \geq 11$ maximum sum-connectivity indices, and the n-vertex trees with the fourth, the fifth, the sixth, and the seventh for $n \geq 8$, and the eighth for $n \geq 13$ minimum sum-connectivity indices.

1. Introduction

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. For $u \in V(G)$, let $d_G(u)$ or $d(u)$ denote the degree of u in G. The Randić connectivity index (or product-connectivity index) of G is defined as [4]

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u)d_G(v)}}.$$

The Randić connectivity index is one of the most successful molecular descriptors in structure-property and structure-activity relationships studies, see [4, 5, 6].

A variant of Randić connectivity index is the sum-connectivity index. For a graph G, it is defined as [10]

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u)+d_G(v)}}.$$

The use of sum-connectivity index in structure-property and structure-activity relationships studies has been investigated in [2, 3, 7]. Some mathematical properties of the sum-connectivity index have also been established, see [1, 8, 9, 10] and the survey [3]. In particular, the trees with the first three minimum and maximum sum-connectivity indices were determined in [10].

In this paper, we determine the n-vertex trees with the fourth for $n \geq 7$, the fifth for $n \geq 10$, the sixth, and the seventh for $n \geq 11$ maximum sum-connectivity indices, and the n-vertex trees with the fourth, the fifth, the sixth, and the seventh for $n \geq 8$, and the eighth for $n \geq 13$ minimum sum-connectivity indices.

2. Lemmas

A path $u_1u_2\dots u_r$ in a graph G is said to be a pendant path at u_1 if $d_G(u_1) \geq 3, d_G(u_i) = 2$ for $i = 2, \dots, r-1$, and $d_G(u_r) = 1$. Let $N_G(u)$ be the set of neighbors of vertex u in G.

We need some lemmas that will be used later.

Lemma 1. *[10] Let Q be a connected graph with at least two vertices. For integers a, b with $a \geq b \geq 1$, let G_1 be the graph obtained from Q by attaching two paths P_a and P_b to $u \in V(Q)$, G_2 be the graph obtained from Q by attaching a path P_{a+b} to $u \in V(Q)$, then $\chi(G_2) > \chi(G_1)$.*

Lemma 2. *For $n \geq 6$, let T be an n-vertex tree with exactly five pendant paths, then*

$$\chi(T) \leq \frac{n-13}{2} + \frac{2}{\sqrt{6}} + \frac{5}{\sqrt{3}} + \sqrt{5}.$$

Proof. Denote by Δ the maximum degree of T. Clearly, $\Delta = 3, 4, 5$. Let $\phi(n) = \frac{n-13}{2} + \frac{2}{\sqrt{6}} + \frac{5}{\sqrt{3}} + \sqrt{5}$.

Case 1. $\Delta = 5$. Obviously, T is a tree obtained by attaching five paths to a single vertex. Denote by s the number of pendant paths of length one in T. Note that $\frac{1}{\sqrt{6}} + \frac{1}{2} - \frac{1}{\sqrt{7}} - \frac{1}{\sqrt{3}} < 0$. Then

$$\begin{aligned}
\chi(T) &= \frac{s}{\sqrt{6}} + (5-s)\left(\frac{1}{\sqrt{7}} + \frac{1}{\sqrt{3}}\right) + \frac{n-1-5-(5-s)}{2} \\
&= \left(\frac{1}{\sqrt{6}} + \frac{1}{2} - \frac{1}{\sqrt{7}} - \frac{1}{\sqrt{3}}\right)s + \frac{n-11}{2} + \frac{5}{\sqrt{7}} + \frac{5}{\sqrt{3}} \\
&\leq \frac{n-11}{2} + \frac{5}{\sqrt{7}} + \frac{5}{\sqrt{3}} \\
&< \phi(n).
\end{aligned}$$

Case 2. $\Delta = 4$. Then T is a tree obtained by attaching two and three paths to the two end vertices say u and v of a path, respectively. Denote by s_1 (s_2, respectively) the number of pendant paths of length one at u (v, respectively). Note that $\frac{1}{\sqrt{5}} + \frac{1}{2} - \frac{1}{\sqrt{6}} - \frac{1}{\sqrt{3}} < 0$ and $1 - \frac{1}{\sqrt{5}} - \frac{1}{\sqrt{3}} < 0$. If $uv \in E(T)$, then $n \geq 7$ and

$$\begin{aligned}
\chi(T) &= \frac{s_1}{2} + (2-s_1)\left(\frac{1}{\sqrt{5}} + \frac{1}{\sqrt{3}}\right) + \frac{1}{\sqrt{7}} + \frac{s_2}{\sqrt{5}} + (3-s_2)\left(\frac{1}{\sqrt{6}} + \frac{1}{\sqrt{3}}\right) \\
&\quad + \frac{n-1-2-(2-s_1)-1-3-(3-s_2)}{2} \\
&= \left(1 - \frac{1}{\sqrt{5}} - \frac{1}{\sqrt{3}}\right) s_1 + \left(\frac{1}{\sqrt{5}} + \frac{1}{2} - \frac{1}{\sqrt{6}} - \frac{1}{\sqrt{3}}\right) s_2 \\
&\quad + \frac{n-12}{2} + \frac{1}{\sqrt{7}} + \frac{3}{\sqrt{6}} + \frac{2}{\sqrt{5}} + \frac{5}{\sqrt{3}} \\
&\leq \frac{n-12}{2} + \frac{1}{\sqrt{7}} + \frac{3}{\sqrt{6}} + \frac{2}{\sqrt{5}} + \frac{5}{\sqrt{3}} < \phi(n),
\end{aligned}$$

and if $uv \notin E(T)$, then $n \geq 8$ and

$$\begin{aligned}
\chi(T) &= \frac{s_1}{2} + (2-s_1)\left(\frac{1}{\sqrt{5}} + \frac{1}{\sqrt{3}}\right) + \frac{1}{\sqrt{5}} + \frac{1}{\sqrt{6}} + \frac{s_2}{\sqrt{5}} \\
&\quad + (3-s_2)\left(\frac{1}{\sqrt{6}} + \frac{1}{\sqrt{3}}\right) + \frac{n-1-2-(2-s_1)-2-3-(3-s_2)}{2} \\
&= \left(1 - \frac{1}{\sqrt{5}} - \frac{1}{\sqrt{3}}\right) s_1 + \left(\frac{1}{\sqrt{5}} + \frac{1}{2} - \frac{1}{\sqrt{6}} - \frac{1}{\sqrt{3}}\right) s_2 \\
&\quad + \frac{n-13}{2} + \frac{4}{\sqrt{6}} + \frac{3}{\sqrt{5}} + \frac{5}{\sqrt{3}} \\
&\leq \frac{n-13}{2} + \frac{4}{\sqrt{6}} + \frac{3}{\sqrt{5}} + \frac{5}{\sqrt{3}} < \phi(n).
\end{aligned}$$

Case 3. $\Delta = 3$. Then there are exactly three vertices say u_1, u_2 and u_3 with maximum degree three in T. Suppose without loss of generality that u_2 lies in the path from u_1 to u_3. Denote by t_i the number of pendant paths of length one at u_i, where $i = 1, 2, 3$. Note that $1 - \frac{1}{\sqrt{5}} - \frac{1}{\sqrt{3}} < 0$. If u_1u_2, $u_2u_3 \in E(T)$, then $n \geq 8$ and

$$\begin{aligned}
\chi(T) &= \frac{t_1}{2} + (2-t_1)\left(\frac{1}{\sqrt{5}} + \frac{1}{\sqrt{3}}\right) + \frac{1}{\sqrt{6}} + \frac{t_2}{2} + (1-t_2)\left(\frac{1}{\sqrt{5}} + \frac{1}{\sqrt{3}}\right) \\
&\quad + \frac{1}{\sqrt{6}} + \frac{t_3}{2} + (2-t_3)\left(\frac{1}{\sqrt{5}} + \frac{1}{\sqrt{3}}\right) \\
&\quad + \frac{n-1-2-(2-t_1)-1-1-(1-t_2)-1-2-(2-t_3)}{2} \\
&= \left(1 - \frac{1}{\sqrt{5}} - \frac{1}{\sqrt{3}}\right)(t_1+t_2+t_3) \\
&\quad + \frac{n-13}{2} + \frac{2}{\sqrt{6}} + \frac{5}{\sqrt{3}} + \sqrt{5}
\end{aligned}$$

$$\leq \quad \frac{n-13}{2}+\frac{2}{\sqrt{6}}+\frac{5}{\sqrt{3}}+\sqrt{5}=\phi(n),$$

if $u_1u_2 \in E(T)$ and $u_2u_3 \notin E(T)$, or if $u_1u_2 \notin E(T)$ and $u_2u_3 \in E(T)$, then $n \geq 9$ and

$$\begin{aligned}
\chi(T) &= \frac{t_1}{2}+(2-t_1)\left(\frac{1}{\sqrt{5}}+\frac{1}{\sqrt{3}}\right)+\frac{2}{\sqrt{5}}+\frac{t_2}{2}+(1-t_2)\left(\frac{1}{\sqrt{5}}+\frac{1}{\sqrt{3}}\right)\\
&\quad +\frac{1}{\sqrt{6}}+\frac{t_3}{2}+(2-t_3)\left(\frac{1}{\sqrt{5}}+\frac{1}{\sqrt{3}}\right)\\
&\quad +\frac{n-1-2-(2-t_1)-2-1-(1-t_2)-1-2-(2-t_3)}{2}\\
&= \left(1-\frac{1}{\sqrt{5}}-\frac{1}{\sqrt{3}}\right)(t_1+t_2+t_3)\\
&\quad +\frac{n-14}{2}+\frac{1}{\sqrt{6}}+\frac{7}{\sqrt{5}}+\frac{5}{\sqrt{3}}\\
&\leq \frac{n-14}{2}+\frac{1}{\sqrt{6}}+\frac{7}{\sqrt{5}}+\frac{5}{\sqrt{3}}<\phi(n),
\end{aligned}$$

and if u_1u_2, $u_2u_3 \notin E(T)$, then $n \geq 10$ and

$$\begin{aligned}
\chi(T) &= \frac{t_1}{2}+(2-t_1)\left(\frac{1}{\sqrt{5}}+\frac{1}{\sqrt{3}}\right)+\frac{2}{\sqrt{5}}+\frac{t_2}{2}+(1-t_2)\left(\frac{1}{\sqrt{5}}+\frac{1}{\sqrt{3}}\right)\\
&\quad +\frac{2}{\sqrt{5}}+\frac{t_3}{2}+(2-t_3)\left(\frac{1}{\sqrt{5}}+\frac{1}{\sqrt{3}}\right)\\
&\quad +\frac{n-1-2-(2-t_1)-2-1-(1-t_2)-2-2-(2-t_3)}{2}\\
&= \left(1-\frac{1}{\sqrt{5}}-\frac{1}{\sqrt{3}}\right)(t_1+t_2+t_3)\\
&\quad +\frac{n-15}{2}+\frac{9}{\sqrt{5}}+\frac{5}{\sqrt{3}}\\
&\leq \frac{n-15}{2}+\frac{9}{\sqrt{5}}+\frac{5}{\sqrt{3}}<\phi(n).
\end{aligned}$$

The result follows by combining Cases 1–3. □

3. The trees with large sum-connectivity indices

The trees with the first three maximum sum-connectivity indices have been determined in [10].

Lemma 3. *[10] Among the trees with n vertices,*

(i) for $n \geq 4$, P_n is the unique tree with the maximum sum-connectivity index, which is equal to $\frac{n-3}{2}+\frac{2}{\sqrt{3}}$*;*

(ii) for $n \geq 7$, the trees with a single vertex of maximum degree three, each of which is adjacent to three vertices of degree two and without vertices of degree at least four are the unique trees with the second maximum sum-connectivity index, which is equal to $\frac{n-7}{2} + \frac{3}{\sqrt{5}} + \sqrt{3}$*;*

(iii) for $n \geq 7$, the trees with a single vertex of maximum degree three, adjacent to two vertices of degree two and one vertex of degree one, and without vertices of degree at least four are the unique trees with the third maximum sum-connectivity index, which is equal to $\frac{n-5}{2} + \frac{2}{\sqrt{5}} + \frac{2}{\sqrt{3}}$*.*

Now we extend the above results to determine the trees with the fourth, the fifth, the sixth and the seventh maximum sum-connectivity indices.

Theorem 1. *Among the trees with n vertices,*

(i) for $n \geq 7$, the trees with a single vertex of maximum degree three, adjacent to one vertex of degree two and two vertices of degree one are the trees with the fourth maximum sum-connectivity index, which is equal to $\frac{n-3}{2} + \frac{1}{\sqrt{5}} + \frac{1}{\sqrt{3}}$*;*

(ii) for $n \geq 10$, the trees with exactly two adjacent vertices of maximum degree three, each of which is adjacent to two vertices of degree two are the trees with the fifth maximum sum-connectivity index, which is equal to $\frac{n-10}{2} + \frac{1}{\sqrt{6}} + \frac{4}{\sqrt{5}} + \frac{4}{\sqrt{3}}$*;*

(iii) for $n \geq 11$, the trees with exactly two nonadjacent vertices of maximum degree three, each of which is adjacent to three vertices of degree two are the trees with the sixth maximum sum-connectivity index, which is equal to $\frac{n-11}{2} + \frac{6}{\sqrt{5}} + \frac{4}{\sqrt{3}}$*;*

(iv) for $n \geq 11$, the trees with exactly two adjacent vertices of maximum degree three, one of which is adjacent to two vertices of degree two, and the other one is adjacent to one vertex of degree two and one vertex of degree one are the trees with the seventh maximum sum-connectivity index, which is equal to $\frac{n-8}{2} + \frac{1}{\sqrt{6}} + \frac{3}{\sqrt{5}} + \sqrt{3}$*.*

Proof. Let T be an n-vertex tree different from the trees with the first three maximum sum-connectivity indices as shown in Lemma 3, where $n \geq 7$. Let $\varphi(n) = \frac{n-8}{2} + \frac{1}{\sqrt{6}} + \frac{3}{\sqrt{5}} + \sqrt{3}$.

Case 1. There are at least five pendant paths in T. By Lemmas 1 and 2, $\chi(T) \leq \leq \frac{n-13}{2} + \frac{2}{\sqrt{6}} + \frac{5}{\sqrt{3}} + \sqrt{5} < \varphi(n)$.

Case 2. There are exactly three pendant paths in T. Then T is a tree with a single vertex of maximum degree three, each is adjacent to one vertex of degree two and two vertices of degree one, whose sum-connectivity index is equal to $\frac{n-3}{2} + \frac{1}{\sqrt{5}} + \frac{1}{\sqrt{3}} > \varphi(n)$.

Case 3. There are exactly four pendant paths in T. Denote by q the number of pendant paths of the length at least two in T. If there is a single vertex of degree four in T, then T is a tree obtained by attaching q paths with at least two vertices and $4-q$ pendant vertices to a single vertex, and thus

$$\begin{aligned}\chi(T) &= \left(\frac{1}{\sqrt{6}}+\frac{1}{\sqrt{3}}\right)q+\frac{4-q}{\sqrt{5}}+\frac{n-1-2q-(4-q)}{2}\\ &< \frac{n-5}{2}+\frac{4}{\sqrt{5}}+0.04q\\ &\le \frac{n-5}{2}+\frac{4}{\sqrt{5}}+0.04\times 4\\ &< \varphi(n).\end{aligned}$$

Suppose that there are exactly two vertices, say u, v, of maximum degree three in T.

Case 3.1. $uv \in E(T)$. Then

$$\begin{aligned}\chi(T) &= \left(\frac{1}{\sqrt{5}}+\frac{1}{\sqrt{3}}\right)q+\frac{4-q}{2}+\frac{1}{\sqrt{6}}+\frac{n-1-2q-(4-q)-1}{2}\\ &= \frac{n-2}{2}+\frac{1}{\sqrt{6}}+\left(\frac{1}{\sqrt{5}}+\frac{1}{\sqrt{3}}-1\right)q.\end{aligned}$$

If $q = 1, 2$, then

$$\begin{aligned}\chi(T) &= \frac{n-2}{2}+\frac{1}{\sqrt{6}}+\left(\frac{1}{\sqrt{5}}+\frac{1}{\sqrt{3}}-1\right)q\\ &< \frac{n-2}{2}+\frac{1}{\sqrt{6}}+0.025q\\ &\le \frac{n-2}{2}+\frac{1}{\sqrt{6}}+0.025\times 2\\ &< \varphi(n).\end{aligned}$$

If $q = 4$, then $n \ge 10$ and $\chi(T) = \frac{n-10}{2}+\frac{1}{\sqrt{6}}+\frac{4}{\sqrt{5}}+\frac{4}{\sqrt{3}} > \varphi(n)$. If $q = 3$, then $n \ge 9$ and $\chi(T) = \frac{n-8}{2}+\frac{1}{\sqrt{6}}+\frac{3}{\sqrt{5}}+\sqrt{3} = \varphi(n)$.

Case 3.2. $uv \notin E(T)$. Then

$$\begin{aligned}\chi(T) &= \left(\frac{1}{\sqrt{5}}+\frac{1}{\sqrt{3}}\right)q+\frac{4-q}{2}+\frac{2}{\sqrt{5}}+\frac{n-1-2q-(4-q)-2}{2}\\ &= \frac{n-3}{2}+\frac{2}{\sqrt{5}}+\left(\frac{1}{\sqrt{5}}+\frac{1}{\sqrt{3}}-1\right)q.\end{aligned}$$

If $q = 1, 2, 3$, then

$$\chi(T) = \frac{n-3}{2}+\frac{2}{\sqrt{5}}+\left(\frac{1}{\sqrt{5}}+\frac{1}{\sqrt{3}}-1\right)q$$

$$
\begin{aligned}
&< \frac{n-3}{2} + \frac{2}{\sqrt{5}} + 0.025q \\
&\le \frac{n-3}{2} + \frac{2}{\sqrt{5}} + 0.025 \times 3 \\
&< \varphi(n).
\end{aligned}
$$

If $q = 4$, then $n \ge 11$ and $\chi(T) = \frac{n-11}{2} + \frac{6}{\sqrt{5}} + \frac{4}{\sqrt{3}} > \varphi(n)$.

By combining Cases 1–3, if $\chi(T) \ge \varphi(n)$, then $\chi(T)$ can only be $\frac{n-3}{2} + \frac{1}{\sqrt{5}} + \frac{1}{\sqrt{3}}$ for $n \ge 7$, $\frac{n-10}{2} + \frac{1}{\sqrt{6}} + \frac{4}{\sqrt{5}} + \frac{4}{\sqrt{3}}$ for $n \ge 10$, $\frac{n-11}{2} + \frac{6}{\sqrt{5}} + \frac{4}{\sqrt{3}}$ for $n \ge 9$, and $\varphi(n) = \frac{n-8}{2} + \frac{1}{\sqrt{6}} + \frac{3}{\sqrt{5}} + \sqrt{3}$ for $n \ge 11$. It is easily checked that

$$
\begin{aligned}
\frac{n-3}{2} + \frac{1}{\sqrt{5}} + \frac{1}{\sqrt{3}} &> \frac{n-10}{2} + \frac{1}{\sqrt{6}} + \frac{4}{\sqrt{5}} + \frac{4}{\sqrt{3}} \\
&> \frac{n-11}{2} + \frac{6}{\sqrt{5}} + \frac{4}{\sqrt{3}} \\
&> \frac{n-8}{2} + \frac{1}{\sqrt{6}} + \frac{3}{\sqrt{5}} + \sqrt{3}.
\end{aligned}
$$

Now the result follows from Lemma 3. □

4. The trees with small sum-connectivity indices

First we present the following transformation.

Lemma 4. *Let H be a connected graph with $u, v \in V(H)$ such that $d_H(u) = d_H(v) = t \ge 1$. Let $H_{a,b}$ be the graph obtained from H by attaching a and b pendant vertices to u and v, respectively. Let $r = \max\{d_H(w) : w \in N_H(u)\}$, and $s = \min\{d_H(w) : w \in N_H(v)\}$. If $r \le s$ and $a \ge b \ge 1$, then $\chi(H_{a+1,b-1}) < \chi(H_{a,b})$.*

Proof. It is easily seen that

$$
\begin{aligned}
&\chi(H_{a+1,b-1}) - \chi(H_{a,b}) = \\
= \; & \frac{a+1}{\sqrt{a+t+2}} - \frac{a}{\sqrt{a+t+1}} + \frac{b-1}{\sqrt{b+t}} - \frac{b}{\sqrt{b+t+1}} \\
& + \sum_{w \in N_G(u)} \left(\frac{1}{\sqrt{d_H(w)+a+t+1}} - \frac{1}{\sqrt{d_H(w)+a+t}} \right) \\
& + \sum_{w \in N_G(v)} \left(\frac{1}{\sqrt{d_H(w)+b+t-1}} - \frac{1}{\sqrt{d_H(w)+b+t}} \right)
\end{aligned}
$$

$$
\begin{aligned}
\leq\ & \frac{a+1}{\sqrt{a+t+2}} - \frac{a}{\sqrt{a+t+1}} + \frac{b-1}{\sqrt{b+t}} - \frac{b}{\sqrt{b+t+1}} \\
& + t\left(\frac{1}{\sqrt{a+t+r+1}} - \frac{1}{\sqrt{a+t+r}}\right) \\
& + t\left(\frac{1}{\sqrt{b+t+s-1}} - \frac{1}{\sqrt{b+t+s}}\right).
\end{aligned}
$$

For fixed $t \geq 1$, let $f(x,y) = \dfrac{x}{\sqrt{x+t+1}} + \dfrac{t}{\sqrt{x+t+y}}$, where $x \geq 1, y \geq 1$. Then

$$
\frac{\partial^2 f(x,y)}{\partial x^2} = -(\frac{x}{4}+t+1)(x+t+1)^{-\frac{5}{2}} + \frac{3t}{4}(x+t+y)^{-\frac{5}{2}} < 0,
$$

and

$$
\frac{\partial^2 f(x,y)}{\partial x \partial y} = \frac{3}{4} t (x+t+y)^{-\frac{5}{2}} > 0.
$$

Thus $\dfrac{\partial f(x,y)}{\partial x}$ is strictly decreasing for $x \geq 1$, and strictly increasing for $y \geq 1$. Now by Lagrange's Mean Value Theorem, for some $a_1 \in (a, a+1)$ and $b_1 \in (b-1, b)$,

$$
\begin{aligned}
& \chi(H_{a+1,b-1}) - \chi(H_{a,b}) \\
\leq\ & (f(a+1,r) - f(a,r)) - (f(b,s) - f(b-1,s)) \\
=\ & \left.\frac{\partial f(x,r)}{\partial x}\right|_{x=a_1} - \left.\frac{\partial f(x,s)}{\partial x}\right|_{x=b_1} \\
\leq\ & \left.\frac{\partial f(x,s)}{\partial x}\right|_{x=a_1} - \left.\frac{\partial f(x,s)}{\partial x}\right|_{x=b_1} < 0,
\end{aligned}
$$

from which we have $\chi(H_{a+1,b-1}) < \chi(H_{a,b})$. □

Let $T_n(n_1, n_2, n_3)$ be the n-vertex tree obtained from $P_5 = v_0v_1v_2v_3v_4$ by attaching n_i pendant vertices to v_i for $i = 1, 2, 3$, where $n_1 + n_2 + n_3 - 5$, $n_1 \geq n_3 \geq 0$, $n_2 \geq 0$.

Lemma 5. *Let $T = T_n(n_1, n_2, n_3)$, where $n_1 + n_2 + n_3 - 5$, $n_1 \geq n_3 \geq 0$, $n_2 \geq 0$ and $n \geq 7$. If $(n_1, n_2, n_3) \neq (n-5, 0, 0), (0, n-5, 0), (n-6, 0, 1)$, then $\chi(T) > \chi(T_n(n-6, 0, 1))$.*

Proof. By Lemma 4, if $n_2 = 0$, then $\chi(T) > \chi(T_n(n-6,0,1))$, and if $n_2 \geq 1$, then

$$
\chi(T) \geq \chi(T_n(n_1+n_3, n_2, 0)) \geq \begin{cases} \chi(T_n(n-6,1,0)) & \text{for } n_1+n_3 \geq n_2, \\ \chi(T_n(1,n-6,0)) & \text{for } n_1+n_3 < n_2. \end{cases}
$$

By direct calculation,

$$
\begin{aligned}
& \chi(T_n(n-6,1,0)) - \chi(T_n(n-6,0,1)) \\
=\ & \left(\frac{n-5}{\sqrt{n-3}} + \frac{1}{\sqrt{n-1}} + \frac{1}{\sqrt{5}} + \frac{1}{2} + \frac{1}{\sqrt{3}}\right)
\end{aligned}
$$

$$
\begin{aligned}
& -\left(\frac{n-5}{\sqrt{n-3}}+\frac{1}{\sqrt{n-2}}+\frac{1}{\sqrt{5}}+1\right) \\
= & \frac{1}{\sqrt{n-1}}-\frac{1}{\sqrt{n-2}}+\frac{1}{\sqrt{3}}-\frac{1}{2}>0
\end{aligned}
$$

and

$$
\begin{aligned}
& \chi(T_n(1,n-6,0))-\chi(T_n(n-6,0,1)) \\
= & \left(\frac{n-6}{\sqrt{n-3}}+\frac{1}{\sqrt{n-2}}+\frac{1}{\sqrt{n-1}}+1+\frac{1}{\sqrt{3}}\right) \\
& -\left(\frac{n-5}{\sqrt{n-3}}+\frac{1}{\sqrt{n-2}}+\frac{1}{\sqrt{5}}+1\right) \\
= & -\frac{1}{\sqrt{n-3}}+\frac{1}{\sqrt{n-1}}+\frac{1}{\sqrt{3}}-\frac{1}{\sqrt{5}}>0.
\end{aligned}
$$

Then the result follows easily. □

Lemma 6. *For $x \geq 6$, let*

$$
\begin{aligned}
f_1(x) &= \frac{x-6}{\sqrt{x-4}}-\frac{x-5}{\sqrt{x-3}}-\frac{1}{\sqrt{x-2}}+\frac{1}{\sqrt{x}}, \\
f_2(x) &= \frac{x-5}{\sqrt{x-3}}-\frac{x-6}{\sqrt{x-2}}-\frac{2}{\sqrt{x-1}}, \\
f_3(x) &= \frac{x-5}{\sqrt{x-3}}-\frac{x-4}{\sqrt{x-2}}-\frac{1}{\sqrt{x-1}}+\frac{1}{\sqrt{x}}, \\
f_4(x) &= \frac{x-5}{\sqrt{x-3}}-\frac{x-5}{\sqrt{x-2}}-\frac{2}{\sqrt{x-1}}+\frac{1}{\sqrt{x}}.
\end{aligned}
$$

Then $f_i(x)$ is strictly increasing for all $i = 1, 2, 3, 4$.

Proof. We only show that $f_1(x)$ is increasing for $x \geq 6$. The proof for the other three cases is similar.

Let $g_1(x) = \frac{x-6}{\sqrt{x-4}} - \frac{1}{\sqrt{x-2}} - \frac{1}{\sqrt{x-1}}$. Then $g_1''(x) = -\frac{x+2}{4}(x-4)^{-\frac{5}{2}} - \frac{3}{4}(x-2)^{-\frac{5}{2}} - \frac{3}{4}(x-1)^{-\frac{5}{2}} < 0$, and thus $g_1^{'}(x)$ is strictly decreasing for $x \geq 6$. It is easily checked that $f_1(x) = g_1(x) - g_1(x+1)$. Now we have $f_1'(x) = g_1'(x) - g_1'(x+1) > 0$, i.e., $f_1(x)$ is strictly increasing for $x \geq 6$. □

Let $S_{n,p}$ be the n-vertex tree formed by attaching $p-1$ pendant vertices to an end vertex of the path P_{n-p+1}.

Lemma 7. *[10] Let T be a tree with n vertices and p pendant vertices, where $3 \leq p \leq n-2$. Then*

$$
\chi(T) \geq \frac{1}{\sqrt{p+2}} + \frac{p-1}{\sqrt{p+1}} + \frac{1}{\sqrt{3}} + \frac{n-p-2}{2}
$$

with equality if and only if $T \cong S_{n,p}$.

Lemma 8. *[1] Let G be a connected graph with $uv \in E(G)$, where $d_G(u)$, $d_G(v) \geq 2$, and u and v have no common neighbor in G. Let G_1 be the graph obtained from G by deleting the edge uv, identifying u and v, which is denoted by w, and attaching a pendent vertex to w. Then $\chi(G) > \chi(G_1)$.*

Let $T_{n,a}$ be the n-vertex tree obtained by attaching a and $n-a-2$ pendant vertices to the two vertices of an edge, respectively, where $a \geq n-a-2$, i.e., $\lceil (n-2)/2 \rceil \leq a \leq n-3$.

Lemma 9. *[10] $\chi(T_{n,n-3}) < \chi(T_{n,n-4}) < \ldots < \chi(T_{n,\lceil (n-2)/2 \rceil})$.*

The trees with the first three minimum sum-connectivity indices have been determined in [10].

Lemma 10. *[10] Among the trees with n vertices, for $n \geq 4$, $S_{n,n-1} \cong S_n$, and $S_{n,n-2} \cong T_{n,n-3}$ are, respectively, the unique trees with the minimum and the second minimum sum-connectivity indices, which are, respectively, equal to $\frac{n-1}{\sqrt{n}}$ and $\frac{n-3}{\sqrt{n-1}} + \frac{1}{\sqrt{n}} + \frac{1}{\sqrt{3}}$, while for $n \geq 6$, $T_{n,n-4}$ is the unique tree with the third minimum sum-connectivity index, which is equal to $\frac{n-4}{\sqrt{n-2}} + \frac{1}{\sqrt{n}} + 1$.*

Now we extend the above results to determine the trees with the fourth, the fifth, the sixth, the seventh, and the eighth minimum sum-connectivity indices.

Theorem 2. *Among the trees with n vertices, for $n \geq 6$.*

(i) For $n = 6$, $T_6(1,0,0)$, and $T_6(0,1,0)$ are respectively the unique trees with the fourth, and the fifth minimum sum-connectivity indices, which are equal to $\frac{1}{\sqrt{5}} + \frac{1}{\sqrt{3}} + \frac{3}{2}$, and $\frac{2}{\sqrt{5}} + \frac{2}{\sqrt{3}} + \frac{1}{2}$, respectively;

(ii) For $n = 7$, $T_7(2,0,0)$, $T_7(0,2,0)$, and $T_7(1,0,1)$ are respectively the unique trees with the fourth, the fifth, and the sixth minimum sum-connectivity indices, which are equal to $\frac{1}{\sqrt{6}} + \frac{3}{\sqrt{5}} + \frac{1}{2} + \frac{1}{\sqrt{3}}$, $\frac{2}{\sqrt{6}} + \frac{2}{\sqrt{5}} + \frac{2}{\sqrt{3}}$, and $\frac{2}{\sqrt{5}} + 2$, respectively;

(iii) For $n = 8, 9$, $T_{n,n-5}$, $T_n(n-5,0,0)$, $T_n(0,n-5,0)$, and $T_n(n-6,0,1)$ are respectively, the unique trees with the fourth, the fifth, the sixth and the seventh minimum sum-connectivity indices, which are equal to $\frac{n-5}{\sqrt{n-3}} + \frac{1}{\sqrt{n}} + \frac{3}{\sqrt{5}}$, $\frac{n-4}{\sqrt{n-2}} + \frac{1}{\sqrt{n-1}} + \frac{1}{2} + \frac{1}{\sqrt{3}}$, $\frac{n-5}{\sqrt{n-2}} + \frac{2}{\sqrt{n-1}} + \frac{2}{\sqrt{3}}$, and $\frac{n-5}{\sqrt{n-3}} + \frac{1}{\sqrt{n-2}} + + \frac{1}{\sqrt{5}} + 1$, respectively;

(iv) For $n = 10, 11, 12$, $T_n(n-5,0,0)$, $T_{n,n-5}$, $T_n(0,n-5,0)$, and $T_{n,n-6}$ are respectively, the unique trees with the fourth, the fifth, the sixth and the seventh minimum sum-connectivity indices, which are equal to $\frac{n-4}{\sqrt{n-2}} + \frac{1}{\sqrt{n-1}} + \frac{1}{2} + \frac{1}{\sqrt{3}}$,

$\dfrac{n-5}{\sqrt{n-3}}+\dfrac{1}{\sqrt{n}}+\dfrac{3}{\sqrt{5}}$, $\dfrac{n-5}{\sqrt{n-2}}+\dfrac{2}{\sqrt{n-1}}+\dfrac{2}{\sqrt{3}}$, *and* $\dfrac{n-6}{\sqrt{n-4}}+\dfrac{1}{\sqrt{n}}+\dfrac{4}{\sqrt{6}}$, *respectively, and* $T_{12,5}$ *is the unique tree with the eighth minimum sum-connectivity index, which is equal to* $\dfrac{1}{\sqrt{12}}+\dfrac{10}{\sqrt{7}}$*;*

(v) For $n \geq 13$, $T_n(n-5,0,0)$, $T_n(0,n-5,0)$, *and* $T_{n,n-5}$ *are respectively, the unique trees with the fourth, the fifth, the sixth minimum sum-connectivity indices, which are equal to* $\dfrac{n-4}{\sqrt{n-2}}+\dfrac{1}{\sqrt{n-1}}+\dfrac{1}{2}+\dfrac{1}{\sqrt{3}}$, $\dfrac{n-5}{\sqrt{n-2}}+\dfrac{2}{\sqrt{n-1}}+\dfrac{2}{\sqrt{3}}$, *and* $\dfrac{n-5}{\sqrt{n-3}}+\dfrac{1}{\sqrt{n}}+\dfrac{3}{\sqrt{5}}$*, respectively;*

(vi) For $n = 13, 14, 15$, $T_{n,n-6}$ *is the unique tree with the seventh minimum sum-connectivity index, which is equal to* $\dfrac{n-6}{\sqrt{n-4}}+\dfrac{1}{\sqrt{n}}+\dfrac{4}{\sqrt{6}}$, *and for* $n \geq 16$, $T_n(n-6,0,1)$ *is the unique tree with the seventh minimum sum-connectivity index, which is equal to* $\dfrac{n-5}{\sqrt{n-3}}+\dfrac{1}{\sqrt{n-2}}+\dfrac{1}{\sqrt{5}}+1$*;*

(vii) For $n = 13, 14, 15$, $T_n(n-6,0,1)$ *is the unique tree with the eighth minimum sum-connectivity index, which is equal to* $\dfrac{n-5}{\sqrt{n-3}}+\dfrac{1}{\sqrt{n-2}}+\dfrac{1}{\sqrt{5}}+1$, *and for* $n \geq 16$, $T_{n,n-6}$ *is the unique tree with the eighth minimum sum-connectivity index, which is equal to* $\dfrac{n-6}{\sqrt{n-4}}+\dfrac{1}{\sqrt{n}}+\dfrac{4}{\sqrt{6}}$.

Proof. Let T be an n-vertex tree different from the trees with the first three minimum sum-connectivity indices as shown in Lemma 10 for $n \geq 6$. Denote by p the number of pendant vertices in T. Obviously, $p \leq n-2$. Let $\psi(n) = \dfrac{n-5}{\sqrt{n-3}}+\dfrac{1}{\sqrt{n-2}}+\dfrac{1}{\sqrt{5}}+1$. Note that $\psi(n) = \chi(T_n(n-6,0,1))$ if $n \geq 7$.

Case 1. $p \leq n-4$. If $p = 2$, then by Lemma 3 (i), $\chi(T) > \psi(n)$. If $p \geq 3$, then by Lemmas 7 and 8, we have

$$\begin{aligned}\chi(T) \geq \chi(S_{n,p}) \geq \chi(S_{n,n-4}) &= \frac{n-5}{\sqrt{n-3}}+\frac{1}{\sqrt{n-2}}+\frac{1}{\sqrt{3}}+1\\ &> \psi(n).\end{aligned}$$

Case 2. $p-2$. Then $T \cong T_{n,a}$ with $\lceil (n-2)/2 \rceil \leq a \leq n-5$, notice that $n \geq 8$. For $n \geq 8$, by Lemma 8, $\chi(T_{n,n-5}) < \chi(T_n(n-6,0,1)) = \psi(n)$. If $a \leq n-6$, then $n \geq 10$ and by Lemma 9,

$$\chi(T_{n,a}) \geq \chi(T_{n,n-6}) = \frac{n-6}{\sqrt{n-4}}+\frac{1}{\sqrt{n}}+\frac{4}{\sqrt{6}}.$$

Note that

$$\chi(T_{n,n-6}) - \psi(n) =$$

$$\begin{aligned} &= \frac{n-6}{\sqrt{n-4}} + \frac{1}{\sqrt{n}} - \frac{n-5}{\sqrt{n-3}} - \frac{1}{\sqrt{n-2}} + \frac{4}{\sqrt{6}} - \frac{1}{\sqrt{5}} - 1 \\ &= f_1(n) + \frac{4}{\sqrt{6}} - \frac{1}{\sqrt{5}} - 1. \end{aligned}$$

Now by Lemma 6, $\chi(T_{n,n-6}) > \psi(n)$ for $n \geq 16$, and $\chi(T_{n,n-6}) < \psi(n)$ for $10 \leq n \leq 15$. Obviously, $\chi(T_{n,n-7}) > \chi(T_{n,n-6}) > \psi(n)$ for $n \geq 16$. Note that $\chi(T_{n,n-7}) = \frac{n-7}{\sqrt{n-5}} + \frac{1}{\sqrt{n}} + \frac{5}{\sqrt{7}}$. By direct calculation, we find that $\chi(T_{n,n-7}) < \psi(n)$ for $n = 12$ and $\chi(T_{n,n-7}) > \psi(n)$ for $n = 13, 14, 15$. It follows that $\chi(T) \leq \psi(n)$ if and only if $T \cong T_{n,n-5}$ for $n \geq 8$, $T_{n,n-6}$ for $10 \leq n \leq 15$, or $T_{n,n-7}$ for $n = 12$.

Case 3. $p - 3$. Then $T \cong T_n(n_1, n_2, n_3)$, where $n_1 + n_2 + n_3 - 5$, $n_1 \geq n_3 \geq 0$, $n_2 \geq 0$. If $(n_1, n_2, n_3) \neq (n-5, 0, 0), (0, n-5, 0), (n-6, 0, 1)$, then by Lemma 5, we have $\chi(T) > \psi(n)$. Note that

$$\begin{aligned} &\psi(n) - \chi(T_n(0, n-5, 0)) = \\ &= \frac{n-5}{\sqrt{n-3}} - \frac{n-6}{\sqrt{n-2}} - \frac{2}{\sqrt{n-1}} + \frac{1}{\sqrt{5}} + 1 - \frac{2}{\sqrt{3}} \\ &= f_2(n) + \frac{1}{\sqrt{5}} + 1 - \frac{2}{\sqrt{3}} > 0 \end{aligned}$$

and that $\chi(T_n(n-5, 0, 0)) - \chi(T_n(0, n-5, 0)) = \frac{1}{\sqrt{n-2}} - \frac{1}{\sqrt{n-1}} + \frac{1}{2} - \frac{1}{\sqrt{3}} < 0$. By Lemma 6, we have $\chi(T_n(n-5, 0, 0)) < \chi(T_n(0, n-5, 0)) < \psi(n)$ for $n \geq 6$.

By combining Cases 1–3, if $\chi(T) \leq \psi(n)$, then $T \cong T_{n,n-5}$ for $n \geq 8$, $T_{n,n-6}$ for $10 \leq n \leq 15$, $T_n(n-5, 0, 0)$ for $n \geq 6$, $T_n(0, n-5, 0)$ for $n \geq 6$, $T_n(n-6, 0, 1)$ for $n \geq 7$, and $T_{n,n-7}$ for $n = 12$. Moreover, we have $\chi(T_n(n-5, 0, 0)) < \chi(T_n(0, n-5, 0))$ for $n \geq 6$, $\chi(T_n(0, n-5, 0)) < \chi(T_n(n-6, 0, 1))$ for $n \geq 7$, $\chi(T_{n,n-6}) > \chi(T_n(n-6, 0, 1))$ for $n \geq 16$, and $\chi(T_{n,n-6}) < \chi(T_n(n-6, 0, 1))$ for $13 \leq n \leq 15$. Now (i) and (ii) follow from Lemma 10. Suppose that $n \geq 8$. Note that

$$\begin{aligned} &\chi(T_{n,n-5}) - \chi(T_n(n-5, 0, 0)) = \\ &= \frac{n-5}{\sqrt{n-3}} + \frac{1}{\sqrt{n}} - \frac{n-4}{\sqrt{n-2}} - \frac{1}{\sqrt{n-1}} + \frac{3}{\sqrt{5}} - \frac{1}{2} - \frac{1}{\sqrt{3}} \\ &= f_3(n) + \frac{3}{\sqrt{5}} - \frac{1}{2} - \frac{1}{\sqrt{3}} \end{aligned}$$

and that

$$\begin{aligned} &\chi(T_{n,n-5}) - \chi(T_n(0, n-5, 0)) = \\ &= \frac{n-5}{\sqrt{n-3}} + \frac{1}{\sqrt{n}} - \frac{n-5}{\sqrt{n-2}} - \frac{2}{\sqrt{n-1}} + \frac{3}{\sqrt{5}} - \frac{2}{\sqrt{3}} \\ &= f_4(n) + \frac{3}{\sqrt{5}} - \frac{2}{\sqrt{3}}. \end{aligned}$$

By Lemma 6, we have $\chi(T_n(n-5,0,0)) < \chi(T_{n,n-5})$ for $n \geq 10$, $\chi(T_n(n-5,0,0)) > \chi(T_{n,n-5})$ for $n = 8, 9$, $\chi(T_n(0,n-5,0)) < \chi(T_{n,n-5})$ for $n \geq 13$, and $\chi(T_n(0,n-5,0)) > \chi(T_{n,n-5})$ for $8 \leq n \leq 12$. By direct calculation, $\chi(T_n(0,n-5,0)) < \chi(T_{n,n-6})$ for $n = 10, 11, 12$. Recall that $\chi(T_{n,n-5}) < \chi(T_{n,n-6}) < \chi(T_{n,n-7})$ for $n \geq 12$. Thus, we find that:

$$\chi(T_{n,n-5}) < \chi(T_n(n-5,0,0)) < \chi(T_n(0,n-5,0)) < \chi(T_n(n-6,0,1))$$

for $n = 8, 9$;

$$\chi(T_n(n-5,0,0)) < \chi(T_{n,n-5}) < \chi(T_n(0,n-5,0)) < \chi(T_{n,n-6})$$

for $n = 10, 11$;

$$\chi(T_n(n-5,0,0)) < \chi(T_{n,n-5}) < \chi(T_n(0,n-5,0)) < \chi(T_{n,n-6}) < \chi(T_{n,n-7})$$

for $n = 12$;

$$\begin{aligned} \chi(T_n(n-5,0,0)) &< \chi(T_n(0,n-5,0)) < \chi(T_{n,n-5}) \\ &< \begin{cases} \chi(T_{n,n-6}) < \chi(T_n(n-6,0,1)) & \text{for } n = 13, 14, 15 \\ \chi(T_n(n-6,0,1)) < \chi(T_{n,n-6}) & \text{for } n \geq 16. \end{cases} \end{aligned}$$

Now the results (iii)–(vii) follow from Lemma 10. □

Acknowledgement. The second author (corresponding author) was supported the Guangdong Provincial Natural Science Foundation of China (No. S2011010005539).

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