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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 $n \geq 14$.

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* $1 \leq j \leq \lfloor \frac{n}{2} \rfloor$;
(2) $Q_{P_n}(v_j) > Q_{P_n}(v_{j+1})$ *for* $1 \leq j \leq \lfloor \frac{n}{2} \rfloor$;
(3) $Q_{P_n}(v_j) > Q_{P_n}(v_{n-k})$ *for* $1 \leq j < k \leq \lfloor \frac{n}{2} \rfloor$.

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 $H(G_{k,m}) > H(G_{k-1,m+1})$.*