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On the first extended zeroth-order connectivity index of trees

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Abstract

The first extended zeroth-order connectivity index of a graph G is defined as ${}^0\chi_1(G)=\sum_{v\in V(G)} D_v^{-1/2}$, where $V(G)$ is the vertex set of G, and D_v is the sum of degrees of neighbors of vertex v in G. We give a sharp lower bound for the first extended zeroth-order connectivity index of trees with given numbers of vertices and pendant vertices, and characterize the extremal trees. We also determine the *n*-vertex trees with the first three smallest first extended zeroth-order connectivity indices.

Keywords: Zeroth-order connectivity index; extended zeroth-order connectivity index; trees, pendant vertices; degree of vertices

1. Introduction

Topological indices are graph invariants used for quantitative structure-property relationship and quantitative structure-activity relationship (Trinajstić, 1992). The extended zeroth-order connectivity index belongs to the class of topological indices (Bonchev and Kier, 1992).

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. For $v\in V(G)$, $\Gamma_G(v)$ denotes the set of its (first) neighbors in G and the degree of v is $d_v=d_v(G)=|\Gamma_G(v)|$. Denote by uv or vu the edge of G connecting vertices u and v. We follow (Trinajstić, 1992; Wilson, 1972) for graph-theoretical terminology.

The zeroth-order connectivity index of a graph G is defined as (Randić, 1975; Randić, 2001)

$${}^0\chi={}^0\chi(G)=\sum_{v\in V(G)} d_v^{-1/2}.$$

It is used in (Siddhaye et al., 2004) to develop structure-based correlations for physical properties of interest in pharmaceutical chemistry: octanol-water partition coefficient, melting point and water solubility.

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For a nonnegative integer k, Bonchev and Kier (1992) proposed the *k*th extended zeroth-order connectivity index, which for a graph G is defined as

$${}^0\chi_k={}^0\chi_k(G)=\sum_{v\in V(G)}\left({}^kd_v\right)^{-1/2},$$

where ${}^0d_v=d_v$ and ${}^kd_v=\sum_{u\in\Gamma(v)} {}^{k-1}d_u$ for $k\geq 1$. Obviously, ${}^0\chi_0={}^0\chi$. Toropov et al. (1997) showed that the extended zeroth-order connectivity indices may be used for structure-property studies. We gave in (Zhou and Trinajstić, 2009) various lower and upper bounds for the first extended zeroth-order connectivity index ${}^0\chi_1$ and the first extended first-order connectivity index ${}^1\chi_1$ in terms of graph parameters such as the number of vertices, the number of edges, and the first Zagreb index.

In this paper, we establish further properties for the first extended zeroth-order connectivity index of trees. We give a sharp lower bound for the first extended zeroth-order connectivity index of trees with given numbers of vertices and pendant vertices (vertices of degree one), and characterize the extremal trees. Then we determine the *n*-vertex trees with the first three smallest first extended zeroth-order connectivity indices for $n\geq 6$.

2. Preliminaries

Let $S_{n,p}$ be the tree obtained by attaching $p-1$ pendant vertices to an end vertex of the path P_{n+1-p}, where $2 \le p \le n-1$.

Lemma 1. Let T be a tree with n vertices and p pendant vertices, where $3 \le p \le n-3$. If u is a pendant neighbor of vertex v in T, then

$$
\begin{aligned}
&{}^0\chi_1(T) - {}^0\chi_1(T-u) \\
&\ge \frac{p-2}{\sqrt{p}} - \frac{p-2}{\sqrt{p-1}} + \frac{1}{\sqrt{2+p}}
\end{aligned}
$$

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

Proof: Let r be the number of vertices of T in $\Gamma_T(v)$ of degree at least two. Obviously, $r \ge 1$. Let z be such a vertex. Let $d_w = d_w(T)$ and $\Gamma(w) = \Gamma_T(w)$ for $w \in V(T)$.

Case 1. $r = 1$. Then v has exactly $d_v - 1$ neighbors of degree one in T and thus $\sum_{w\in\Gamma(v)\setminus\{u\}} d_w \ge d_v$ with equality if and only if v has one neighbor of degree two. Moreover, since $p < n-2$, there is a vertex in $\Gamma(z)\setminus\{v\}$ of degree at least two, implying that $\sum_{t\in\Gamma(z)\setminus\{v\}} d_t \ge 2$ with equality if and only if $d_t = d_z = 2$ for the neighbor t of z different from v. It is easily seen that $\frac{1}{\sqrt{x}} - \frac{1}{\sqrt{x-1}}$ is increasing for $x > 1$. Thus

$$
\begin{aligned}
&{}^0\chi_1(T) - {}^0\chi_1(T-u) \\
&= \frac{1}{\sqrt{d_v}} + \left(\frac{1}{\sqrt{1+\sum_{w\in\Gamma(v)\setminus\{u\}} d_w}} - \frac{1}{\sqrt{\sum_{w\in\Gamma(v)\setminus\{u\}} d_w}} \right) \\
&\quad + \sum_{w\in\Gamma(v)\setminus\{u\}} \left(\frac{1}{\sqrt{d_v + \sum_{t\in\Gamma(w)\setminus\{v\}} d_t}} - \frac{1}{\sqrt{d_v - 1 + \sum_{t\in\Gamma(w)\setminus\{v\}} d_t}} \right) \\
&= \frac{1}{\sqrt{d_v}} + \left(\frac{1}{\sqrt{1+\sum_{w\in\Gamma(v)\setminus\{u\}} d_w}} - \frac{1}{\sqrt{\sum_{w\in\Gamma(v)\setminus\{u\}} d_w}} \right) \\
&\quad + (d_v - 2)\left(\frac{1}{\sqrt{d_v}} - \frac{1}{\sqrt{d_v - 1}} \right) \\
&\quad + \left(\frac{1}{\sqrt{d_v + \sum_{t\in\Gamma(z)\setminus\{v\}} d_t}} - \frac{1}{\sqrt{d_v - 1 + \sum_{t\in\Gamma(z)\setminus\{v\}} d_t}} \right) \\
&\ge \frac{1}{\sqrt{d_v}} + \left(\frac{1}{\sqrt{1+d_v}} - \frac{1}{\sqrt{d_v}} \right) \\
&\quad + (d_v - 2)\left(\frac{1}{\sqrt{d_v}} - \frac{1}{\sqrt{d_v - 1}} \right) \\
&\quad + \frac{1}{\sqrt{d_v + 2}} - \frac{1}{\sqrt{d_v - 1 + 2}} \\
&= \frac{d_v - 2}{\sqrt{d_v}} - \frac{d_v - 2}{\sqrt{d_v - 1}} + \frac{1}{\sqrt{d_v + 2}}
\end{aligned}
$$

with equality if and only if $\sum_{w\in\Gamma(v)\setminus\{u\}} d_w = d_v$ and $\sum_{t\in\Gamma(z)\setminus\{v\}} d_t = 2$, i.e., v has one neighbor of degree two, and all other neighbors have degree one, and the degree two neighbor of v has a neighbor (different from v) of degree two.

Case 2. $r \ge 2$. Then $\sum_{w\in\Gamma(v)\setminus\{u\}} d_w \ge d_v + r - 1$ and $\sum_{t\in\Gamma(z)\setminus\{v\}} d_t \ge 1$. Similarly as above, we have

$$
\begin{aligned}
&{}^0\chi_1(T) - {}^0\chi_1(T-u) \\
&= \frac{1}{\sqrt{d_v}} + \left(\frac{1}{\sqrt{1 + \sum_{w \in \Gamma(v)\backslash\{u\}} d_w}} - \frac{1}{\sqrt{\sum_{w \in \Gamma(v)\backslash\{u\}} d_w}} \right) \\
&+ \sum_{w \in \Gamma(v)\backslash\{u\}} \left(\frac{1}{\sqrt{d_v + \sum_{t \in \Gamma(w)\backslash\{v\}} d_t}} - \frac{1}{\sqrt{d_v - 1 + \sum_{t \in \Gamma(w)\backslash\{v\}} d_t}} \right) \\
&\geq \frac{1}{\sqrt{d_v}} + \left(\frac{1}{\sqrt{1 + d_v + r - 1}} - \frac{1}{\sqrt{d_v + r - 1}} \right) \\
&+ (d_v - r - 1)\left(\frac{1}{\sqrt{d_v}} - \frac{1}{\sqrt{d_v - 1}} \right) \\
&+ r\left(\frac{1}{\sqrt{d_v + 1}} - \frac{1}{\sqrt{d_v - 1 + 1}} \right).
\end{aligned}
$$

Let $m(r)$ be the right-most expression of the above inequality. Note that

$$
\begin{aligned}
&m(2) - \left(\frac{d_v - 2}{\sqrt{d_v}} - \frac{d_v - 2}{\sqrt{d_v - 1}} + \frac{1}{\sqrt{d_v + 2}} \right) \\
&= \frac{d_v - 4}{\sqrt{d_v}} - \frac{d_v - 3}{\sqrt{d_v - 1}} + \frac{1}{\sqrt{d_v + 2}} + \frac{1}{\sqrt{d_v + 1}} \\
&- \left(\frac{d_v - 2}{\sqrt{d_v}} - \frac{d_v - 2}{\sqrt{d_v - 1}} + \frac{1}{\sqrt{d_v + 2}} \right) \\
&= \frac{1}{\sqrt{d_v + 1}} + \frac{1}{\sqrt{d_v - 1}} - \frac{2}{\sqrt{d_v}} > 0
\end{aligned}
$$

and $m(r)$ is increasing for $r \geq 2$. Then

$$
\begin{aligned}
&{}^0\chi_1(T) - {}^0\chi_1(T-u) \\
&= m(r) \geq m(2) \\
&> \frac{d_v - 2}{\sqrt{d_v}} - \frac{d_v - 2}{\sqrt{d_v - 1}} + \frac{1}{\sqrt{d_v + 2}}.
\end{aligned}
$$

Combining Cases 1 and 2, we have

$$
\begin{aligned}
&{}^0\chi_1(T) - {}^0\chi_1(T-u) \\
&\geq \frac{d_v - 2}{\sqrt{d_v}} - \frac{d_v - 2}{\sqrt{d_v - 1}} + \frac{1}{\sqrt{d_v + 2}}
\end{aligned}
$$

with equality if and only if among the d_v neighbors of v, one has degree two, and others have degree one, and the degree two neighbor of v has a neighbor (different from v) of degree two. Let

$$
f(x) = \frac{x-2}{\sqrt{x}} - \frac{x-2}{\sqrt{x-1}} + \frac{1}{\sqrt{x+2}}
$$

for $x \geq 2$. Taking the derivative of $f(x)$,

$$
\begin{aligned}
f'(x) &= \frac{1}{2}(x+2)x^{-\frac{3}{2}} - \frac{1}{2}(x+2)^{-\frac{3}{2}} \\
&- \frac{x}{2}(x-1)^{-\frac{3}{2}}.
\end{aligned}
$$

Note that $(1+t)^{-\frac{3}{2}} \geq 1 - \frac{3}{2}t$ for $|t| \leq 1$. Then

$$
\begin{aligned}
&2x^{\frac{3}{2}} f'(x) \\
&= (x+2) - \left(1 + \frac{2}{x}\right)^{-\frac{3}{2}} - x\left(1 - \frac{1}{x}\right)^{-\frac{3}{2}} \\
&\leq (x+2) - \left(1 - \frac{3}{2} \cdot \frac{2}{x}\right) - x\left(1 + \frac{3}{2} \cdot \frac{1}{x}\right) \\
&= -\frac{1}{2} + \frac{3}{x} \leq 0,
\end{aligned}
$$

and thus $f(x)$ is decreasing for $x \geq 6$. By direct calculation, $f(3) > f(4) > f(5) > f(6)$. Since $d_v \leq p$, we have

$$
\begin{aligned}
&{}^0\chi_1(T) - {}^0\chi_1(T-u) \\
&\geq f(d_v) \geq f(p) \\
&= \frac{p-2}{\sqrt{p}} - \frac{p-2}{\sqrt{p-1}} + \frac{1}{\sqrt{2+p}}
\end{aligned}
$$

with equalities if and only if $d_v = p$, and v has $p-1$ pendant neighbors, i.e., $T \cong S_{n,p}$.

3. Results

Proposition 1. Let T be a tree with n vertices and p pendant vertices, where $3 \leq p \leq n-3$. Then

$$
\begin{aligned}
{}^0\chi_1(T) &\geq \frac{1}{\sqrt{p+1}} + \frac{p-1}{\sqrt{p}} + \frac{1}{\sqrt{p+2}} \\
&+ \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}} + \frac{n-p-3}{2}
\end{aligned}
$$

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

Proof: It is easy to check that the result is true for $n=6$. Suppose that $n \geq 7$ and the result is true for trees with $n-1$ vertices. Let T be a tree with n vertices and p pendant vertices, where $3 \leq p \leq n-3$. Let $d_z = d_z(T)$ and $\Gamma(z) = \Gamma_T(z)$ for $z \in V(T)$. Choose $u, v \in V(T)$ such that u is a pendant neighbor of v and d_v is as large as possible.

First suppose that $d_v = 2$. Then $p \leq \frac{n-1}{2} \leq n-4$. Let $\Gamma(v) \setminus \{u\} = \{w\}$. Then $d_w \geq 2$ and $\sum_{t \in \Gamma(w)\setminus\{v\}} d_t \geq d_w$. Thus

$$\begin{aligned}
&{}^0\chi_1(T) - {}^0\chi_1(T-u) \\
&= \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{1+d_w}} - \frac{1}{\sqrt{d_w}} \\
&\quad + \frac{1}{\sqrt{\sum_{t \in \Gamma(w)\setminus\{v\}} d_t + 2}} - \frac{1}{\sqrt{\sum_{t \in \Gamma(w)\setminus\{v\}} d_t + 1}} \\
&\geq \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{1+d_w}} - \frac{1}{\sqrt{d_w}} \\
&\quad + \frac{1}{\sqrt{d_w+2}} - \frac{1}{\sqrt{d_w+1}} \\
&\geq \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}} + \frac{1}{2} - \frac{1}{\sqrt{3}} = \frac{1}{2}.
\end{aligned}$$

Note that $T-u$ possesses p pendant vertices. By the induction hypothesis and the choice of v, we have

$$\begin{aligned}
{}^0\chi_1(T-u) > \frac{1}{\sqrt{p+1}} + \frac{p-1}{\sqrt{p}} + \frac{1}{\sqrt{p+2}} \\
+ \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}} + \frac{(n-1)-p-3}{2}
\end{aligned}$$

and then

$$\begin{aligned}
{}^0\chi_1(T) &\geq {}^0\chi_1(T-u) + \frac{1}{2} \\
&> \frac{1}{\sqrt{p+1}} + \frac{p-1}{\sqrt{p}} + \frac{1}{\sqrt{p+2}} \\
&\quad + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}} + \frac{n-p-3}{2}.
\end{aligned}$$

Next suppose that $d_v \geq 3$ and $p \geq 3$. Then $T-u$ possesses $p-1$ pendant vertices. By Lemma 1 and the induction hypothesis, we have

$$\begin{aligned}
&{}^0\chi_1(T-u) \\
&\geq \frac{1}{\sqrt{p}} + \frac{p-2}{\sqrt{p-1}} + \frac{1}{\sqrt{p+1}} + \frac{1}{\sqrt{2}} \\
&\quad + \frac{1}{\sqrt{3}} + \frac{(n-1)-(p-1)-3}{2}
\end{aligned}$$

and then

$$\begin{aligned}
&{}^0\chi_1(T) \\
&\geq {}^0\chi_1(T-u) + \frac{p-2}{\sqrt{p}} - \frac{p-2}{\sqrt{p-1}} \\
&\quad + \frac{1}{\sqrt{p+2}} \\
&\geq \frac{1}{\sqrt{p}} + \frac{p-2}{\sqrt{p-1}} + \frac{1}{\sqrt{p+1}} \\
&\quad + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}} + \frac{n-p-3}{2} \\
&\quad + \frac{p-2}{\sqrt{p}} - \frac{p-2}{\sqrt{p-1}} + \frac{1}{\sqrt{p+2}} \\
&= \frac{1}{\sqrt{p+1}} + \frac{p-1}{\sqrt{p}} + \frac{1}{\sqrt{p+2}} \\
&\quad + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}} + \frac{n-p-3}{2}
\end{aligned}$$

with equalities if and only if $T-u \cong S_{n-1,p-1}$ and $d_v = p$, i.e., $T \cong S_{n,p}$.

Let $T_{n,a}$ be the tree obtained by attaching a and $n-a-2$ pendant vertices to the two vertices of the path P_2, respectively. A tree with n vertices and $n-2$ pendant vertices is of the form $T_{n,a}$ with

$1 \le a \le \left\lfloor \frac{n-2}{2} \right\rfloor$.

Proposition 2. For $1 \le a \le \left\lfloor \frac{n-2}{2} \right\rfloor$,

$$^0\chi_1(T_{n,a}) = \frac{a}{\sqrt{a+1}} + \frac{n-2-a}{\sqrt{n-1-a}} + \frac{2}{\sqrt{n-1}}$$

and

$$^0\chi_1(T_{n,1}) < {}^0\chi_1(T_{n,2}) < \cdots < {}^0\chi_1(T_{n,\lfloor (n-2)/2 \rfloor}).$$

Proof: It is easily seen that

$$^0\chi_1(T_{n,a}) = \frac{a}{\sqrt{a+1}} + \frac{n-2-a}{\sqrt{n-1-a}} + \frac{2}{\sqrt{n-1}}.$$

Let

$$g(x) = \frac{x}{\sqrt{x+1}} + \frac{n-2-x}{\sqrt{n-1-x}} + \frac{2}{\sqrt{n-1}}$$

for $1 \le x \le \left\lfloor \frac{n-2}{2} \right\rfloor$. Taking the derivative of $g(x)$,

$$g'(x) = \frac{1}{2}(x+2)(x+1)^{-\frac{3}{2}} - \frac{1}{2}(n-x)(n-1-x)^{-\frac{3}{2}}.$$

Note that $n-1-x \ge x+1$ and $1 - \frac{1}{n-x} \ge 1 - \frac{1}{x+2}$. Then

$$(n-1-x)\left(1 - \frac{1}{n-x}\right)^2 \ge (x+1)\left(1 - \frac{1}{x+2}\right)^2,$$

from which we have $g'(x) > 0$. Thus $g(x)$ is increasing for $1 \le x \le \left\lfloor \frac{n-2}{2} \right\rfloor$. Then

$$^0\chi_1(T_{n,1}) < {}^0\chi_1(T_{n,2}) < \cdots < {}^0\chi_1(T_{n,\lfloor (n-2)/2 \rfloor}),$$

as desired.

By Propositions 1 and 2, we have

Theorem 1. Let T be a tree with n vertices and p pendant vertices, where $3 \le p \le n-2$. Then

$$^0\chi_1(T) \ge \begin{cases} \frac{1}{\sqrt{p+1}} + \frac{p-1}{\sqrt{p}} + \frac{1}{\sqrt{p+2}} + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}} + \frac{n-p-3}{2} & \text{if } p \le n-3 \\ \frac{n-3}{\sqrt{n-2}} + \frac{1}{\sqrt{n-1}} + \frac{1}{\sqrt{2}} & \text{if } p = n-2 \end{cases}$$

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

Theorem 2. Among n-vertex trees, $S_{n,n-1} \cong S_n$, $S_{n,n-2} \cong T_{n,1}$ are respectively the unique trees with the smallest and the second smallest first extended zeroth-order connectivity indices, which are equal to $\frac{n}{\sqrt{n-1}}$ and $\frac{n-3}{\sqrt{n-2}} + \frac{1}{\sqrt{2}} + \frac{2}{\sqrt{n-1}}$ respectively for $n \ge 4$, while $T_{n,2}$ is the unique tree with the third smallest first extended zeroth-order connectivity index, which is equal to $\frac{n-4}{\sqrt{n-3}} + \frac{2}{\sqrt{3}} + \frac{2}{\sqrt{n-1}}$ for $n \ge 6$.

Proof: The cases $n = 4, 5$ may be easily checked by direct comparison. Suppose that $n \ge 6$. If T is a tree with n vertices and p pendant vertices, where $3 \le p \le n-3$, then by Theorem 1, we have

$$^0\chi_1(T) \ge \frac{1}{\sqrt{p+1}} + \frac{p-1}{\sqrt{p}} + \frac{1}{\sqrt{p+2}} + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}} + \frac{n-p-3}{2}.$$

Let

$$h(x) = \frac{1}{\sqrt{x+1}} + \frac{x-1}{\sqrt{x}} + \frac{1}{\sqrt{x+2}} + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}} + \frac{n-x-3}{2}$$

for $2 \le x \le n-3$. It is easily seen that

$$\begin{aligned}
&h(x+1)-h(x)\\
&=\frac{1}{\sqrt{x}}-\frac{1}{\sqrt{x+1}}+\sqrt{x+1}-\sqrt{x}\\
&\quad+\frac{1}{\sqrt{x+3}}-\frac{1}{\sqrt{x+1}}-\frac{1}{2}\\
&\le\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{2+1}}+\sqrt{2+1}-\sqrt{2}\\
&\quad+\frac{1}{\sqrt{x+3}}-\frac{1}{\sqrt{x+1}}-\frac{1}{2}\\
&<\frac{1}{\sqrt{x+3}}-\frac{1}{\sqrt{x+1}}<0,
\end{aligned}$$

implying that $h(x)$ is decreasing for $2 \le x \le n-3$. Then $h(p) \ge {}^0\chi_1(S_{n,n-3})$ with equality if and only if $p = n-3$, and thus

$$\begin{aligned}
&{}^0\chi_1(T)\\
&\ge h(p)\ge {}^0\chi_1(S_{n,n-3})\\
&=\frac{1}{\sqrt{n-2}}+\frac{n-4}{\sqrt{n-3}}+\frac{1}{\sqrt{n-1}}+\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{3}}\\
&>\frac{n-4}{\sqrt{n-3}}+\frac{2}{\sqrt{3}}+\frac{2}{\sqrt{n-1}}={}^0\chi_1(T_{n,2}).
\end{aligned}$$

By Proposition 2, the first extended zeroth-order connectivity index of *n*-vertex trees with $n-2$ pendant vertices may be ordered as

$${}^0\chi_1(T_{n,1})<{}^0\chi_1(T_{n,2})<\cdots<{}^0\chi_1(T_{n,\lfloor (n-2)/2\rfloor}).$$

Obviously, an *n*-vertex tree with $n-1$ pendant vertices is the star S_n and an *n*-vertex tree with two pendant vertices is the path P_n. Note that

$${}^0\chi_1(P_n)=\sqrt{2}+\frac{2}{\sqrt{3}}+\frac{n-4}{2}$$

and

$${}^0\chi_1(S_n)=\frac{n}{\sqrt{n-1}}.$$

It is easily seen that $t(x)=\frac{x-3}{\sqrt{x-2}}-\frac{x-2}{\sqrt{x-1}}$ is increasing for $x \ge 6$. Then

$$\begin{aligned}
&{}^0\chi_1(T_{n,1})-{}^0\chi_1(S_n)\\
&=\frac{n-3}{\sqrt{n-2}}+\frac{1}{\sqrt{2}}+\frac{2}{\sqrt{n-1}}-\frac{n}{\sqrt{n-1}}\\
&=\frac{n-3}{\sqrt{n-2}}-\frac{n-2}{\sqrt{n-1}}+\frac{1}{\sqrt{2}}\\
&\ge t(6)+\frac{1}{\sqrt{2}}\\
&=\frac{3}{2}-\frac{4}{\sqrt{5}}+\frac{1}{\sqrt{2}}\\
&>0
\end{aligned}$$

and

$$\begin{aligned}
&{}^0\chi_1(P_n)-{}^0\chi_1(T_{n,2})\\
&=\sqrt{2}+\frac{2}{\sqrt{3}}+\frac{n-4}{2}\\
&\quad-\left(\frac{n-4}{\sqrt{n-3}}+\frac{2}{\sqrt{3}}+\frac{2}{\sqrt{n-1}}\right)\\
&=\left(\sqrt{2}-\frac{2}{\sqrt{n-1}}\right)+\left(\frac{n-4}{2}-\frac{n-4}{\sqrt{n-3}}\right)\\
&>0.
\end{aligned}$$

Thus ${}^0\chi_1(P_n)>{}^0\chi_1(T_{n,2})$ and ${}^0\chi_1(T_{n,1})>{}^0\chi_1(S_n)$. The result follows.

We note that the fact that S_n is the unique *n*-vertex tree with the smallest first extended zeroth-order connectivity index has been known in (Zhou and Trinajstić, 2009), by a different reasoning.

4. Comment

As suggested by one referee, we may go further to study some other extremal problems such as trees with given matching number or maximal vertex degree, and characterize trees with minimal or maximal values of the first extended zeroth-order connectivity indices.

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