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Trees with the seven smallest and eight greatest Harary indices ☆

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A R T I C L E I N F O

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A B S T R A C T

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 $n \geq 14$.

1. Introduction

The Harary index of a graph G, denoted by $H(G)$, was been independently by Plavšićet 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].

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Let $\gamma(G, k)$ be the number of vertex pairs of the graph G that are at distance k. Then

$$H(G) = \sum_{k\geq 1} \frac{1}{k}\gamma(G, k). \tag{1.1}$$

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 $N_G(v)$ the neighbors of v in G. $d_G(v) = |N_G(v)|$ 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 pendent vertex. An edge $e = uv$ incident with the pendent vertex v is a pendent 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 $\mathcal{T}(n)$ 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 $\mathcal{T}(n)$ (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 $\mathcal{T}(n)$ with $n \geq 20$ and the seventh smallest hyper-Wiener indices of trees in $\mathcal{T}(n)$ 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 $\mathcal{T}(n)$ with $n \geq 16$, which are all molecular trees, and the first up to eighth greatest Harary indices of trees in $\mathcal{T}(n)$ 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 $Q_G(v) = \sum_{u\in V(G)} \frac{d_G(u,v)}{d_G(u,v)+1}$. For convenience, sometimes we write $Q_G(v)$ as $Q_{V(G)}(v)$. Note that the function $f(x) = \frac{x}{x+1}$ 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) $Q_{P_n}(v_j) = Q_{P_n}(v_{n-j})$ *for* $1 \leq j \leq \left\lfloor \frac{n}{2} \right\rfloor$;
(2) $Q_{P_n}(v_j) > Q_{P_n}(v_{j+1})$ *for* $1 \leq j \leq \left\lfloor \frac{n}{2} \right\rfloor$;
(3) $Q_{P_n}(v_j) > Q_{P_n}(v_{n-k})$ *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 pendent vertex of G with $uv \in E(G)$. Then we have $H(G) = H(G-v) + n - 1 - Q_{G-v}(u)$.*

Proof. By the definitions of Harary index and $Q_G(u)$, we have

$$\begin{aligned} H(G) &= \sum_{u,v\in V(G-v)} \frac{1}{d_G(u,v)} + \sum_{x\in V(G-v)} \frac{1}{d_G(x,v)} \\ &= H(G-v) + \sum_{x\in V(G-v)} \frac{1}{d_G(x,u)+1} \\ &= H(G-v) + \sum_{x\in V(G-v)} \left(1 - \frac{d_G(x,u)}{d_G(x,u)+1}\right) \\ &= H(G-v) + n - 1 - Q_{G-v}(u), \end{aligned}$$

completing the proof of the lemma. □

Corollary 2.1. *Let G_1 and G_2 be two graphs of same order and with v_i as a pendent vertex of G_i and $u_iv_i \in E(G_i)$ 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 $P : v(=v_0)v_1v_2\cdots v_k$ and $Q : v(=u_0)u_1u_2\cdots u_m$ 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 $H(G_{k,m}) > H(G_{k-1,m+1})$.*

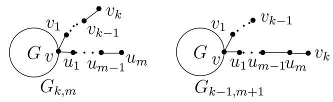

Fig. 1. The graphs $G_{k,m}$ and $G_{k-1,m+1}$.

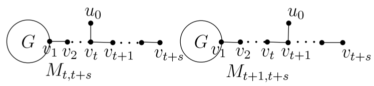

Fig. 2. The graphs $M_{t,t+s}$ and $M_{t+1,t+s}$.

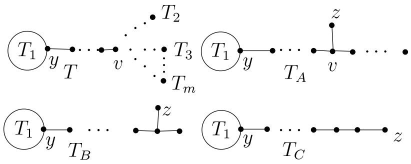

Fig. 3. The trees T, T_A, T_B and T_C.

Proof. By Lemma 2.2, we have

$$\begin{aligned}
&H(G_{k,m}) = H(G_{k-1,m}) + n + k + m - 1 - Q_{G_{k-1,m}}(v_{k-1}),\\
&H(G_{k-1,m+1}) = H(G_{k-1,m}) + n + k + m - 1 - Q_{G_{k-1,m}}(u_m), \quad \text{and}\\
&H(G_{k,m}) - H(G_{k-1,m+1}) \;=\; Q_{G_{k-1,m}}(u_m) - Q_{G_{k-1,m}}(v_{k-1})\\
&\qquad\qquad\qquad\qquad\quad\;\, = \; Q_{G-v}(u_m) - Q_{G-v}(v_{k-1}) \quad \text{by Lemma 2.1(1)}\\
&\qquad\qquad\qquad\qquad\quad\;\, > \; 0.
\end{aligned}$$

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 $M_{t,t+s} = G' + v_tu_0$ and $M_{t+i,t+s} = G' + v_{t+i}u_0$ where $1 \le i \le s$ and u_0 is a new vertex not in G'. As two examples, $M_{t,t+s}$ and $M_{t+1,t+s}$ 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

$$\begin{aligned}
&H(M_{t,t+s}) = H(G') + n + t + s - 1 - Q_{G'}(v_t),\\
&H(M_{t+1,t+s}) = H(G') + n + t + s - 1 - Q_{G'}(v_{t+1}), \quad \text{and,}\\
&H(M_{t,t+s}) - H(M_{t+1,t+s}) = Q_{G'}(v_{t+1}) - Q_{G'}(v_t).
\end{aligned}$$

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

$$\begin{aligned}
H(M_{t,t+s}) - H(M_{t+1,t+s}) &= Q_{V_1}(v_{t+1}) - Q_{V_1}(v_t) + Q_{V_2}(v_{t+1}) - Q_{V_2}(v_t)\\
&> Q_{V_2}(v_{t+1}) - Q_{V_2}(v_t)\\
(\text{since } d_{M_{t+1,t+s}}(v_{t+1}, x) &= d_{M_{t,t+s}}(v_t, x) + 1 \quad \text{for any vertex } x \text{ in } G)\\
&> 0.
\end{aligned}$$

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 $H(M_{t,t+s}) > H(M_{t+i,t+s})$ for $1 \le i \le s$.*

Recall that a vertex v of a tree T is called a *branching point* of T if $d(v) \ge 3$. 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 $d(v) = m \ge 3$. Suppose that all components of $T - v$ except T_1 are paths. Then $H(T) \ge H(T_A) \ge H(T_B) > H(T_C)$ 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 $H(T_B) > H(T_C)$ and $H(T) \ge H(T_A)$ with the equality holding if and only if $T \cong T_A$. Now it suffices to prove that $H(T_A) \ge H(T_B)$ with the equality holding if and only if $T_A \cong T_B$.

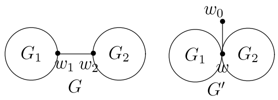

Fig. 4. The graphs G and G' in Lemma 2.8.

Considering the structures of T_A and T_B, from Corollary 2.2, the desired result holds clearly, completing the proof of this lemma. $\square$

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 $H(G) = H(G_1) + H(G_2) + \sum_{x\in V(G_1-u)} \sum_{y\in V(G_2-u)} \frac{1}{d_{G_1}(x,u)+d_{G_2}(u,y)}$.*

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*

$$H(G) = \sum_{i=1}^{2} H(G_i) + 1 + \sum_{x\in V(G_1)} \frac{1}{d_G(x, w_1) + 1} + \sum_{y\in V(G_2)} \frac{1}{d_G(w_2, y) + 1} + \sum_{x\in V(G_1-w_1), y\in V(G_2-w_2)} \frac{1}{d_{G_1}(x, w_1) + 1 + d_{G_2}(w_2, v)}.$$

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

$$\begin{aligned} H(G) &= \sum_{i=1}^{2} H(G_i) + 1 + \sum_{x\in V(G_1)} \frac{1}{d_{G_1}(x, w_1) + 1} + \sum_{y\in V(G_2)} \frac{1}{d_{G_2}(w_2, y) + 1} \\ &\quad + \sum_{x\in V(G_1-w_1), y\in V(G_2-w_2)} \frac{1}{d_{G_1}(x, w_1) + 1 + d_{G_2}(w_2, v)}, \\ H(G') &= H(G_1 \bullet G_2) + H(K_1) + 1 + \sum_{x\in V(G_1\bullet G_2)} \frac{1}{d_{G'}(x, w_0)} \\ &= H(G_1) + H(G_2) + \sum_{x\in V(G_1)} \sum_{y\in V(G_2)} \frac{1}{d_{G_1}(x, u) + d_{G_2}(u, y)} + 1 + \sum_{x\in V(G_1\bullet G_2)} \frac{1}{d_{G'}(x, w_0)} \\ &= H(G_1) + H(G_2) + 1 + \sum_{x\in V(G_1)} \frac{1}{d_{G_1}(x, w) + 1} + \sum_{y\in V(G_2)} \frac{1}{d_{G_2}(w, y) + 1} \\ &\quad + \sum_{x\in V(G_1), y\in V(G_2)} \frac{1}{d_{G_1}(x, w) + d_{G_2}(w, y)}, \quad \text{and} \end{aligned}$$

$$H(G') - H(G) = \sum_{x\in V(G_1), y\in V(G_2)} \left[\frac{1}{d_{G_1}(x, w) + d_{G_2}(w, y)} - \frac{1}{d_{G_1}(x, w) + d_{G_2}(w, y) + 1} \right] > 0.$$

Therefore the proof for this lemma is completed. $\square$

Let G_1, G_2 be two connected graphs with $V(G_1) \bigcap V(G_2) = \{v\}$. Let G_1vG_2 be a new graph with $V(G_1) \bigcup V(G_2)$ as its vertex set and $E(G_1) \bigcup E(G_2)$ 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 $H(GvT_l) \leq H(GvS_l)$ where v is identified with the center of the star S_l in GvS_l. Moreover, the above equality holds if and only if $T_l \cong S_l$.*

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 three 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 $H(G_1^*) > H(G)$ or $H(G_2^*) > H(G)$.*

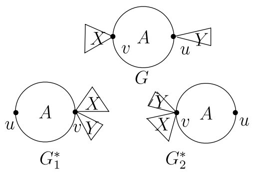

Fig. 5. The graphs G, G_1^* and G_2^* in Lemma 2.9.

Proof. For convenience, we set $B_i = H(G_i^*) - H(G)$ for $i = 1, 2$. Then we have

$$\begin{aligned} H(G) &= \sum_{x,y\in V(X)} \frac{1}{d_G(x,y)} + \sum_{x,y\in V(Y)} \frac{1}{d_G(x,y)} + \sum_{x,y\in V(A)} \frac{1}{d_G(x,y)} + \sum_{x\in V(X-v),y\in V(Y-u)} \frac{1}{d_G(x,y)} \\ &\quad + \sum_{x\in V(A),y\in V(Y-u)} \frac{1}{d_G(x,y)} + \sum_{x\in V(A),y\in V(X-v)} \frac{1}{d_G(x,y)}. \end{aligned}$$

$$\begin{aligned} B_1 &= \sum_{x\in V(X-v),y\in V(Y-u)} \left[\frac{1}{d_{G_1^*}(x,y)} - \frac{1}{d_G(x,y)}\right] + \sum_{x\in V(A),y\in V(Y-u)} \left[\frac{1}{d_{G_1^*}(x,y)} - \frac{1}{d_G(x,y)}\right] \\ &> \sum_{x\in V(A),y\in V(Y-u)} \left[\frac{1}{d_A(x,v)+d_Y(u,y)} - \frac{1}{d_A(x,u)+d_Y(u,y)}\right] \\ &= \sum_{x\in V(A-u-v)} \frac{d_A(x,u)-d_A(x,v)}{(d_A(x,v)+d_Y(u,y))(d_A(x,u)+d_Y(u,y))} \\ &> \sum_{x\in V(A-u-v)} \frac{d_A(x,u)-d_A(x,v)}{(D(A)+D(Y))(D(A)+D(Y))} > \sum_{x\in V(A-u-v)} \frac{d_A(x,u)-d_A(x,v)}{4D(G)^2} \end{aligned} \tag{2.1}$$

$$\begin{aligned} B_2 &= \sum_{x\in V(X-v),y\in V(Y-u)} \left[\frac{1}{d_{G_2^*}(x,y)} - \frac{1}{d_G(x,y)}\right] + \sum_{x\in V(X-v),y\in V(A)} \left[\frac{1}{d_{G_2^*}(x,y)} - \frac{1}{d_G(x,y)}\right] \\ &> \sum_{x\in V(X-v),y\in V(A)} \left[\frac{1}{d_X(x,v)+d_A(u,y)} - \frac{1}{d_X(x,v)+d_A(v,y)}\right] \\ &= \sum_{y\in V(A-u-v)} \frac{d_A(y,v)-d_A(y,u)}{(d_X(x,v)+d_A(u,y))(d_X(x,v)+d_A(v,y))} \\ &> \sum_{x\in V(A-u-v)} \frac{d_A(x,v)-d_A(x,u)}{(D(X)+D(A))(D(X)+D(A))} > \sum_{x\in V(A-u-v)} \frac{d_A(x,v)-d_A(x,u)}{4D(G)^2}. \end{aligned} \tag{2.2}$$

If $B_1 \le 0$, by (2.1), we have $\sum_{x\in V(H-u-v)} \frac{d_H(x,u)-d_H(x,v)}{4D(G)^2} < 0$. 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_k} is $l_k > 1$, we write it as $n_k^{l_k}$ 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 $s - 1$ 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 $r \le t$, $p_1 \ge p_2 \ge \cdots \ge p_{r-1}$ and $q_1 \ge q_2 \ge \cdots \ge q_{r-1}$. 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 $T = T_n\left(\left\lceil \frac{k}{2} \right\rceil, \left\lfloor \frac{k}{2} \right\rfloor, 1^{n-k-1}\right)$.

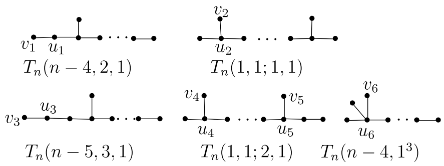

Fig. 6. The five trees in Lemma 3.1.

From Lemma 2.8 and the induction hypothesis, we have

$$H\left(T_n\left(\left\lceil\frac{k}{2}\right\rceil, \left\lfloor\frac{k}{2}\right\rfloor, 1^{n-k-1}\right)\right) < H\left(T_n\left(\left\lceil\frac{k-1}{2}\right\rceil, \left\lfloor\frac{k-1}{2}\right\rfloor, 1^{n-k}\right)\right) < H(S_n),$$

finishing the proof for the right inequality.

Next we turn to the proof of the left inequality. We prove it by induction on Δ, i.e., the maximum degree of T in $\mathcal{T}(n)$.If $\Delta = 2$, there exists only one tree P_n in $\mathcal{T}(n)$ and there is nothing to prove. For $\Delta = 3$, by using repeatedly Lemma 2.2, any tree T in $\mathcal{T}(n)$ 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 $\mathcal{T}(n)$ 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 $\mathcal{T}(n)$ 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 $A_1 = H(T_n(1, 1; 1, 1)) - H(T_n(n-4, 2, 1)), A_2 = H(T_n(n-5, 3, 1)) - H(T_n(1, 1; 1, 1)), A_3 = H(T_n(1, 1; 2, 1)) - H(T_n(n-5, 3, 1))$ and $A_4 = H(T_n(n-4, 1^3)) - H(T_n(1, 1; 2, 1))$.

By Lemma 2.2, we have

$$H(T_n(n-4, 2, 1)) = H(T_{n-1}(n-3, 1^2)) + n - 1 - Q_{T_{n-1}(n-3,1^2)}(u_1),$$

$$H(T_n(1, 1; 1, 1)) = H(T_{n-1}(n-3, 1^2)) + n - 1 - Q_{T_{n-1}(n-3,1^2)}(u_2),$$

$$H(T_n(n-5, 3, 1)) = H(T_{n-1}(n-5, 2, 1)) + n - 1 - Q_{T_{n-1}(n-5,2,1)}(u_3),$$

$$\begin{aligned} H(T_n(1, 1; 2, 1)) &= H(T_{n-1}(n-5, 2, 1)) + n - 1 - Q_{T_{n-1}(n-5,2,1)}(u_4) \\ &= H(T_{n-1}(n-4, 1^2)) + n - 1 - Q_{T_{n-1}(n-4,1^2)}(u_5), \end{aligned}$$

$$H(T_n(n-4, 1^3)) = H(T_{n-1}(n-4, 1^2)) + n - 1 - Q_{T_{n-1}(n-4,1^2)}(u_6).$$

So we have

$$\begin{aligned} Q_{T_{n-1}(n-3,1^2)}(u_1) - Q_{T_{n-1}(n-3,1^2)}(u_2) &= \frac{1}{2} + \frac{2}{3} \times 2 + \frac{3}{4} + \cdots + \frac{n-5}{n-4} + \frac{n-4}{n-3} + \frac{n-3}{n-2} \\ &\quad - \left(\frac{1}{2} \times 2 + \frac{2}{3} + \frac{3}{4} + \cdots + \frac{n-5}{n-4} + \frac{n-4}{n-3} \times 2\right) \\ &= \frac{2}{3} - \frac{1}{2} + \left(\frac{n-3}{n-2} - \frac{n-4}{n-3}\right) > 0. \end{aligned}$$

Thus, we get $A_1 > 0$ from Corollary 2.1.

Set $A_2^{(1)} = H(T_{n-1}(n-5, 2, 1)) - H(T_{n-1}(n-3, 1^2))$ and $A_2^{(2)} = Q_{T_{n-1}(n-3,1^2)}(u_2) - Q_{T_{n-1}(n-5,2,1)}(u_3)$. Then $A_2 = A_2^{(1)} + A_2^{(2)}$. Similarly, we obtain

$$A_2^{(1)} = \frac{n-4}{n-3} - \frac{2}{3},$$

$$\begin{aligned} A_2^{(2)} &= \frac{1}{2}\times 2+\frac{2}{3}+\frac{3}{4}+\cdots+\frac{n-5}{n-4}+\frac{n-4}{n-3}\times 2-\left(\frac{1}{2}+\frac{2}{3}+\frac{3}{4}\times 2+\cdots+\frac{n-4}{n-3}+\frac{n-3}{n-2}\right)\\ &= -\frac{1}{4}-\left(\frac{n-3}{n-2}-\frac{n-4}{n-3}\right). \end{aligned}$$

So we have

$$\begin{aligned} A_2 &= A_2^{(1)}+A_2^{(2)}\\ &= \frac{1}{12}-\frac{1}{n-3}-\frac{1}{(n-2(n-3))} > 0 \quad \text{for } n \geq 16. \end{aligned}$$

As shown in Fig. 6, by the definition of $Q_G(u)$,

$$\begin{aligned} Q_{T_{n-1}(n-5,2,1)}(u_3)-Q_{T_{n-1}(n-5,2,1)}(u_4) &= \frac{1}{2}+\frac{2}{3}+\frac{3}{4}\times 2+\cdots+\frac{n-5}{n-4}+\frac{n-4}{n-3}+\frac{n-3}{n-2}\\ &\quad -\left(\frac{1}{2}\times 2+\frac{2}{3}+\frac{3}{4}\times 2+\cdots+\frac{n-5}{n-6}+\frac{n-5}{n-4}\times 2+\frac{n-4}{n-3}\right)\\ &= \frac{1}{4}+\left(\frac{n-3}{n-2}-\frac{n-5}{n-4}\right) > 0,\\ Q_{T_{n-1}(n-4,1^2)}(u_5)-Q_{T_{n-1}(n-4,1^2)}(u_6) &= \frac{1}{2}\times 2+\frac{2}{3}\times 2+\frac{3}{4}\times 2+\frac{4}{5}+\cdots+\frac{n-6}{n-5}+\frac{n-5}{n-4}\times 2\\ &\quad -\left(\frac{1}{2}\times 3+\frac{2}{3}+\frac{3}{4}+\cdots+\frac{n-5}{n-4}+\frac{n-4}{n-3}\right)\\ &= \frac{1}{6}-\frac{1}{(n-3)(n-4)} > 0. \end{aligned}$$

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

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 $T \in \mathcal{T}(n) \setminus \{T_n(n-3, 1^2), T_n(n-4, 2, 1), T_n(n-5, 3, 1), T_n(n-4, 1^3)\}$ 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

$$\begin{aligned} H(T) &= H(T_n(n_1, n_2, \ldots, n_m)) \geq H(T_n(n_1+n_m-1, n_2, \ldots, 1))\\ &> H(T_n(n_1+n_m, n_2, \ldots, n_{m-1}))\\ &> \cdots > H\left(T_n\left(n_1+\sum_{i=5}^{m} n_i, n_2, n_3, n_4\right)\right)\\ &> H\left(T_n\left(n_1+\sum_{i=5}^{m} n_i+n_4-1, n_2, n_3, 1\right)\right)\\ &> H\left(T_n\left(n_1+\sum_{i=5}^{m} n_i+n_4+n_3-2, n_2, 1, 1\right)\right)\\ &> H\left(T_n\left(n_1+\sum_{i=5}^{m} n_i+n_4+n_3+n_2-3, 1, 1, 1\right)\right) = H(T_n(n-4, 1^3)). \end{aligned}$$

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 $H(T) > H(T_n(n-6, 4, 1))$ since $T \notin \{T_n(n-3, 1^2), T_n(n-4, 2, 1), T_n(n-5, 3, 1)\}$. Applying Lemma 2.2 to the pendent 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_6 of $T_n(n-4, 1^3)$ as shown in Fig. 6, by Corollary 2.1 and a direct calculation, we have $H(T_n(n-6, 4, 1)) > H(T_n(n-4, 1^3))$.

If $n_3 \geq 2$, then by Lemma 2.3, it follows that $H(T) > H(T_n(n-5, 2, 2))$. Similarly, applying Lemma 2.2 to one pendent vertex at distance 2 from the 3-degree vertex of $T_n(n-5, 2, 2)$ and to the vertex v_6 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 $T = T_n(n_1, n_2, n_3) \notin \{T_n(n-3, 1^2), T_n(n-4, 2, 1), T_n(n-5, 3, 1)\}$, which completes the proof of this lemma. □

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 subcase, $2 \leq p_1 + p_2 \leq 3$. From the choice of T, $T = T_n(2, 1; 2, 1)$. 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

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

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 $d(u_1) = m$ 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_m 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 $n_{m-1}, n_m \geq 3$. Without loss of generality, assume that $n_{m-1} \geq n_m$.

Subcase 1.1. $n_1 + n_2 + \cdots + n_{m-2} \geq 2$.

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

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

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

Subcase 1.2. $n_1 + n_2 + \cdots + n_{m-2} = 1$.

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

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

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. □

Combing 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

$$H(T_2) = n - 1 + \frac{1}{2}\binom{n-2}{2} + \frac{1}{3}(n-3),$$
$$H(T_3) = n - 1 + \frac{1}{2}\left[n - 2 + \binom{n-4}{2} + 1\right] + \frac{2}{3}(n-4),$$
$$H(T_4) = n - 1 + \frac{1}{2}\left[\binom{n-3}{2} + 2\right] + \frac{2}{3}(n-5) + \frac{1}{4},$$
$$H(T_5) = n - 1 + \frac{1}{2}\left[\binom{n-3}{2} + 2\right] + \frac{1}{3}(n-3) + \frac{1}{4}(n-4),$$
$$H(T_6) = n - 1 + \frac{1}{2}\left[n - 2 + \binom{n-5}{2} + \binom{3}{2}\right] + \frac{3}{3}(n-5),$$
$$H(T_7) = n - 1 + \frac{1}{2}\left[\binom{n-4}{2} + 4\right] + \frac{1}{3}[3(n-6) + 3] + \frac{2}{4},$$
$$H(T_8) = n - 1 + \frac{1}{2}\left[\binom{n-4}{2} + 3\right] + \frac{1}{3}[3(n-7) + 6] + \frac{3}{4}.$$

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]:

$$M_1(G) = \sum_{v \in V(G)} d_G(v)^2.$$

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 Δ. 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

$$\begin{aligned}
H(T) &\leq \frac{n(n-1)}{6} + \frac{n-1}{2} + \frac{1}{12}M_1(T) \\
&\leq \max\left\{\frac{(n-1)(n+3)}{6} + \frac{(n-1)(n-7)}{12} + \frac{(n-1)^2}{12(n-7)}, \frac{(n-1)(n+3)}{6} + \frac{(n-1)(n+3)}{24}\right\} \\
&= \max\left\{\frac{3n^2 - 4n + 1}{12} + \frac{(n-1)^2}{12(n-7)}, \frac{5(n-1)(n+3)}{24}\right\} \\
&< 2n - 6 + \frac{n^2 - 9n + 29}{4} = H(T_8).
\end{aligned}$$

This completes the proof of this lemma. $\square$

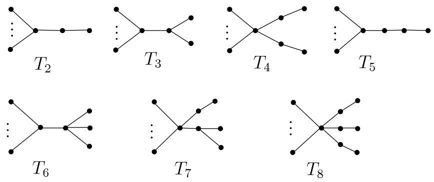

Fig. 7. The trees $T_2, T_3, \ldots, T_8$.

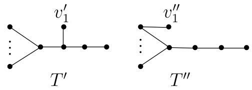

Fig. 8. The trees T' and T''.

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 $T \cong S_n(\Delta-1, n-\Delta-1)$. Note that $4 \leq n-\Delta-1 \leq 5 < \Delta-1$ since $\Delta \in \{n-6, n-5\}$. By Lemma 2.9, again, $H(S_n(\Delta-1, n-\Delta-1))$ reaches its maximum value at $\Delta = n-5$. From Eq. (1.1), we have

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

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 $T_0 = T_{n-1}(1^{n-5}, 3)$ 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

$$H(T'') = n-1+\frac{1}{2}\left[\binom{n-5}{2}+n-2\right]+\frac{1}{3}(2n-9)+\frac{1}{4}(n-4)+\frac{1}{5}.$$

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 $T \in \mathcal{T}(n) \setminus \{S_n, T_2, T_3, T_4, T_5, T_6, T_t, T_8\}$. Then*

$$H(T) < H(T_8) < H(T_7) < H(T_6) < H(T_5) < H(T_4) < H(T_3) < H(T_2) < H(S_n).$$

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 $T_n(1, 1; 2, 1), T_n(n-4, 1^3), T_n(n-5, 3, 1), T_n(1, 1; 1, 1), T_n(n-4, 2, 1), T_n(n-3, 1^2), P_n$ 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 $T_n(n-4, 1^3), T_n(1, 1; 2, 1)$ 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 (minimal or maximal) 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 (minimal or maximal) 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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References

[1] R. Balakrishnan, N. Sridharan, K.V. Iyer, Wiener index of graphs with more than one cut-vertex, Appl. Math. Lett. 21 (2008) 922–927.
[2] J.A. Bondy, U.S.R. Murty, Graph Theory with Applications, Macmillan Press, New York, 1976.
[3] K.C. Das, Maximizing the sum of the squares of the degrees of a graph, Discrete Math. 285 (2004) 57–66.
[4] K.C. Das, B. Zhou, N. Trinajstić, Bounds on Harary index, J. Math. Chem. 46 (2009) 1369–1376.
[5] H. Deng, The trees on $n > 9$ vertices with the first to seventeenth greatest Wiener indices are chemical trees, MATCH Commun. Math. Comput. Chem. 57 (2007) 393–402.
[6] A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: theory and applications, Acta Appl. Math. 66 (2001) 211–249.
[7] A. Dobrynin, I. Gutman, S. Klavžar, P. Žiget, Wiener index of hexagonal systems, Acta Appl. Math. 72 (2002) 247–294.
[8] E. Estrada, L. Rodriguez, Matrix algebraic manipulation of molecular graphs. 2. Harary- and MTI-like molecular descriptors, MATCH Commun. Math. Comput. Chem. 35 (1997) 157–167.
[9] L. Feng, A. Ilić, Zagreb, Harary and hyper-Wiener indices of graphs with a given matching number, Appl. Math. Lett. 23 (2010) 943–948.
[10] B. Furtula, I. Gutman, Ž. Tomović, A. Vesel, I. Pesek, Wiener-type topological indices of phenylenes, Indian J. Chem. Sec. A 41 (2002) 1767–1772.
[11] X. Guo, H. Dong, Ordering trees by their Wiener indices, J. Xiamen Univ. Natur. Sci. 44 (2005) 297–298.
[12] I. Gutman, A property of the Wiener number and its modifications, Indian J. Chem. Sec. A 36 (1997) 128–132.
[13] I. Gutman, Relation between hyper-Wiener and Wiener index, Chem. Phys. Lett. 364 (2002) 352–356.
[14] I. Gutman, K.C. Das, The first Zagreb index 30 years after, MATCH Commun. Math. Comput. Chem. 50 (2004) 83–92.
[15] I. Gutman, B. Furtula, Hyper-Wiener index vs. Wiener index. Two highly correlated structure-descriptors, Monatsh. Chem. 134 (2003) 975–981.
[16] I. Gutman, B. Furtula, J. Belić, Note on the hyper-Wiener index, J. Serb. Chem. Soc. 68 (2003) 943–948.
[17] I. Gutman, O.E. Polansky, Mathematical Concepts in Organic Chemistry, Springer, Berlin, 1986, 127–141.
[18] I. Gutman, J. Rada, O. araujo, The Wiener index of starlike trees and a related partial order, MATCH Commun. Math. Comput. Chem. 42 (2000) 145–154.
[19] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, Chem. Phys. Lett. 17 (1972) 535–538.
[20] O. Ivanciuc, T.S. Balaban, A.T. Balaban, Reciprocal distance matrix, related local vertex invariants and topological indices, J. Math. Chem. 12 (1993) 309–318.
[21] D.J. Klein, I. Lukovits, I. Gutman, On the definition of the hyper-Wiener index for cycle-containing structures, J. Chem. Inf. Comput. Sci. 35 (1995) 50–52.
[22] M. Liu, B. Liu, Trees with the seven smallest and fifteen greatest hyper-Wiener indices, MATCH Commun. Math. Comput. Chem. 63 (2010) 151–170.
[23] M. Liu, B. Liu, Q. Li, Erratum to 'The trees on vertices with the first to seventeenth greatest Wiener indices are chemical trees', MATCH Commun. Math. Comput. Chem. 64 (2010) 743–756.
[24] B. Lučić, A. Miličević, S. Nikolić, N. Trinajstić, Harary index—twelve years later, Croat. Chem. Acta 75 (2002) 847–868.
[25] Z. Mihalic, D. Veljan, D. Amic, S. Nikolić, D. Plavšić, N. Trinajstić, The distance marix in chemistry, J. Math. Chem. 11 (1992) 223–258.
[26] S. Nikolić, N. Trinajstić, The Wiener index: development and applications, Croat. Chem. Acta 68 (1995) 105–129.
[27] D. Plavšić, S. Nikolić, N. Trinajstić, Z. Mihalić, On the Harary index for the characterization of chemical graphs, J. Math. Chem. 12 (1993) 235–250.
[28] M. Randić, Novel molecular descriptor for structure–property studies, Chem. Phys. Lett. 211 (1993) 478–483.
[29] R. Todeschini, V. Consonni, Handbook of Molecular Descriptors, Wiley-VCH, Weinheim, 2000, pp. 497–502.
[30] R. Todeschini, V. Consonni, Molecular Descriptors for Chemoinformatics, vols. I–II, Wiley-VCH, Weinheim, 2009, pp. 934–938.
[31] N. Trinajstić, Chemical Graph Theory, CRC Press, Boca Raton, FL, 1992.
[32] N. Trinajstić, S. Nikolić, S. Basak, I. Lukovits, Distance indices and their Hyper-counterparts: intercorrelation and use in the structure–property modeling, SAR QSAR Environ. Res. 12 (2001) 31–54.
[33] H. Wiener, Structural determination of paraffin boiling point, J. Am. Chem. Soc. 69 (1947) 17–20.
[34] K. Xu, N. Trinajstić, Hyper-Wiener and Harary indices of graphs with cut edges, Util. Math. 84 (2011) 153–163.
[35] K. Xu, K.C. Das, Extremal unicyclic and bicyclic graphs with respect to Harary index, Bull. Malays. Math. Sci. Soc. (in press).
[36] K. Xu, K.C. Das, On Harary index of graphs, Discrete Appl. Math. 159 (2011) 1631–1640.
[37] B. Zhou, X. Cai, N. Trinajstić, On the Harary index, J. Math. Chem. 44 (2008) 611–618.
[38] B. Zhou, I. Gutman, Relations between Wiener, hyper-Wiener and Zagreb indices, Chem. Phys. Lett. 394 (2004) 93–95.