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Research article

The Sombor index and coindex of two-trees

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Abstract: The Sombor index of a graph G, introduced by Ivan Gutman, is defined as the sum of the weights $\sqrt{d_G(u)^2 + d_G(v)^2}$ of all edges uv of G, where $d_G(u)$ denotes the degree of vertex u in G. The Sombor coindex was recently defined as $\overline{SO}(G) = \sum_{uv\notin E(G)} \sqrt{d_G(u)^2 + d_G(v)^2}$. As a new vertex-degree-based topological index, the Sombor index is important because it has been proved to predict certain physicochemical properties. Two-trees are very important structures in complex networks. In this paper, the maximum and second maximum Sombor index, the minimum and second minimum Sombor coindex of two-trees and the extremal two-trees are determined, respectively. Besides, some problems are proposed for further research.

Keywords: Sombor index; Sombor coindex; two-tree
Mathematics Subject Classification: 05C09, 05C92

1. Introduction

Throughout this paper, let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. Let $|V(G)|$ and $|E(G)|$ denote the order and the number of edges of G, respectively. If two vertices u, v are adjacent, we write $u \sim v$; if u, v are non-adjacent, we write $u \nsim v$. Let $N_G(v)$ be the set of all vertices adjacent to v and $d_G(v) = |N_G(v)|$ be the degree of a vertex $v \in V(G)$. If there is no confusion from the context, we abbreviate $d_G(v)$ by $d(v)$. The complement $\overline{G}$ of a graph G is the graph with vertex set $V(G)$, in which two vertices are adjacent if and only if they are not adjacent in G. Let K_n, $K_{a,b}$ be the complete graph of order n, complete bipartite graph of order $a + b$, respectively.

In the chemical and pharmaceutical sciences, topological indices are graph invariants that play a significant role [24]. Molecular models can be used to study chemical graphs in which vertices represent atoms and edges between vertices represent chemical bonds. In recent years, many topological indices have been introduced and applied in various fields of science including structural chemistry, theoretical chemistry, environmental chemistry, etc. [5, 10]. There are several types of topological indices, one of the most important being vertex-degree-based topological indices. For instance, Ivan Gutman introduced the Sombor index, defined as [9]:

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d_G(u)^2 + d_G(v)^2}.$$

The Sombor coindex was first considered in [19] and was recently defined as [18]:

$$\overline{SO}(G) = \sum_{uv \notin E(G)} \sqrt{d_G(u)^2 + d_G(v)^2}.$$

Determining the extreme values of topological indices of different graph classes has always been the focus and hot research issue of chemical graph theory, and the results provide mathematical methods and tools for analyzing the structures of compounds with physical or chemical properties. It is verified that the Sombor index has good prediction and identification ability for the simulation of alkane vaporization entropy and vaporization enthalpy [20]. Recently, the Sombor index has a good application in networks [2, 21]. At present, the research on topological indices mainly includes graph operations, indices of graphs and (in)equalities, the correlation results can be found in [1, 3, 6–8, 11, 14–17].

The two-tree T_t was defined in [4] as follows: (1) $T_0 \cong K_2$ where K_2 is a two-tree with 2 vertices; (2) T_t ($t \geq 1$) is a two-tree obtained from T_{t-1} by adding a new vertex adjacent to the two end vertices of one edge. Two-trees are very important structures in complex networks, such as generalized Farey graph and fractal scale-free network [27]. At present, the extreme values of the Randić index, Harmonic index, Multiplicative Sum Zagreb index and ABC index of two-trees have been determined (see [12, 13, 22, 23, 25, 26]), while the extreme values of the Sombor (co)index of two-trees are unknown. In order to perfect the extreme values of two-trees under different indices, we consider the extreme values of the Sombor (co)index of two-trees.

The organization of this paper is as follows: In Section 2, the maximum and second maximum Sombor index, the minimum and second minimum Sombor coindex of two-trees are determined, respectively. Moreover, the two-trees with these extreme Sombor (co)index are characterized. In Section 3, some problems are proposed for further research.

2. Extreme Sombor index and Sombor coindex of two-trees

In this section, the maximum and second maximum Sombor index, the minimum and second minimum Sombor coindex of two-trees are determined by mathematical induction and analytical structure method.

It is clear that T_t ($t \geq 1$) has at least two vertices of degree 2 and $|V(T_t)| = t + 2$. Let X_n denote the graph obtained from $K_{2,n-2}$ by joining an edge between the two vertices of degree $n-2$ and L_n denote the graph obtained from X_{n-1} by adding a new vertex and connecting it with a 2-degree vertex and a $(n-2)$-degree vertex. Both X_n, L_n (see Figures 1, 2) are two-trees.

We first prove some lemmas in preparation for the main results.

By the definition of the Sombor index and Sombor coindex, we have the following results.

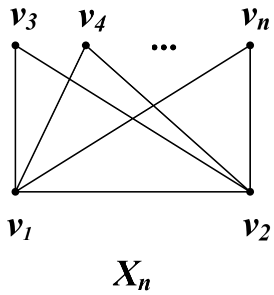


Figure 1. The two-tree X_n.

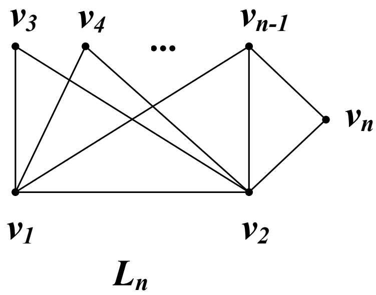


Figure 2. The two-tree L_n.

Proposition 2.1. *The Sombor index and Sombor coindex of two-trees X_n and L_n are*

$$SO(X_n) = \sqrt{2}(n-1) + 2(n-2)\sqrt{(n-1)^2+4}, \quad \overline{SO}(X_n) = \sqrt{2}(n-2)(n-3),$$

$$\begin{aligned} SO(L_n) = &(n-4)\sqrt{(n-2)^2+4} + (n-3)\sqrt{(n-1)^2+4} + \sqrt{(n-1)^2+(n-2)^2} \\ &+ \sqrt{13} + \sqrt{(n-1)^2+9} + \sqrt{(n-2)^2+9}, \end{aligned}$$

$$\overline{SO}(L_n) = \sqrt{2}(n-3)(n-4) + \sqrt{(n-2)^2+4} + \sqrt{13}(n-4).$$

Proof. Firstly, it is easy to check that $d_{X_n}(v_1) = d_{X_n}(v_2) = n-1$, $d_{X_n}(v_i) = 2$ for $3 \le i \le n$, $E(X_n) = \{v_1v_2, v_1v_3, v_1v_4, \cdots, v_1v_n, v_2v_3, v_2v_4, \cdots, v_2v_n\}$ and $E(\overline{X_n})$ is composed by the edges formed by any two vertices in $\{v_3, v_4, \cdots, v_n\}$. Then we have

$$\begin{aligned} SO(X_n) &= \sum_{uv \in E(X_n)} \sqrt{d_G(u)^2 + d_G(v)^2} = \sqrt{(n-1)^2+(n-1)^2} + 2(n-2)\sqrt{(n-1)^2+2^2}, \\ \overline{SO}(X_n) &= \sum_{uv \notin E(X_n)} \sqrt{d_G(u)^2 + d_G(v)^2} = \binom{n-2}{2}\sqrt{2^2+2^2} = \sqrt{2}(n-2)(n-3). \end{aligned}$$

Secondly, it is easy to check that $d_{L_n}(v_1) = n-2$, $d_{L_n}(v_2) = n-1$, $d_{L_n}(v_i) = 2$ for $i \in \{3, 4, \cdots, n-3, n-2, n\}$, $d_{L_n}(v_{n-1}) = 3$, $E(L_n) = \{v_1v_2, v_1v_3, v_1v_4, \cdots, v_1v_{n-1}, v_2v_3, v_2v_4, \cdots, v_2v_{n-1}, v_2v_n, v_{n-1}v_n\}$, $E(\overline{L_n}) = \{v_1v_n, v_3v_{n-1}, v_4v_{n-1}, \cdots, v_{n-2}v_{n-1}\} \cup E'$, where E' is composed by the edges formed by any two vertices in $\{v_3, v_4, \cdots, v_{n-3}, v_{n-2}, v_n\}$. Then we have

$$\begin{aligned}
SO(L_n) &= \sum_{uv\in E(L_n)} \sqrt{d_G(u)^2 + d_G(v)^2} \\
&= \sqrt{(n-1)^2 + (n-2)^2} + (n-4)\sqrt{(n-2)^2 + 2^2} + (n-3)\sqrt{(n-1)^2 + 2^2} \\
&\quad + \sqrt{2^2 + 3^2} + \sqrt{(n-1)^2 + 3^2} + \sqrt{(n-2)^2 + 3^2}, \\
\overline{SO}(L_n) &= \sum_{uv\notin E(L_n)} \sqrt{d_G(u)^2 + d_G(v)^2} \\
&= \binom{n-3}{2}\sqrt{2^2 + 2^2} + \sqrt{(n-2)^2 + 2^2} + (n-4)\sqrt{2^2 + 3^2} \\
&= \sqrt{2}(n-3)(n-4) + \sqrt{(n-2)^2 + 4} + \sqrt{13}(n-4).
\end{aligned}$$

□

Lemma 2.2. *Let* $f(x,y) = \sqrt{x^2 + y^2} - \sqrt{(x-1)^2 + (y-1)^2}$*,* $2 \le x, y \le n$ *for some* $n \ge 3$*. Then* $f(x,y) \le \sqrt{2}$ *with equality holds if and only if* $x = y$*. Moreover, if* $x < y$*, then* $f(x,y)$ *is monotonic increasing with* x *and* $f(x,y) \le f(n-1,n)$*.*

Proof. We prove this conclusion in two-dimensional plane rectangular coordinate system. It is clear that $\sqrt{x^2 + y^2}$, $\sqrt{(x-1)^2 + (y-1)^2}$ represent the distance between the coordinate (x,y) and $(0,0)$, $(1,1)$, respectively. Then (x,y), $(0,0)$, $(1,1)$ form a triangle. Let e_1, e_2, e_3 represent the edges between (x,y) and $(0,0)$, (x,y) and $(1,1)$, $(0,0)$ and $(1,1)$, respectively. At this time, the problem is transformed into solving the maximum value of $|e_1| - |e_2|$ where $|e_i|$ represents the length of e_i $(i = 1,2,3)$. From the properties of triangles, we know that the difference value between the lengths of any two edges is less than the third edge. Thus $|e_1| - |e_2| < |e_3| = \sqrt{2}$ if $(0,0)$, $(1,1)$, (x,y) are not collinear. If $(0,0)$, $(1,1)$, (x,y) are collinear, then we have $x = y$ and $|e_1| - |e_2| = |e_3| = \sqrt{2}$ by $x \ge 2$, $y \ge 2$. Thus, $f(x,y) \le \sqrt{2}$ with equality holds if and only if $x = y$.

When $y > x \ge 2$, we have $x^2(y-1)^2 - (x-1)^2y^2 = (2xy - (x+y))(y-x) > 0$. Then,

$$\begin{aligned}
\frac{\partial f(x,y)}{\partial x} &= \frac{x}{\sqrt{x^2 + y^2}} - \frac{x-1}{\sqrt{(x-1)^2 + (y-1)^2}} \\
&= \frac{\sqrt{x^2(x-1)^2 + x^2(y-1)^2} - \sqrt{x^2(x-1)^2 + (x-1)^2y^2}}{\sqrt{x^2 + y^2}\sqrt{(x-1)^2 + (y-1)^2}} > 0.
\end{aligned}$$

Moreover,

$$\frac{\partial f(y-1,y)}{\partial y} = \frac{\sqrt{(2y-1)^2\big((y-2)^2 + (y-1)^2\big)} - \sqrt{(2y-3)^2\big((y-1)^2 + y^2\big)}}{\sqrt{(y-1)^2 + y^2}\sqrt{(y-2)^2 + (y-1)^2}} > 0$$

by $(2y-1)^2\big((y-2)^2 + (y-1)^2\big) - (2y-3)^2\big((y-1)^2 + y^2\big) = 4(y-1) > 0$. Thus, $f(x,y) \le f(y-1,y) \le f(n-1,n)$. □

Lemma 2.3. *Let* $g(x,y) = \sqrt{x^2 + y} - \sqrt{(x-1)^2 + y}$*,* $G(x,y) = g(x,y) - g(x-1,y)$*, where* $x, y > 0$*. Then,*

(i) $g(x, y)$ *is monotonic increasing with x;*
(ii) $g(x, y)$ *is monotonic decreasing with y;*
(iii) $G(x, y)$ *is monotonic decreasing with x and* $G(x, y) > 0$*.*

Proof. We consider the derivative of $g(x, y)$,

$$\frac{\partial g}{\partial x} = \frac{x}{\sqrt{x^2 + y}} - \frac{x - 1}{\sqrt{(x - 1)^2 + y}} = \frac{\sqrt{x^2(x - 1)^2 + yx^2} - \sqrt{x^2(x - 1)^2 + y(x - 1)^2}}{\sqrt{x^2 + y}\sqrt{(x - 1)^2 + y}} > 0,$$

$$\frac{\partial g}{\partial y} = \frac{1}{2}\left(\frac{1}{\sqrt{x^2 + y}} - \frac{1}{\sqrt{(x - 1)^2 + y}}\right) = \frac{\sqrt{(x - 1)^2 + y} - \sqrt{x^2 + y}}{\sqrt{x^2 + y}\sqrt{(x - 1)^2 + y}} < 0.$$

Hence, $g(x, y)$ is monotonic increasing with x and monotonic decreasing with y, and $G(x, y) > 0$ is naturally.

Besides, by

$$\frac{\partial^2 g}{\partial x^2} = \partial_x(\frac{x}{\sqrt{x^2 + y}}) - \partial_x(\frac{x - 1}{\sqrt{(x - 1)^2 + y}}) = y(\frac{1}{(x^2 + y)^{\frac{3}{2}}} - \frac{1}{((x - 1)^2 + y)^{\frac{3}{2}}}) < 0,$$

we know that $\frac{\partial g}{\partial x}$ is monotonic decreasing with x and thus the third claim holds. □

Now we determine the maximum Sombor index of two-trees.

Theorem 2.4. *Let G be a two-tree of order* $n \geq 2$*. Then,*

$$SO(G) \leq \sqrt{2}(n - 1) + 2(n - 2)\sqrt{(n - 1)^2 + 4},$$

with equality holds if and only if $G \cong X_n$*.*

Proof. We prove this result by induction on n.

When $n = 2, 3, 4$, it is clear that $G \cong X_2, X_3, X_4$, respectively.

Assume that the result holds for $n - 1$ ($n \geq 5$). Choose a vertex w of degree 2 from the graph G, then $G - w$ is a two-tree of order $n - 1$. By the induction hypothesis, $SO(G - w) \leq SO(X_{n-1})$ with equality holds if and only if $G - w \cong X_{n-1}$. In the following we prove that $SO(G) \leq SO(X_n)$.

Let u and v be two vertices adjacent to the vertex w in G. Let $d(u) = a, d(v) = b$ and $N_G(u) \setminus \{v, w\} = \{u_1, u_2, \cdots, u_{a-2}\}$, $N_G(v) \setminus \{u, w\} = \{v_1, v_2, \cdots, v_{b-2}\}$. By the construction of G, we know that $3 \leq a, b \leq n - 1$. Combining with Lemmas 2.2 and 2.3, we have

$$\begin{aligned} SO(G) =& SO(G - w) + \left(\sqrt{a^2 + 4} + \sqrt{b^2 + 4}\right) + \left(\sqrt{a^2 + b^2} - \sqrt{(a - 1)^2 + (b - 1)^2}\right) \\ &+ \sum_{i=1}^{a-2}\left(\sqrt{a^2 + d(u_i)^2} - \sqrt{(a - 1)^2 + d(u_i)^2}\right) + \sum_{j=1}^{b-2}\left(\sqrt{b^2 + d(v_j)^2} - \sqrt{(b - 1)^2 + d(v_j)^2}\right) \\ \leq& SO(X_{n-1}) + 2\sqrt{(n - 1)^2 + 4} + \sqrt{2} + \sum_{i=1}^{n-3}\left(\sqrt{(n - 1)^2 + d(u_i)^2} - \sqrt{(n - 2)^2 + d(u_i)^2}\right) \\ &+ \sum_{j=1}^{n-3}\left(\sqrt{(n - 1)^2 + d(v_j)^2} - \sqrt{(n - 2)^2 + d(v_j)^2}\right) \end{aligned}$$

$$
\begin{aligned}
&\leq SO(X_{n-1}) + 2\sqrt{(n-1)^2+4} + \sqrt{2} + 2(n-3)\Big(\sqrt{(n-1)^2+4} - \sqrt{(n-2)^2+4}\Big)\\
&=[2(n-3)\sqrt{(n-2)^2+4} + \sqrt{2}(n-2)] + \sqrt{2} + 2(n-2)\sqrt{(n-1)^2+4}\\
&\quad - 2(n-3)\sqrt{(n-2)^2+4}\\
&=2(n-2)\sqrt{(n-1)^2+4} + \sqrt{2}(n-1)\\
&=SO(X_n).
\end{aligned}
$$

For the first inequality, $\sqrt{a^2+4} + \sqrt{b^2+4} \leq \sqrt{(n-1)^2+4} + \sqrt{(n-1)^2+4}$ is obvious. $\sqrt{a^2+b^2} - \sqrt{(a-1)^2+(b-1)^2} \leq \sqrt{2}$ holds by Lemma 2.2. $\sum_{i=1}^{a-2}\Big(\sqrt{a^2+d(u_i)^2} - \sqrt{(a-1)^2+d(u_i)^2}\Big) \leq \sum_{i=1}^{n-3}\Big(\sqrt{(n-1)^2+d(u_i)^2} - \sqrt{(n-2)^2+d(u_i)^2}\Big)$ holds by (i) of Lemma 2.3 and $a \leq n-1$. The rest part of the first inequality holds by the similar reason.

For the second inequality, the two sum terms are similar and we only consider the first one. In fact,

$$
\Big(\sqrt{(n-1)^2+d(u_i)^2} - \sqrt{(n-2)^2+d(u_i)^2}\Big) \leq \Big(\sqrt{(n-1)^2+4} - \sqrt{(n-2)^2+4}\Big)
$$

holds by (ii) of Lemma 2.3 and $d(u_i) \geq 2$.

Combining with the above arguments, $SO(G) \leq SO(X_n)$ and the equality holds if and only if $G - w \cong X_{n-1}$, $a = b = n-1$ and $d(u_i) = d(v_i) = 2$ for $1 \leq i \leq n-3$, which implies $G \cong X_n$.

Then the result holds for n, and we complete the proof. □

Next we determine the second maximum Sombor index of two-trees.

Theorem 2.5. *Let G be a two-tree of order $n \geq 5$ and $G \ncong X_n$. Then*

$$
\begin{aligned}
SO(G) \leq &(n-4)\sqrt{(n-2)^2+4} + (n-3)\sqrt{(n-1)^2+4} + \sqrt{(n-1)^2+(n-2)^2}\\
&+ \sqrt{13} + \sqrt{(n-1)^2+9} + \sqrt{(n-2)^2+9},
\end{aligned}
$$

with equality holds if and only if $G \cong L_n$.

Proof. We prove this result by induction on n.

When $n = 5$, G can only be isomorphic to L_5 and X_5, thus $G \cong L_5$ by $G \ncong X_5$.

Assume that the result holds for $n-1$ ($n \geq 6$). We choose one vertex w of degree 2 from G such that $G-w \ncong X_{n-1}$, then $G-w$ is a two-tree of order $n-1$. By the induction hypothesis, $SO(G-w) \leq SO(L_{n-1})$ with equality holds if and only if $G - w \cong L_{n-1}$. In the following we prove that $SO(G) \leq SO(L_n)$ and the equality holds if and only if $G \cong L_n$.

Let u and v be two vertices adjacent to the vertex w in G. Since $n \geq 6$, from the definition of two-trees we know that there must exist a vertex p with $d(p) \geq 3$ which is adjacent to u and v (otherwise $G - w \cong X_{n-1}$). Let $d(u) = a, d(v) = b, d(p) = c$ and $N_G(u) \setminus \{v, w, p\} = \{u_1, u_2, \cdots, u_{a-3}\}$, $N_G(v) \setminus \{u, w, p\} = \{v_1, v_2, \cdots, v_{b-3}\}$. Then $3 \leq a, b, c \leq n-1$ and $d(u_i) \geq 2$, $d(v_j) \geq 2$ for $1 \leq i \leq a-3$, $1 \leq j \leq b-3$. Without loss of generality, we assume that $a \leq b$.

Let

$$
\begin{aligned}
f(x,y,z) =&\Big(\sqrt{x^2+4} + \sqrt{y^2+4}\Big) + \Big(\sqrt{x^2+y^2} - \sqrt{(x-1)^2+(y-1)^2}\Big)\\
&+ \Big(\sqrt{x^2+z^2} - \sqrt{(x-1)^2+z^2}\Big) + \Big(\sqrt{y^2+z^2} - \sqrt{(y-1)^2+z^2}\Big)\\
&+ \sum_{i=1}^{x-3}\Big(\sqrt{x^2+d(u_i)^2} - \sqrt{(x-1)^2+d(u_i)^2}\Big) + \sum_{j=1}^{y-3}\Big(\sqrt{y^2+d(v_j)^2} - \sqrt{(y-1)^2+d(v_j)^2}\Big).
\end{aligned}
$$

Then we have

$$SO(G) = SO(G-w) + f(a,b,c). \tag{2.1}$$

Next we complete the proof by the following two cases.

Case 1: $b \le c$.

Then $c \le n-2$ since $p \nsim w$ and $a \le b \le c \le n-2$, and thus $f(a,b,c) \le f(c,c,c)$ by Lemmas 2.2 and 2.3. From (i) and (ii) of Lemma 2.3, we have $g(c,c^2) < g(n-2,9)$ by $n \ge 6$. Then by (2.1), Lemmas 2.2 and 2.3, we have

$$\begin{aligned}
SO(G) \le& SO(L_{n-1}) + f(c,c,c)\\
\le& SO(L_{n-1}) + 2\sqrt{c^2+4} + \sqrt{2} + 2\Big(\sqrt{c^2+c^2} - \sqrt{(c-1)^2+c^2}\Big)\\
&+ 2\sum_{i=1}^{c-3}\Big(\sqrt{c^2+4} - \sqrt{(c-1)^2+4}\Big)\\
<& SO(L_{n-1}) + 2\sqrt{(n-2)^2+4} + \sqrt{2} + 2\Big(\sqrt{(n-2)^2+9} - \sqrt{(n-3)^2+9}\Big)\\
&+ 2(n-5)\Big(\sqrt{(n-2)^2+4} - \sqrt{(n-3)^2+4}\Big)\\
=& \Big[(n-5)\sqrt{(n-3)^2+4} + (n-4)\sqrt{(n-2)^2+4} + \sqrt{(n-2)^2+(n-3)^2}\\
&+ \sqrt{(n-2)^2+9} + \sqrt{(n-3)^2+9} + \sqrt{13}\Big] + 2\sqrt{(n-2)^2+4} + \sqrt{2}\\
&+ 2\Big(\sqrt{(n-2)^2+9} - \sqrt{(n-3)^2+9}\Big) + 2(n-5)\Big(\sqrt{(n-2)^2+4} - \sqrt{(n-3)^2+4}\Big)\\
=& 3(n-4)\sqrt{(n-2)^2+4} - (n-5)\sqrt{(n-3)^2+4} + \sqrt{(n-2)^2+(n-3)^2}\\
&+ 3\sqrt{(n-2)^2+9} - \sqrt{(n-3)^2+9} + \sqrt{2} + \sqrt{13}.
\end{aligned}$$

Let $A_1 = 3(n-4)\sqrt{(n-2)^2+4} - (n-5)\sqrt{(n-3)^2+4} + \sqrt{(n-2)^2+(n-3)^2} + 3\sqrt{(n-2)^2+9} - \sqrt{(n-3)^2+9} + \sqrt{2} + \sqrt{13}$. Then

$$\begin{aligned}
SO(L_n) - A_1 =& (n-3)\sqrt{(n-1)^2+4} + (n-5)\sqrt{(n-3)^2+4} - 2(n-4)\sqrt{(n-2)^2+4}\\
&+ \sqrt{(n-1)^2+(n-2)^2} - \sqrt{(n-2)^2+(n-3)^2} + \sqrt{(n-1)^2+9}\\
&+ \sqrt{(n-3)^2+9} - 2\sqrt{(n-2)^2+9} - \sqrt{2}.
\end{aligned}$$

Let $x = n-1, y = 4$ $(n \ge 6)$ in Lemma 2.3. Then we have

$$\begin{aligned}
&(n-3)\sqrt{(n-1)^2+4} + (n-5)\sqrt{(n-3)^2+4} - 2(n-4)\sqrt{(n-2)^2+4}\\
=& 2g(n-1,4) + (n-5)G(n-1,4)\\
\ge& 2g(5,4) + G(5,4)\\
>& 1.8725.
\end{aligned}$$

It is easy to check that for $n \ge 6$, $\sqrt{(n-1)^2+(n-2)^2} - \sqrt{(n-2)^2+(n-3)^2} > 0$, and $\sqrt{(n-1)^2+9} + \sqrt{(n-3)^2+9} - 2\sqrt{(n-2)^2+9} = G(n-1,9) > 0$ by Lemma 2.3. Hence $SO(L_n) - A_1 > 1.8725 - \sqrt{2} > 0$, and then $SO(G) < A_1 < SO(L_n)$.

Case 2: $b > c$.

Then we have $b \le n-1$ and $\max\{a, c\} \le n-2$ (otherwise, $a = b = n-1$, which implies $G \cong X_n$).

If $a < b$, then $a \le n-2$, $b \le n-1$. By (2.1), Lemmas 2.2 and 2.3, we have

$$
\begin{aligned}
SO(G) \le & SO(L_{n-1}) + f(n-2, n-3, 3) \\
\le & SO(L_{n-1}) + \left(\sqrt{(n-2)^2+4} + \sqrt{(n-1)^2+4}\right) + \left(\sqrt{(n-2)^2+(n-1)^2}\right. \\
& \left. - \sqrt{(n-3)^2+(n-2)^2}\right) + \left(\sqrt{(n-2)^2+9} - \sqrt{(n-3)^2+9}\right) \\
& + \left(\sqrt{(n-1)^2+9} - \sqrt{(n-2)^2+9}\right) + (n-5)\left(\sqrt{(n-2)^2+4} - \sqrt{(n-3)^2+4}\right) \\
& + (n-4)\left(\sqrt{(n-1)^2+4} - \sqrt{(n-2)^2+4}\right) \\
= & (n-3)\sqrt{(n-1)^2+4} + (n-4)\sqrt{(n-2)^2+4} + \sqrt{(n-1)^2+(n-2)^2} \\
& + \sqrt{13} + \sqrt{(n-1)^2+9} + \sqrt{(n-2)^2+9} \\
= & SO(L_n).
\end{aligned}
$$

The equality holds if and only if $G - w \cong L_{n-1}$, $a = n-2$, $b = n-1$, $c = 3$, $d(u_i) = d(v_j) = 2$ for $1 \le i \le a-3$ and $1 \le j \le b-3$, which implies $G \cong L_n$.

If $a = b$, then $a = b \le n-2$. By (2.1), Lemmas 2.2 and 2.3, we have

$$
\begin{aligned}
SO(G) \le & SO(L_{n-1}) + f(a, a, c) \\
\le & SO(L_{n-1}) + f(n-2, n-2, 3) \\
\le & SO(L_{n-1}) + 2\sqrt{(n-2)^2+4} + \sqrt{2} + 2\left(\sqrt{(n-2)^2+9} - \sqrt{(n-3)^2+9}\right) \\
& + 2(n-5)\left(\sqrt{(n-2)^2+4} - \sqrt{(n-3)^2+4}\right) \\
= & A_1.
\end{aligned}
$$

Thus $SO(G) \le A_1 < SO(L_n)$ by Case 1.

Combining the two cases, we have $SO(G) \le SO(L_n)$ and the equality holds if and only if $G \cong L_n$. Thus the result holds for n, and we complete the proof. □

Next we consider the minimum Sombor coindex of two-trees.

Theorem 2.6. *Let G be a two-tree of order $n \ge 2$. Then,*

$$\overline{SO}(G) \ge \sqrt{2}(n-2)(n-3),$$

with equality holds if and only if $G \cong X_n$.

Proof. We prove this result by induction on n.

When $n = 2, 3, 4$, G can only be isomorphic to X_2, X_3, X_4, respectively.

Assume that the result holds for $n-1$ ($n \ge 5$). Let w be a vertex of G with degree 2. Then $G - w$ is a two-tree of order $n-1$. By the induction hypothesis, $\overline{SO}(G-w) \ge \overline{SO}(X_{n-1})$ with equality holds if and only if $G - w \cong X_{n-1}$. In the following we prove that $\overline{SO}(G) \ge \overline{SO}(X_n)$.

Let $N_G(w) = \{u, v\}$, $V(G)\backslash\{u, v, w\} = \{t_1, t_2, \cdots, t_{n-3}\}$ and $d(u) = a, d(v) = b$. Then $3 \leq a, b \leq n-1$, $d(t_i) \geq 2$ for $1 \leq i \leq n-3$, $\sqrt{x^2 + y^2} - \sqrt{(x-1)^2 + y^2} > 0$ for $3 \leq x \leq n-1$, and

$$\begin{aligned}\overline{SO}(G) =&\overline{SO}(G-w) + \sum_{t_i \nsim u}\left(\sqrt{a^2 + d(t_i)^2} - \sqrt{(a-1)^2 + d(t_i)^2}\right)\\ &+ \sum_{t_i \nsim v}\left(\sqrt{b^2 + d(t_i)^2} - \sqrt{(b-1)^2 + d(t_i)^2}\right) + \sum_{i=1}^{n-3}\sqrt{4 + d(t_i)^2}\\ \geq&\overline{SO}(X_{n-1}) + \sqrt{8}(n-3)\\ =&\overline{SO}(X_n).\end{aligned}$$

If $a = b = n-1$, then the first two summations are equal to 0 since no vertices are non-adjacent to u, v.

Thus $\overline{SO}(G) \geq \overline{SO}(X_n)$ with equality holds if and only if $G - w \cong X_{n-1}$, $a = b = n-1$ and $d(t_i) = 2$ for $1 \leq i \leq n-3$, which implies $G \cong X_n$. Then the result holds for n, and we complete the proof. □

Finally, we consider the second minimum Sombor coindex of two-trees.

Lemma 2.7. *Let* $h(x, y) = \sqrt{y^2 + x^2} - \sqrt{(y-1)^2 + x^2} + \sqrt{4 + x^2}$ *where* $x > 0, y \geq 3$. *Then* $h(x, y)$ *is monotonic increasing with* x.

Proof. The derivative of function $h(x, y)$ with respect to x is

$$h'(x) = \frac{x}{\sqrt{y^2 + x^2}} - \frac{x}{\sqrt{(y-1)^2 + x^2}} + \frac{x}{\sqrt{4 + x^2}}.$$

Then $h'(x) > 0$ since

$$\frac{1}{\sqrt{4 + x^2}} - \frac{1}{\sqrt{(y-1)^2 + x^2}} = \frac{\sqrt{(y-1)^2 + x^2} - \sqrt{4 + x^2}}{\sqrt{(y-1)^2 + x^2}\sqrt{4 + x^2}} \geq 0.$$

□

Theorem 2.8. *Let* G *ba a two-tree of order* $n \geq 5$ *and* $G \ncong X_n$. *Then,*

$$\overline{SO}(G) \geq \sqrt{2}(n-3)(n-4) + \sqrt{(n-2)^2 + 4} + \sqrt{13}(n-4),$$

with equality holds if and only if $G \cong L_n$.

Proof. We prove the result by induction on n.

For $n = 5$, G can only be isomorphic to L_5.

Assume that the result holds for $n-1$ ($n \geq 6$). Let w be a vertex of G with degree 2 such that $G - w \ncong X_{n-1}$. Then $G - w$ is a two-tree of order $n-1$. By the induction hypothesis, $\overline{SO}(G-w) \geq \overline{SO}(L_{n-1})$ with equality holds if and only if $G - w \cong L_{n-1}$. In the following we prove that $\overline{SO}(G) \geq \overline{SO}(L_n)$.

Let $N_G(w) = \{u, v\}$, $d(u) = a$ and $d(v) = b$. Then $3 \leq a, b \leq n-1$. From the definition of two-trees and $G \ncong X_n$, there must exist a vertex p with $d(p) = c \geq 3$ such that $p \sim u$ and $p \sim v$. Let $V(G) \setminus \{u, v, w\} = \{t_1, t_2, \cdots, t_{n-5}, t_{n-4}, p\}$. Without loss of generality, we assume $a \leq b$. By $G \ncong X_n$, we have $a \leq n-2$. Then by Lemmas 2.2, 2.3 and 2.7, we have

$$\begin{aligned}
\overline{SO}(G) =&\overline{SO}(G-w) + \sum_{t_i \nsim u}\left(\sqrt{a^2+d(t_i)^2} - \sqrt{(a-1)^2+d(t_i)^2}\right) \\
&+ \sum_{t_i \nsim v}\left(\sqrt{b^2+d(t_i)^2} - \sqrt{(b-1)^2+d(t_i)^2}\right) + \sum_{i=1}^{n-4}\sqrt{4+d(t_i)^2} + \sqrt{4+c^2} \\
\geq&\overline{SO}(L_{n-1}) + \sum_{t_i \nsim u}\left(\sqrt{a^2+d(t_i)^2} - \sqrt{(a-1)^2+d(t_i)^2}\right) + \sum_{i=1}^{n-4}\sqrt{4+d(t_i)^2} + \sqrt{4+c^2} \quad (2.2) \\
=&\overline{SO}(L_{n-1}) + \sum_{t_i \nsim u}\left(\sqrt{a^2+d(t_i)^2} - \sqrt{(a-1)^2+d(t_i)^2} + \sqrt{4+d(t_i)^2}\right) \\
&+ \sum_{t_i \sim u}\sqrt{4+d(t_i)^2} + \sqrt{4+c^2} \\
\geq&\overline{SO}(L_{n-1}) + \sum_{t_i \nsim u}\left(\sqrt{a^2+4} - \sqrt{(a-1)^2+4} + \sqrt{4+4}\right) + \sum_{t_i \sim u}\sqrt{4+4} + \sqrt{4+3^2} \quad (2.3) \\
=&\overline{SO}(L_{n-1}) + \sum_{t_i \nsim u}\left(\sqrt{a^2+4} - \sqrt{(a-1)^2+4}\right) + 2\sqrt{2}(n-4) + \sqrt{13} \\
\geq&\overline{SO}(L_{n-1}) + \left(\sqrt{(n-2)^2+4} - \sqrt{(n-3)^2+4}\right) + 2\sqrt{2}(n-4) + \sqrt{13} \quad (2.4) \\
=& \sqrt{2}(n-3)(n-4) + \sqrt{13}(n-4) + \sqrt{(n-2)^2+4} \\
=&\overline{SO}(L_n).
\end{aligned}$$

The (2.2) holds by $\sum_{t_i \nsim v}\left(\sqrt{b^2+d(t_i)^2} - \sqrt{(b-1)^2+d(t_i)^2}\right) \geq 0$ and $\overline{SO}(G-w) \geq \overline{SO}(L_{n-1})$, where the equality holds if and only if $b = n-1$ and $G - w \cong L_{n-1}$.

By Lemma 2.7, we have $h(d(t_i), a)$ is monotonic increasing with $d(t_i)$. Thus (2.3) holds, where the equality holds if and only if $d(p) = 3$, $d(t_i) = 2$ for $1 \leq i \leq n-4$.

It is not difficult to find that $\sum\limits_{t_i \nsim u}\left(\sqrt{a^2+4} - \sqrt{(a-1)^2+4}\right)$ has $n-1-a$ summation terms by $d(u) = a$ and $d_G(u) + d_{\overline{G}}(u) = n-1$. Then for $a \leq n-3$, by $n-1-a \geq 2$ and $\sqrt{a^2+4} - \sqrt{(a-1)^2+4} \geq \sqrt{3^2+4} - \sqrt{2^2+4} > 0.776$, we have

$$\sum_{t_i \nsim u}\left(\sqrt{a^2+4} - \sqrt{(a-1)^2+4}\right) = (n-1-a)(\sqrt{a^2+4} - \sqrt{(a-1)^2+4}) > 1.$$

For $a = n-2$,

$$\sum_{t_i \nsim u}\left(\sqrt{a^2+4} - \sqrt{(a-1)^2+4}\right) = \sqrt{(n-2)^2+4} - \sqrt{(n-3)^2+4} < 1,$$

since $\sqrt{(n-2)^2+4} - \sqrt{(n-3)^2+4}$ represents the difference between the distance from the coordinate $(n-2, 2)$ to the coordinates $(0, 0)$ and $(1, 0)$. Thus (2.4) holds, where the equality holds if and only if $a = n-2$.

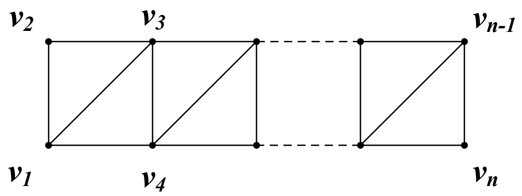
Thus $\overline{SO}(G) \geq \overline{SO}(L_n)$ with equality holds if and only if $G - w \cong L_{n-1}$, $a = n-2$, $b = n-1$, $c = 3$ and $d(t_i) = 2$ for $1 \leq i \leq n-4$, which implies $G \cong L_n$.

Then the result holds for n, and we complete the proof. □

3. Conclusions

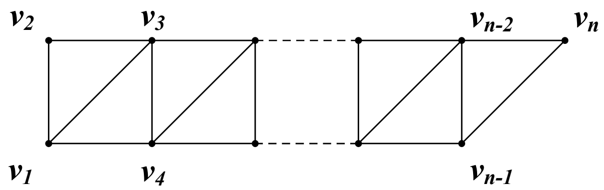
In this paper, we focus on the Sombor (co)index of two-trees (a very important structure in complex networks). The maximum and second maximum Sombor index, the minimum and second minimum Sombor coindex of two-trees are determined, respectively. Besides, the two-trees with these extreme Sombor (co)index are characterized.

However, the minimum Sombor index and the maximum Sombor coindex of two-trees are unknown. By calculating the degree sequence of X_n and L_n, it is not difficult to find that there is a big difference $((n-1)-2)$ between their vertex degrees. Therefore, considering the other extreme cases, we guess that the two-tree corresponding to the minimum Sombor index (or the maximum Sombor coindex) should minimize the difference between $d_G(u)$ and $d_G(v)$ for any $uv \in E(G)$ as much as possible. Combining with Lemmas 2.2 and 2.3, we conjecture that these two extreme values will be contributed by the two-tree H_n^1 (Figure 3) if n is even or H_n^2 (Figure 4) if n is odd.



n is even

Figure 3. The two-tree H_n^1.



n is odd

Figure 4. The two-tree H_n^2.

Conjecture 3.1. *Let G be a two-tree of order n. Then,*

$$SO(G) \geq 6\sqrt{2}n + 2\sqrt{13} + 4\sqrt{5} + 20 - 33\sqrt{2},$$
$$\overline{SO}(G) \leq 2\sqrt{2}n^2 + (10 - 26\sqrt{2}n + 4\sqrt{5})n + 89\sqrt{2} + 2\sqrt{13} - 20\sqrt{5} - 60,$$

with equality holds if and only if $G \cong H_n^i$ ($i = 1$ *if n is even,* $i = 2$ *if n is odd*).

It is not difficult to find that the extremal two-trees in this paper are the same as that in [12, 13, 22, 23, 25, 26], which raises a question naturally, whether the extremal two-trees for other unstudied vertex-degree-based topological indices are the same as X_n, L_n. The work of this paper promotes the study of this problem. At the same time, the proofs of the extremal two-trees are different for different indices, it is a question worth studying to find a method to determine the extremal two-trees for any indices.

Use of AI tools declaration

The authors declare they have not used Artificial Intelligence (AI) tools in the creation of this article.

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Conflict of interest

The authors declare that they have no conflicts of interest.

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