Trees with the seven smallest and eight greatest Harary indices✩

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ABSTRACT

The Harary index is defined as the sum of reciprocals of distances between all pairs of vertices of a connected graph. In this paper, we determined the first up to seventh smallest Harary indices of trees of order \( n \geq 16 \) and the first up to eighth greatest Harary indices of trees of order \( n \geq 14 \).

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1. Introduction

The Harary index of a graph \( G \), denoted by \( H(G) \), was been independently by Plavšić et al. [27] and by Ivanciuc et al. [20] in 1993. It was named in honor of Professor Frank Harary on the occasion of his 70th birthday. The Harary index is defined as follows:

\[
H = H(G) = \sum_{u,v \in V(G)} \frac{1}{d_G(u,v)}
\]

where the summation goes over all pairs of vertices of \( G \) and \( d_G(u,v) \) denotes the distance of the two vertices \( u \) and \( v \) in the graph \( G \) (i.e., the number of edges in a shortest path connecting \( u \) and \( v \)). Mathematical properties and applications of \( H \) are reported in [4,8,9,24,34–37].

Another two related distance-based topological indices of the graph \( G \) are the Wiener index \( W(G) \) and the hyper-Wiener index \( WW(G) \). As an oldest topological index, the Wiener index of a (molecular) graph \( G \), first introduced by Wiener [33] in 1947, was defined as

\[
W(G) = \sum_{u,v \in V(G)} d_G(u,v)
\]

with the summation going over all pairs of vertices of \( G \). The hyper-Wiener index of \( G \), first introduced by Randić [28] in 1993, is nowadays defined as [21]:

\[
WW(G) = \frac{1}{2} \sum_{u,v \in V(G)} d_G(u,v) + \frac{1}{2} \sum_{u,v \in V(G)} d_G(u,v)^2.
\]

Mathematical properties and applications of the Wiener index and hyper-Wiener index are extensively reported in the literature [1,6,7,9,10,17,13,12,16,15,22,25,26,29–32,38].
Let $\gamma(G, k)$ be the number of vertex pairs of the graph $G$ that are at distance $k$. Then
\begin{equation}
H(G) = \sum_{k=1}^{\Delta} \frac{1}{k} \gamma(G, k).
\end{equation}

All graphs considered in this paper are finite and simple. Let $G$ be a graph with vertex set $V(G)$ and edge set $E(G)$. For a vertex $v \in V(G)$, we denote by $N_v(v)$ the neighbors of $v$ in $G$. $d_G(v) = |N_v(v)|$ is called the degree of $v$ in $G$ or is written as $d(v)$ for short. In particular, $\Delta = \Delta(G)$ is called the maximum degree of vertices of $G$. A vertex $v$ of degree 1 is called a pendant vertex. An edge $e = uv$ incident with the pendant vertex $v$ is a pendant edge. For a subset $W$ of $V(G)$, let $G - W$ be the subgraph of $G$ obtained by deleting the vertices of $W$ and the edges incident with them. Similarly, for a subset $E'$ of $E(G)$, we denote by $G - E'$ the subgraph of $G$ obtained by deleting the edges of $E'$. If $W = \{v\}$ and $E' = \{xy\}$, the subgraphs $G - W$ and $G - E'$ will be written as $G - v$ and $G - xy$ for short, respectively. The diameter of the graph $G$ will be denoted by $D(G)$. In the following we denote by $P_n$ and $S_n$ the path graph and the star graph with $n$ vertices, respectively. For other undefined notations and terminology from graph theory, the readers are referred to [2].

Let $T(n)$ be the set of trees of order $n$. A molecular tree is a tree of maximum degree at most 4. It models the skeleton of an acyclic molecule [31]. Gutman et al. [18] first gave a partial order to Wiener index among starlike trees. After then, Deng [5], Liu and Liu [23] determined the seventeenth Wiener indices of trees of order $n \geq 28$. And the trees with the first up to fifteenth smallest Wiener indices among trees of order $n$ were determined by Guo and Dong [11]. Gutman [12] characterized the extremal (maximal and minimal) hyper-Wiener indices of trees in $T(n)$ (they are attained at $P_n$ and $S_n$, respectively). Very recently, Liu and Liu [22] determined the fifteenth greatest hyper-Wiener indices of trees in $T(n)$ with $n \geq 20$ and the seventh smallest hyper-Wiener indices of trees in $T(n)$ with $n \geq 17$. Das et al. [4] and Zhou et al. [37] gave some nice bounds of Harary index. In this paper we identify the first up to seventh smallest Harary indices of trees in $T(n)$ with $n \geq 18$, which are all molecular trees, and the first up to eighth greatest Harary indices of trees in $T(n)$ with $n \geq 14$.

2. Some lemmas

In this section we list or prove some lemmas as basic but necessary preliminaries, which will be used in the subsequent proofs.

First, for a graph $G$ with $v \in V(G)$, we define $Q_C(v) = \sum_{u \in V(G)} \frac{d(u, v)}{d(u, v) + 1}$. For convenience, sometimes we write $Q_C(v)$ as $Q_C(v(G))$. Note that the function $f(x) = \frac{1}{x+1}$ is strictly increasing for $x \geq 1$. Thus the lemma below follows immediately.

**Lemma 2.1.** Suppose that $P_n = v_1v_2 \cdots v_n$ is a path where the vertices $v_i$ and $v_{i+1}$ are adjacent for $i = 1, 2, 3, \ldots, n - 1$. Then we have
1. $Q_{C_n}(v_i) = Q_{P_n}(v_{n+1})$ for $1 \leq j \leq \left\lfloor \frac{n}{2} \right\rfloor$;
2. $Q_{C_n}(v_j) > Q_{P_n}(v_{j+1})$ for $1 \leq j \leq \left\lfloor \frac{n}{2} \right\rfloor$;
3. $Q_{C_n}(v_j) > Q_{P_n}(v_{j-k})$ for $1 \leq j < k \leq \left\lfloor \frac{n}{2} \right\rfloor$.

**Lemma 2.2.** Let $G$ be a graph of order $n$ and $v$ be a pendant vertex of $G$ with $uv \in E(G)$. Then we have $H(G) = H(G - v) + n - 1 - Q_{C_{G-v}}(u)$.

**Proof.** By the definitions of Harary index and $Q_C(u)$, we have
$$H(G) = \sum_{u,v \in V(G-v)} \frac{1}{d_G(u, v)} + \sum_{x \in V(G-v)} \frac{1}{d_G(x, v)}$$
$$= H(G - v) + \sum_{x \in V(G-v)} \frac{1}{d_G(x, u) + 1}$$
$$= H(G - v) + \sum_{x \in V(G-v)} \left(1 - \frac{d_G(x, u)}{d_G(x, u) + 1}\right)$$
$$= H(G - v) + n - 1 - Q_{C_{G-v}}(u),$$
completing the proof of the lemma.

**Corollary 2.1.** Let $G_1$ and $G_2$ be two graphs of same order and with $v_1$ as a pendant vertex of $G_i$ and $u_i v_i \in E(G_i)$ for $i = 1, 2$. If $H(G_2 - v_2) \geq H(G_1 - v_1)$ and $Q_{G_1-v_1}(u_1) \geq Q_{G_2-v_2}(u_2)$, then $H(G_2) \geq H(G_1)$ with the equality holding if and only if the above two equalities hold simultaneously.

Let $G$ be a graph with $v \in V(G)$. As shown in Fig. 1, for two integers $m \geq k \geq 1$, let $G_{k,m}$ be the graph obtained from $G$ by attaching at $v$ two new paths $P : v = v_0 \rightarrow v_1 \rightarrow v_2 \cdots \rightarrow v_k$ and $Q : v = u_0 \rightarrow u_1 \rightarrow u_2 \cdots \rightarrow u_m$ of lengths $k$ and $m$, where $v_1, v_2, \ldots, v_k$ and $u_1, u_2, \ldots, u_m$ are distinct new vertices. Suppose that $G_{k-1,m+1} = G_{k,m} - v_{k-1}v_k + u_mv_k$. A related graph transformation is given in the following lemma.

**Lemma 2.3.** Let $G \neq K_1$ be a connected graph of order $n$ and $v \in V(G)$. If $m \geq k \geq 1$, then $H(G_{k,m}) > H(G_{k-1,m+1})$. 

Let $G$ be a connected graph of order $n$.

**Lemma 2.1.** Let $G$ be a connected graph of order $n$.

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**Proof.** By Lemma 2.2, we have

\[
H(G_{k,m}) = H(G_{k-1,m}) + n + k + m - 1 - Q_{G_{k-1,m}}(v_{k-1}),
\]

\[
H(G_{k-1,m+1}) = H(G_{k-1,m}) + n + k + m - 1 - Q_{G_{k-1,m}}(u_m),
\]

and

\[
H(G_{k,m}) - H(G_{k-1,m+1}) = Q_{G_{k-1,m}}(u_m) - Q_{G_{k-1,m}}(v_{k-1})
\]

\[
> 0.
\]

Note that the latter inequality holds because of the fact that $d_G(x, u_m) > d_G(x, v_{k-1})$ for any vertex $x$ in $G$. \(\square\)

Suppose that $G$ is a graph with $v_1 \in V(G)$, and $v_2, v_3, \ldots, v_{t+s}$ are distinct new vertices (not in $G$). Let $G'$ be the graph obtained from $G$ by attaching at $v_1$ a new path $P : v_1v_2 \cdots v_{t+s}$. Let $M_{t,s} = G' + v_1u_0$ and $M_{t+1,s} = G' + v_{t+1}u_0$ where $1 \leq i \leq s$ and $u_0$ is a new vertex not in $G'$. As two examples, $M_{t,s}$ and $M_{t+1,s}$ are shown in Fig. 2.

**Lemma 2.4.** Let $G$ be a connected graph of order $n > 1$. If $t > s > 1$, then $H(M_{t,t+s}) > H(M_{t+1,t+s})$.

**Proof.** By Lemma 2.2, we have

\[
H(M_{t,t+s}) = H(G') + n + t + s - 1 - Q_G(v_1),
\]

\[
H(M_{t+1,t+s}) = H(G') + n + t + s - 1 - Q_G(v_1 + 1), \quad \text{and,}
\]

\[
H(M_{t,t+s}) - H(M_{t+1,t+s}) = Q_G(v_1 + 1) - Q_G(v_1).
\]

Set $V_1 = V(G) \setminus \{v_1\}$ and $V(G') \setminus V_1 = V_2$. Then we have

\[
H(M_{t,t+s}) - H(M_{t+1,t+s}) = Q_G(v_1 + 1) - Q_G(v_1).
\]

(since $d_{M_{t+1,t+s}}(v_{t+1}, x) = d_{M_{t,t+s}}(v_t, x) + 1$ for any vertex $x$ in $G$)

\[
> 0.
\]

Note that the latter inequality holds by Lemma 2.1(2) and the hypothesis $t > s > 1$. \(\square\)

By Lemma 2.4, we obtain the next result immediately.

**Corollary 2.2.** Let $G$ be a connected graph of order $n > 1$. If $t > s > 1$, then we have $H(M_{t,t+s}) > H(M_{t+1,t+s})$ for $1 \leq i \leq s$.

Recall that a vertex $v$ of a tree $T$ is called a branching point of $T$ if $d(v) \geq 3$. Moreover, $v$ is said to be an out-branching point if at most one of the components of $T - v$ is not a path; otherwise, $v$ is an in-branching point of $T$. Next we will introduce another graph transformation: $T \longrightarrow T_A \longrightarrow T_B \longrightarrow T_C$ as shown in Fig. 3, where $T$ is a tree of order $n$ and $v$ is an out-branching point of $T$ with $d(v) = m$, and all the components $T_1, T_2, \ldots, T_m$ of $T - v$ except $T_1$ are paths.

**Lemma 2.5.** Let $T$ be a tree of order $n$ with $v$ as its out-branching point, and $d(v) = m \geq 3$. Suppose that all components of $T - v$ except $T_1$ are paths. Then $H(T) \geq H(T_A) \geq H(T_B) > H(T_C)$ with $H(T) = H(T_A)$ (or $H(T_B)$) if and only if $T = T_A$ (or $T_B$).

**Proof.** By Lemma 2.2, it follow that $H(T_A) > H(T_B)$ and $H(T) \geq H(T_A)$ with the equality holding if and only if $T = T_A$. Now it suffices to prove that $H(T_A) \geq H(T_B)$ with the equality holding if and only if $T_A = T_B$.\(\square\)
Let $G$ be a graph and $T$ a tree of order $l$ with $V(T) = \{v\}$. By the definition of Harary index, it is not difficult to obtain the following two lemmas.

**Lemma 2.6.** Let $G$ be a (connected) graph with a cut vertex $u$ such that $G_1$ and $G_2$ are two connected subgraphs of $G$ having $u$ as the only common vertex and $G_1 \bigcup G_2 = G$. Let $|V(G_i)| = n_i$ for $i = 1, 2$. Then $H(G) = H(G_1) + H(G_2) + \sum_{x \in V(G_1)} \sum_{y \in V(G_2)} d_G(x, y)$.

**Lemma 2.7.** Let $G$ be a graph and $w_1w_2 \in E(G)$ a cut edge in $G$, and $G - w_1w_2 = G_1 \bigcup G_2$ with $n_i = |V(G_i)|$ for $i = 1, 2$. Suppose that $w_i \in V(G_i)$ for $i = 1, 2$, then

$\begin{align*}
H(G) &= \sum_{i=1}^{2} H(G_i) + 1 + \sum_{x \in V(G_1)} \frac{1}{d_G(x, w_1)} + \sum_{y \in V(G_2)} \frac{1}{d_G(w_2, y)} \\
&\quad + \sum_{x \in V(G_1), y \in V(G_2)} \frac{1}{d_G(x, w_1) + 1 + d_G(w_2, y)}.
\end{align*}$

**Lemma 2.8** ([34]). Let $w_1w_2 \in E(G)$ be a cut edge in $G$, and $G - w_1w_2 = G_1 \bigcup G_2$ with $n_i = |V(G_i)| \geq 2$ for $i = 1, 2$. Suppose that $w_i \in V(G_i)$ for $i = 1, 2$. Assume that $G'$ is a graph obtained from $G$ by identifying vertex $w_1$ with $w_2$ (the new vertex is labeled as $w$) and attaching at $w$ a pendent vertex $w_0$ (see Fig. 4). Then $H(G) < H(G')$.

**Proof.** For convenience, we set $H(K_1) = 0$ and $G' - w_0 = G_1 \bullet G_2$. From Lemmas 2.6 and 2.7, we have

$\begin{align*}
H(G) &= \sum_{i=1}^{2} H(G_i) + 1 + \sum_{x \in V(G_1)} \frac{1}{d_G(x, w_1)} + \sum_{y \in V(G_2)} \frac{1}{d_G(w_2, y)} \\
&\quad + \sum_{x \in V(G_1), y \in V(G_2)} \frac{1}{d_G(x, w_1) + d_G(w_2, y)}.
\end{align*}$

$\begin{align*}
H(G') &= H(G_1 \bullet G_2) + H(K_1) + 1 + \sum_{x \in V(G_1 \bullet G_2)} \frac{1}{d_G(x, w_0)} \\
&= H(G_1) + H(G_2) + \sum_{x \in V(G_1 \bullet G_2)} \sum_{y \in V(G_2)} \frac{1}{d_G(x, u) + d_G(u, y)} + 1 + \sum_{x \in V(G_1 \bullet G_2)} \frac{1}{d_G(x, w_0)} \\
&= H(G_1) + H(G_2) + \sum_{x \in V(G_1 \bullet G_2)} \sum_{y \in V(G_2)} \frac{1}{d_G(x, u) + d_G(u, y)} + 1 + \sum_{x \in V(G_1 \bullet G_2)} \frac{1}{d_G(x, u)} \\
&\quad + \sum_{x \in V(G_1 \bullet G_2)} \sum_{y \in V(G_2)} \frac{1}{d_G(x, w) + d_G(w, y)}, \quad \text{and}
\end{align*}$

$\begin{align*}
H(G') - H(G) &= \sum_{x \in V(G_1 \bullet G_2)} \left[ \frac{1}{d_G(x, u) + d_G(u, y)} - \frac{1}{d_G(x, u) + d_G(u, y) + 1} \right] > 0.
\end{align*}$

Therefore the proof for this lemma is completed. □

Let $G_1, G_2$ be two connected graphs with $V(G_1) \bigcap V(G_2) = \{v\}$. Let $G_1 \cup G_2$ be a new graph with $V(G_1 \bigcup G_2)$ as its vertex set and $E(G_1 \bigcup G_2)$ as its edge set. By repeating Lemma 2.8, it is not difficult to obtain the following result.

**Corollary 2.3.** Let $G$ be a graph and $T_l$ a tree of order $l$ with $V(G) \bigcap V(T_l) = \{v\}$. Then we have $H(G \cup T_l) \leq H(G \cup S_l)$ where $v$ is identified with the center of the star $S_l$ in $G \cup S_l$. Moreover, the above equality holds if and only if $T_l \equiv S_l$.

**Lemma 2.9** ([34]). Let $A, X$ and $Y$ be three connected graphs with disjoint vertex sets. Suppose that $u, v$ are two vertices of $A$, $v_0$ is a vertex of $X$, $u_0$ is a vertex of $Y$. Let $G$ be the graph obtained from $A, X$ and $Y$ by identifying $v$ with $v_0$ and $u$ with $u_0$, respectively. Let $G_1^*$ be the graph obtained from $A, X$ and $Y$ by identifying two vertices $v, v_0$ and $u_0$, and let $G_2^*$ be the graph obtained from $A, X$ and $Y$ by identifying three vertices $u, v_0$ and $u_0$ (see Fig. 5). Then we have $H(G_1^*) > H(G) > H(G_2^*)$. 

Fig. 4. The graphs $G$ and $G'$ in Lemma 2.8.
For any tree $T$, we set $B_i = H(G_i^*) - H(G)$ for $i = 1, 2$. Then we have

\[
H(G) = \sum_{x \in V(X)} \frac{1}{d_G(x, y)} + \sum_{x \in V(A), y \in V(Y)} \frac{1}{d_G(x, y)} + \sum_{x \in V(X), y \in V(Y)} \frac{1}{d_G(x, y)} + \sum_{x \in V(X), y \in V(Y)} \frac{1}{d_G(x, y)}.
\]

\[
B_1 = \sum_{x \in V(X), y \in V(Y)} \left[ \frac{1}{d_G(x, y)} - \frac{1}{d_G(x, y)} \right] + \sum_{x \in V(A), y \in V(Y)} \left[ \frac{1}{d_G(x, y)} - \frac{1}{d_G(x, y)} \right] + \sum_{x \in V(A), y \in V(Y)} \left[ \frac{1}{d_G(x, y)} - \frac{1}{d_G(x, y)} \right].
\]

\[
B_2 = \sum_{x \in V(X), y \in V(Y)} \left[ \frac{1}{d_G(x, y)} - \frac{1}{d_G(x, y)} \right] + \sum_{x \in V(A), y \in V(Y)} \left[ \frac{1}{d_G(x, y)} - \frac{1}{d_G(x, y)} \right] + \sum_{x \in V(A), y \in V(Y)} \left[ \frac{1}{d_G(x, y)} - \frac{1}{d_G(x, y)} \right].
\]

If $B_1 \leq 0$, by (2.1), we have $\sum_{x \in V(X)} \frac{1}{d_G(x, y)} < 0$. By (2.2), we have $B_2 > 0$. Thus the result in this lemma follows immediately.

In the next lemma, we determine the extremal (maximal and minimal) Harary indices of trees in $\mathcal{T}(n)$. In order to do this, we need some definitions below.

Let $T_n(n_1, n_2, \ldots, n_m)$ be a starlike tree of order $n$ obtained from the star $S_{m+1}$ by replacing its $m$ edges by $m$ paths $P_{n_1}, P_{n_2}, \ldots, P_{n_m}$ with $\sum_{i=1}^{m} n_i = n - 1$. Obviously, any starlike tree has exactly one branching point. If the number of $P_{n_i}$ is $l_i > 1$, we write it as $n_i^l$ in the following. For example, $T_{11}(2, 2, 3, 3)$ will be written as $T_{11}(2^2, 3^2)$ for short. For a tree $T$ of order $n$ with two branching points $v_1$ and $v_2$ and $d(v_1) = r$ and $d(v_2) = t$, if the orders of $r - 1$ components, which are paths, of $T - v_1$ are $p_1, p_2, \ldots, p_{r-1}$, and the orders of $t - 1$ components, which are paths, of $T - v_2$ are $q_1, q_2, \ldots, q_{t-1}$, we write the tree as $T = T_n(p_1, p_2, \ldots, p_{r-1}; q_1, q_2, \ldots, q_{t-1})$ where $r \leq t$, $p_1 \geq p_2 \geq \cdots \geq p_{r-1}$ and $q_1 \geq q_2 \geq \cdots \geq q_{t-1}$. In particular, in $T_n(p_1, p_2, \ldots, p_{r-1}; q_1, q_2, \ldots, q_{t-1})$, if $p_1 = p_2 = \cdots = p_{r-1} = 1 = q_1 = q_2 = \cdots = q_{t-1}$ and $r + t = n$, we denote this tree by $S_n(r - 1, t - 1)$ (i.e., the so-called double star).

**Lemma 2.10.** For any tree $T$ in $\mathcal{T}(n) \setminus \{P_n, S_n\}$, we have $H(P_n) < H(T) < H(S_n)$.

**Proof.** First we prove the right inequality by induction on $d$, i.e., the diameter of $T$.

If $d = 2$, there is only one tree $S_n$ in $\mathcal{T}(n)$, and there is nothing to prove. When $d = 3$, then $T = S_n(a, b)$ for two positive integers $a, b$ with $a + b = n$. By Lemma 2.8, $H(T) = H(S_n(a, b)) < H(S_n)$, and the right inequality holds.

Assume that the right inequality holds for all trees with diameter $d < k$. Suppose that $T$ is a tree with diameter $k$ and Harary index as large as possible. Then, by Corollary 2.3 and Lemmas 2.2 and 2.9, we find that $T = T_n\left(\left\lfloor \frac{k}{2} \right\rfloor, \left\lceil \frac{k}{2} \right\rceil, 1^{n-k-1}\right)$. 

![Fig. 5. The graphs $G, G_1$, and $G_2$ in Lemma 2.9.](image-url)
Similarly, we obtain

\[ H(T_n\left(\frac{k}{2}, \frac{k}{2}, 1^{n-k-1}\right)) < H(T_n\left(\frac{k-1}{2}, \frac{k-1}{2}, 1^{n-k}\right)) < H(S_n), \]

finishing the proof for the right inequality.

Next we turn to the proof of the left inequality. We prove it by induction on \( \Delta \), i.e., the maximum degree of \( T \) in \( T(n) \). If \( \Delta = 2 \), there exists only one tree \( P_2 \) in \( T(n) \) and there is nothing to prove. For \( \Delta = 3 \), by using repeatedly Lemma 2.2, any tree \( T \) in \( T(n) \) can be changed into some tree \( T_n(n_1, n_2, n_3) \). By Lemma 2.5, we claim that \( H(T_n(n_1, n_2, n_3)) \) attains the minimum value at \( T_n(n-3, 1^2) \). Thanks to Lemma 2.5, again, \( H(T_n(n-3, 1^2)) > H(P_n) \), thus the left inequality holds clearly.

Assume that the left inequality holds for all trees with maximum degree \( \Delta < k \). Suppose that \( T \) is a tree in \( T(n) \) and with maximum degree \( k \) and Harary index as small as possible. By Lemmas 2.2 and 2.5, we find that \( T \cong T_n(n-k, 1^{n-k-1}) \).

In view of Lemma 2.5 and the induction hypothesis, we have

\[ H(T_n(n-k, 1^{k-1})) > H(T_n(n-k-1, 1^k)) > H(P_n), \]

completing the proof of the left inequality.

3. Ordering of trees w.r.t. smallest Harary indices

In this section we will determine the first up to seventh smallest Harary indices of trees in \( T(n) \) with \( n \geq 16 \).

**Lemma 3.1.** Suppose that \( n \geq 16 \). Then we have \( H(T_n(n - 4, 1^3)) > H(T_n(1, 1; 2, 1)) > H(T_n(n - 5, 3, 1)) > H(T_n(1, 1; 1, 1)) > H(T_n(n - 4, 2, 1)) > H(T_n(n - 3, 1^2)). \)

**Proof.** By Lemma 2.5, we have \( H(T_n(n - 4, 2, 1)) > H(T_n(n - 3, 1^2)) \).

Now we consider the other four inequalities. For convenience, the trees \( T_n(n - 4, 1^3) \), \( T_n(1, 1; 2, 1) \), \( T_n(n - 5, 3, 1) \), \( T_n(1, 1; 1, 1) \), \( T_n(n - 4, 2, 1) \) are shown in Fig. 6. Set \( A_1 = H(T_n(1, 1; 1, 1)) - H(T_n(n - 4, 2, 1)), A_2 = H(T_n(n - 5, 3, 1)) - H(T_n(n - 4, 2, 1)) \).

By Lemma 2.2, we have

\[ H(T_n(n - 4, 2, 1)) = H(T_n(1, 1; 1, 1) + n - 1 - Q_{T_n-1(n-3,1^2)}(u_1), \]
\[ H(T_n(1, 1; 1, 1)) = H(T_n(n - 4, 1^3)) + n - 1 - Q_{T_n-1(n-3,1^2)}(u_2), \]
\[ H(T_n(n - 5, 3, 1)) = H(T_n(n - 5, 2, 1)) + n - 1 - Q_{T_n-1(n-5,2,1)}(u_3), \]
\[ H(T_n(1, 1; 2, 1)) = H(T_n(n - 5, 2, 1)) + n - 1 - Q_{T_n-1(n-5,2,1)}(u_4) \]
\[ = H(T_n(n - 4, 1^3)) + n - 1 - Q_{T_n-1(n-4,1^3)}(u_5), \]
\[ H(T_n(n - 4, 1^3)) = H(T_n(n - 4, 1^3)) + n - 1 - Q_{T_n-1(n-4,1^3)}(u_6). \]

So we have

\[ Q_{T_n-1(n-3,1^2)}(u_1) - Q_{T_n-1(n-3,1^2)}(u_2) = \frac{1}{2} + \frac{2}{3} + \frac{3}{4} + \cdots + \frac{n-5}{n-4} + \frac{n-4}{n-3} + \frac{n-3}{n-2} - \left( \frac{1}{2} + \frac{2}{3} + \frac{3}{4} + \cdots + \frac{n-5}{n-4} + \frac{n-4}{n-3} + \frac{n-3}{n-2} \right) \]
\[ = \frac{2}{3} \times \left( \frac{n-3}{n-2} - \frac{n-4}{n-3} \right) > 0. \]

Thus, we get \( A_1 > 0 \) from Corollary 2.1.

Set \( A_2 = H(T_n(n-5, 2, 1)) - H(T_n(n-3, 1^2)) \) and \( A_2 = Q_{T_n-1(n-3,1^2)}(u_2) - Q_{T_n-1(n-5,2,1)}(u_3) \). Then \( A_2 = A_2 + A_2^2 \).

Similarly, we obtain

\[ A_2 = \frac{n-4}{n-3} - \frac{2}{3}. \]
So we have

$$A_2 = A_2^{(1)} + A_2^{(2)}$$

$$= \frac{1}{12} - \frac{1}{n-3} - \frac{1}{(n-2(n-3))} > 0 \quad \text{for } n \geq 16.$$  

As shown in Fig. 6, by the definition of $Q_{c}(u)$,

$$Q_{T(n-1)(n-5,2,1)}(u_3) - Q_{T(n-1)(n-5,2,1)}(u_4) = \frac{1}{2} \times 2 + \frac{2}{3} \times 2 + \cdots + \frac{n-5}{n-4} \times 2 - \left(\frac{1}{2} \times 2 + \frac{2}{3} \times 2 + \cdots + \frac{n-5}{n-4} \times 2 \right)$$

$$= \frac{1}{4} - \left(\frac{n-3}{n-2} - \frac{n-4}{n-3}\right) > 0.$$

$$Q_{T(n-1)(n-4,1,2)}(u_5) - Q_{T(n-1)(n-4,1,2)}(u_6) = \frac{1}{2} \times 2 + \frac{2}{3} \times 2 + \frac{3}{4} \times 2 + \cdots + \frac{n-5}{n-4} \times 2$$

$$- \left(\frac{1}{2} \times 2 + \frac{2}{3} \times 2 + \cdots + \frac{n-5}{n-4} \times 2\right)$$

$$= \frac{1}{6} - \frac{1}{(n-3)(n-4)} > 0.$$  

Thanks to Corollary 2.1, it follows that $A_i > 0$ for $i = 3, 4$. Thus the proof of this lemma is completed. \qed

In a similar way as that in the proof of Lemma 3.1, it is not difficult to obtain the following lemma.

**Lemma 3.2.** Let $n \geq 16$. Then $H(T(n, 2, 1; 2, 1)) > H(T(n, 1; 1; 3, 1)) > H(T(n, n-4, 1, 3)).$

**Lemma 3.3.** Suppose that $n \geq 16$. For any tree $T \in T(n) \setminus \{T(n-3, 1^2), T(n-4, 2, 1), T(n-5, 3, 1), T(n-4, 1^3)\}$ and with only one branching point, $H(T) > H(T(n, n-4, 1^3)).$

**Proof.** By hypothesis, we assume that $T = T_n(n_1, n_2, \ldots, n_m)$ with $n_1 \geq n_2 \geq \cdots \geq n_m$. When $m \geq 4$, by Lemma 2.5 and considering $T \neq T_n(n, 4, 1^3)$, it follows that

$$H(T) = H(T_n(n_1, n_2, \ldots, n_m)) \geq H(T_n(n_1, n_m - 1, n_2, \ldots, 1))$$

$$> H(T_n(n_1 + n_m, n_2, \ldots, n_m))$$

$$> \cdots > H\left(T_n\left(n_1 + \sum_{i=5}^{m} n_i, n_2, n_3, n_4\right)\right)$$

$$> H\left(T_n\left(n_1 + \sum_{i=5}^{m} n_i + n_4 - 1, n_2, n_3, 1\right)\right)$$

$$> H\left(T_n\left(n_1 + \sum_{i=5}^{m} n_i + n_4 + n_3 - 2, n_2, 1, 1\right)\right)$$

$$> H\left(T_n\left(n_1 + \sum_{i=5}^{m} n_i + n_4 + n_3 + n_2 - 3, 1, 1, 1\right)\right) = H(T_n(n-4, 1^3)).$$  

For $m = 3$, we have $T = T_n(n_1, n_2, n_3)$. It suffices to consider the following two cases: $n_3 = 1$ and $n_3 \geq 2$.

If $n_3 = 1$, then by Lemma 2.3, it follows that $H(T) > H(T_n(n-6, 4, 1^3))$ since $T \not\in \{T_n(n-3, 1^2), T_n(n-4, 2, 1), T_n(n-5, 3, 1)\}$. Applying Lemma 2.2 to the pendant vertex which is at the distance 4 from the unique 3-degree vertex of the tree $T_n(n-6, 4, 1)$ and to the vertex $v_0$ of $T_n(n-4, 1^3)$ as shown in Fig. 6, by Corollary 2.1 and a direct calculation, we have $H(T_n(n-6, 4, 1^3)) > H(T_n(n-4, 1^3)).$

If $n_3 \geq 2$, then by Lemma 2.3, it follows that $H(T) > H(T_n(n-5, 2, 2, 2))$. Similarly, applying Lemma 2.2 to one pendant vertex at distance 2 from the 3-degree vertex of $T_n(n-5, 2, 2)$ and to the vertex $v_0$ of $T_n(n-4, 1^3)$ as shown in Fig. 6, by Corollary 2.1 and a direct calculation, we have $H(T_n(n-5, 2, 2)) > H(T_n(n-4, 1^3)).$

Thus we claim that $H(T) > H(T_n(n-4, 1^3))$ for any tree $T = T_n(n_1, n_2, n_3) \not\in \{T_n(n-3, 1^2), T_n(n-4, 2, 1), T_n(n-5, 3, 1)\}$, which completes the proof of this lemma. \qed
Lemma 3.4. Suppose that $n \geq 16$. For any tree $T \in \mathcal{T}(n) \setminus \{T_n(1, 1; 1, 1), T_n(1, 1; 2, 1)\}$ and with two branching points, $H(T) > H(T_n(n - 4, 1^3))$.

Proof. By hypothesis, $T = T_n(p_1, p_2, \ldots, p_{r-1}; q_1, q_2, \ldots, q_{t-1})$. According to the degrees of these two branching points, we divide the proof into the following cases.

Case 1. $t \geq 4$.

By Lemma 2.5, it follows that

$$H(T) > H\left(T_n\left(q_1, q_2, \ldots, q_{t-1}, n - \sum_{i=1}^{t-1} q_i - 1\right)\right) \geq H(T_n(n - 4, 1^3)).$$

Case 2. $r = t = 3$.

In this case, $T = T_n(p_1, p_2, q_1, q_2)$. Without loss of generality, assume that $q_1 + q_2 \geq p_1 + p_2$. Since $T \notin \{T_n(1, 1; 1, 1), T_n(1, 1; 2, 1)\}$, then $3 \leq q_1 + q_2 \leq n - 4$. Next we consider the following subcases.

Subcase 2.1. $q_1 + q_2 = 3$.

In this case, $2 \leq p_1 + p_2 \leq 3$. From the choice of $T$, $T = T_n(2, 2; 1, 1)$. By Lemma 3.2, we have $H(T_n(2, 1; 2, 1)) > H(T_n(n - 4, 1^3)).$

Subcase 2.2. $4 \leq q_1 + q_2 \leq n - 4$.

In view of Corollary 2.2 and Lemma 3.2, it follows that

$$H(T) = H(T_n(p_1, p_2, q_1, q_2)) \geq H(T_n(1, 1; q_1 + q_2 - 1, 1)) \geq H(T_n(1, 3, 1)) > H(T_n(n - 4, 1^3)).$$

This completes the proof of this lemma. □

Lemma 3.5. Suppose that $n \geq 16$. For any tree $T \in \mathcal{T}(n)$ and with $k \geq 3$ branching points, we have $H(T) > H(T_n(n - 4, 1^3))$.

Proof. According to the value of $k$, we only need to consider the following two cases.

Case 1. $k = 3$.

In this case, we assume that $u_1, u_2, u_3$ are three branching points of $T$ with $u_1$ as its in-branching point and $u_2, u_3$ as its out-branching points. Let $d(u_i) = m$ and $T_1, T_2, \ldots, T_m$ be the components of $T - u_1$. Suppose that $T_1, T_2, \ldots, T_m$ except $T_m-1, T_n$ are paths and the order of $T_i$ is $n_i$ for $1 \leq i \leq m$. By hypothesis, it follows that $u_2 \in V(T_{m-1})$ and $u_3 \in V(T_m)$ and $n_m - 1, m \geq 3$. Without loss of generality, assume that $n_m - 1, m \geq 3$. By Lemma 2.3, $\sum_{i=1}^{m-2} n_i \geq 2$.

Recall that $n_m - 1, m \geq 3$. By Lemma 2.3,

$$H(T) > H\left(T_n\left(n_m - 1, n_m, \sum_{n=1}^{m-2} n_i\right)\right) \geq H(T_n(n - 6, 3, 2)) > H(T_n(n - 5, 2, 2)) > H(T_n(n - 4, 1^3)).$$

Note that the last inequality holds from the proof of Lemma 3.3.

Subcase 1.2. $n_1 + n_2 + \cdots + n_m = 1$.

This implies that $m = 3$ and $n_1 = 1$. If $n_3 \geq 4$, by Lemma 2.3,

$$H(T) > H(T_n(n_2, n_3, 1)) \geq H(T_n(n - 6, 4, 1)) > H(T_n(n - 4, 1^3)).$$

Note that the last inequality holds from the proof of Lemma 3.3, again. If $n_3 = 3$, by Lemmas 2.5 and 3.2, we obtain

$$H(T) > H(T_n(1, 1; n - 5, 1)) > H(T_n(1, 3, 1)) > H(T_n(n - 4, 1^3)).$$

Case 2. $k > 3$.

We prove this case by induction on $k$. By Case 1, it is true for $k = 3$.

Let $T$ be a tree with $k \geq 4$ branching points. Then $T$ must have an out-branching point. By Lemma 2.5, $H(T) > H(T_c)$ where $T_c$ has $k - 1$ branching points. It follows that $H(T_c) > H(T_n(n - 4, 1^3))$ by the induction hypothesis. So we complete the proof of this lemma. □

Combining Lemma 2.10 with Lemmas 3.1–3.5, one of the main results below follows immediately.

Theorem 3.1. Let $n \geq 16$ and $T \in \mathcal{T}(n) \setminus \{P_n, T_n(n - 3, 1^2), T_n(n - 4, 2, 1), T_n(1, 1; 1, 1), T_n(n - 5, 3, 1), T_n(1, 1; 2, 1), T_n(n - 4, 1^3)\}$. Then $H(T) > H(T_n(n - 4, 1^3)) > H(T_n(1, 1; 2, 1)) > H(T_n(n - 5, 3, 1)) > H(T_n(1, 1; 1, 1)) > H(T_n(n - 4, 2, 1)) > H(T_n(n - 3, 1^2)) > H(P_n)$. 
4. Ordering trees w.r.t. greatest Harary indices

We now turn to the eighth greatest Harary indices of trees from $\mathcal{T}(n)$ with $n \geq 14$. Let $T_1 = S_n$, and let $T_2, T_3, \ldots, T_8$ be the trees of order $n \geq 14$ as shown in Fig. 7. From Eq. (1.1), we have

\[
H(T_2) = n - 1 + \frac{1}{2} \left( \frac{n - 2}{2} \right) + \frac{1}{3} (n - 3),
\]

\[
H(T_3) = n - 1 + \frac{1}{2} \left[ n - 2 + \left( \frac{n - 4}{2} \right) + 1 \right] + \frac{2}{3} (n - 4),
\]

\[
H(T_4) = n - 1 + \frac{1}{2} \left[ \left( \frac{n - 3}{2} \right) + 2 \right] + \frac{2}{3} (n - 5) + \frac{1}{4} (n - 4),
\]

\[
H(T_5) = n - 1 + \frac{1}{2} \left[ \left( \frac{n - 3}{2} \right) + 2 \right] + \frac{1}{3} (n - 3) + \frac{1}{4} (n - 4),
\]

\[
H(T_6) = n - 1 + \frac{1}{2} \left[ \left( \frac{n - 5}{2} \right) + \left( \frac{3}{2} \right) \right] + \frac{3}{3} (n - 5),
\]

\[
H(T_7) = n - 1 + \frac{1}{2} \left[ \left( \frac{n - 4}{2} \right) + 4 \right] + \frac{1}{3} [3(n - 6) + 3] + \frac{2}{4},
\]

\[
H(T_8) = n - 1 + \frac{1}{2} \left[ \left( \frac{n - 4}{2} \right) + 3 \right] + \frac{1}{3} [3(n - 7) + 6] + \frac{3}{4}.
\]

Thus we have the following lemma.

**Lemma 4.1.** Suppose that $n \geq 14$. Then $H(T_2) > H(T_3) > H(T_4) > H(T_5) > H(T_6) > H(T_7) > H(T_8)$.

The first Zagreb index $M_1(G)$ is defined as [19]:

\[
M_1(G) = \sum_{v \in V(G)} d_c(v)^2.
\]

As an important topological index, it has been closely correlated with many chemical and mathematical properties [3, 14, 37].

**Lemma 4.2** ([22]). Let $T$ be a tree of order $n$ with maximum degree $\Delta$. Then

\[
M_1(T) \leq \max \left\{ (n - 1) \left( \Delta + \frac{n - 1}{\Delta} \right), \frac{(n - 1)(n + 3)}{2} \right\}.
\]

**Lemma 4.3** ([37]). Let $G$ be a tree of order $n$ and with $m$ edges, which does not contain triangles or quadrangles. Then we have $H(G) \leq \frac{n(n - 1)}{6} + \frac{m}{2} + \frac{1}{12} M_1(G)$.

**Lemma 4.4.** Let $n \geq 14$. For any tree $T \in \mathcal{T}(n)$ with maximum degree $\Delta \leq n - 7$, we have $H(T) < H(T_8)$.

**Proof.** Let $f(x) = x + \frac{n - 1}{x}$ where $x \in [2, n - 7]$. Then $f'(x) = 1 - \frac{n - 1}{x^2}$. Moreover, it is easily checked that $f(x) \leq \max \left\{ n - 7 + \frac{n - 1}{n - 7}, 2 + \frac{n - 1}{2} \right\}$. Note that $2 \leq \Delta \leq n - 7$. By Lemma 4.2,

\[
M_1(T) \leq \max \left\{ (n - 1)(n - 7) + \frac{(n - 1)^2}{n - 7}, \frac{(n - 1)(n + 3)}{2} \right\}.
\]

Combining Lemma 4.3 with the fact $n \geq 14$, we obtain

\[
H(T) \leq \frac{n(n - 1)}{6} + \frac{n - 1}{2} + \frac{1}{12} M_1(T)
\]

\[
\leq \max \left\{ \frac{(n - 1)(n + 3)}{6} + \frac{(n - 1)(n - 7)}{12} + \frac{(n - 1)^2}{12(n - 7)}, \frac{(n - 1)(n + 3)}{6} + \frac{(n - 1)(n + 3)}{24} \right\}
\]

\[
= \max \left\{ \frac{3n^2 - 4n + 1}{12} + \frac{(n - 1)^2}{12(n - 7)}, \frac{5(n - 1)(n + 3)}{24} \right\}
\]

\[
< 2n - 6 + \frac{n^2 - 9n + 29}{4} = H(T_8).
\]

This completes the proof of this lemma. \qed
Lemma 4.5. Let $n \geq 14$. For any tree $T \in \mathcal{T}(n)$ with maximum degree $\Delta \in \{n - 6, n - 5\}$, we have $H(T) < H(T_8)$.

Proof. Assume that $T \in \mathcal{T}(n)$ with maximum degree $\Delta \in \{n - 6, n - 5\}$ has the Harary index as large as possible. Then $T$ has a star $S_{\Delta+1}$ as an induced subgraph. In view of Corollary 2.3 and Lemma 2.9, we find that $T \cong S_9(\Delta - 1, n - \Delta - 1)$. Note that $4 \leq n - \Delta - 1 \leq 5 < \Delta - 1$ since $\Delta \in \{n - 6, n - 5\}$. By Lemma 2.9, again, $H(S_9(\Delta - 1, n - \Delta - 1))$ reaches its maximum at $\Delta = n - 5$. From Eq. (1.1), we have

$$H(S_9(n - 6, 4)) = n - 1 + \frac{1}{2} \left( n - 2 + \left( \frac{n - 6}{2} \right) + 4 \right) + \frac{4}{3} (n - 6) < H(T_8),$$

which completes the proof of this lemma. □

Lemma 4.6. Let $n \geq 14$. For any tree $T \in \mathcal{T}(n) \setminus \{T_6, T_7, T_8\}$ with maximum degree $\Delta = n - 4$, we have $H(T) < H(T_8)$.

Proof. It is easy to see that there exist only three trees $T_6, T_7, T_8$ in $\mathcal{T}(n)$ and with maximum degree $n - 4$ and diameter 3. By hypothesis, the diameter $D(T) \geq 4$, therefore, $T$ must contain $T_6 = T_{n-1}(1^{n-5}, 3)$ as an induced subgraph.

Assume that $\{v_1\} = V(T) \setminus V(T_0)$. We find that $v_1$ must be adjacent to one vertex of $T$ except the unique vertex of maximum degree. By Lemmas 2.3 and 2.5, we claim that $H(T)$ reaches its maximum value at one of the two trees shown in Fig. 8 (the vertex $v_1$ is labeled as $v_1'$ and $v_1''$ in $T'$ and $T''$, respectively).

Applying Lemma 2.2 to the vertices $v_1'$ and $v_1''$ of $T'$ and $T''$, respectively, considering Corollary 2.1, we obtain $H(T'') > H(T')$. From Eq. (1.1), we have

$$H(T'') = n - 1 + \frac{1}{2} \left( \left( \frac{n - 5}{2} \right) + 1 \right) \left( 2n - 9 \right) + \frac{1}{4} (n - 4) + \frac{1}{5}.$$ 

Moreover, for $n \geq 14$,

$$H(T_8) - H(T'') = \frac{n - 3}{12} - \frac{1}{5} > 0.$$

Therefore, $H(T) < H(T_8)$ for any tree $T \in \mathcal{T}(n) \setminus \{T_6, T_7, T_8\}$ and with maximum degree $\Delta = n - 4$, completing the proof of this lemma. □

Theorem 4.1. Let $n \geq 14$ and $T \in \mathcal{T}(n) \setminus \{S_n, T_2, T_3, T_4, T_5, T_6, T_7, T_8\}$. Then

$$H(T) < H(T_6) < H(T_7) < H(T_8) < H(T_9) < H(T_2) < H(T_2) < H(S_n).$$

Proof. Note that $T_3, T_4, T_5$ are all the trees with maximum degree $\Delta - 3$ and $T_2$ is the only tree with maximum degree $n - 2$. Combining Lemma 2.10 with Lemmas 4.1 and 4.4–4.6, this theorem follows immediately. □

5. Remarks

As three distance-based topological indices of graphs, Wiener index, hyper-Wiener index and Harary index are closely correlated. The relations between them and with other topological indices have been reported by some authors [13,15, 37,38]. For example, in [22], it was pointed out that $T_{n_1}(1, 1; 2, 1), T_{n_1}(n - 4, 1^3), T_{n_1}(n - 5, 3, 1), T_{n_1}(1, 1; 1, 1), T_{n_1}(n - 4, 2, 1), T_{n_1}(n - 3, 1^3), P_n$ are trees from $\mathcal{T}(n)$ where $n \geq 20$ with the seven greatest hyper-Wiener indices, moreover, $S_n, T_2, T_3, T_4, T_5, T_6, T_7, T_8$ except $T_5$ are the ones from $\mathcal{T}(n)$ where $n \geq 17$ with the seventh smallest hyper-Wiener indices. Note that these trees are exactly the extremal ones with respect to Harary index from $\mathcal{T}(n)$ except that $T_{n_1}(n - 4, 1^3), T_{n_1}(1, 1; 2, 1)$ are the trees in this set with seventh, sixth smallest Harary indices, respectively.

We will end the paper with the following remarks, that seem to be worth researching in the future.
Remark 5.1. In what set \( \mathcal{G}(n) \) of connected graphs of order \( n \), are the extremal (maximal or minimal) Harary index and the extremal (maximal or minimal) hyper-Wiener index attained at the same graph?

Remark 5.2. In what set \( \mathcal{G}(n) \) of connected graphs of order \( n \), are the extremal (maximal or minimal) Harary index and the extremal (maximal or minimal) Wiener index attained at the same graph?

Remark 5.3. In what set \( \mathcal{G}(n) \) of connected graphs of order \( n \), are the extremal (maximal or minimal) hyper-Wiener index and the extremal (maximal or minimal) Wiener index attained at the same graph?

Remark 5.4. Which are the further relations among these three topological indices: Wiener index, hyper-Wiener index and Harary index, especially between (hyper-)Wiener index and Harary index?

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