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On Distance–Based Graph Invariants*

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Abstract

Let G be a simple connected graph of order n with m edges and diameter d. Let W, WW, H, and RCW be the Wiener index, hyper-Wiener index, Harary index, and reciprocal complementary Wiener index of G. The multiplicative version of Wiener index (π-index) is equal to the product of the distances between all pairs of vertices. We compare H and RCW. For bipartite graph of order $n > 5$, we prove that $\pi > 2\,WW$. In any connected graph, if $d \geq 4$ and $m \leq \frac{285\,W-6624}{287}$, then $\pi \geq 2\,WW$. Some additional relations between W, WW, H, and RCW are also obtained.

1 Introduction

Let G be a simple connected graph on n vertices with edge set $E(G)$ ($|E(G)| = m$), where the vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$. If the vertices v_i and v_j are adjacent, we write $v_iv_j \in E(G)$. For any vertex $v_i \in V(G)$, let $N_G(v_i)$ be the neighbor set of v_i and then

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the degree of the vertex v_i is equal to $|N_G(v_i)|$, and will be denoted by d_i. The distance between two vertices $v_i, v_j \in V(G)$, denoted by, $d_G(v_i, v_j)$, is defined as the length of a shortest path between v_i and v_j in G. The diameter of the graph G is denoted by d and is defined as $d = \max\{d_G(v_i, v_j) : \ v_i, v_j \in V(G)\}$.

The join $G_1 \vee G_2$ of graphs G_1 and G_2 is the graph obtained from the disjoint union of G_1 and G_2 by adding all edges between $V(G_1)$ and $V(G_2)$. The complement of G is denoted by $\overline{G}$. As usual, K_n, $K_{p,q}$ $(p + q = n)$, P_n, and C_n denote, respectively, the complete graph, the complete bipartite graph, the path, and the cycle graph on n vertices.

The Wiener index of G, defined as

$$W = W(G) = \sum_{\{v_i,v_j\} \subseteq V(G)} d_G(v_i, v_j)\,,$$

is perhaps the most studied topological index, both from a mathematical point of view and of its applications [6, 17, 20, 33, 34, 40].

The hyper-Wiener index is defined for all connected graphs as [32]

$$WW = WW(G) = \frac{1}{2} \sum_{\{v_i,v_j\} \subseteq V(G)} \Big[d_G(v_i, v_j)^2 + d_G(v_i, v_j) \Big].$$

If we denote by $d(G, k)$ the number of vertex pairs of G, whose distance is equal to k, then the hyper-Wiener index of G can be expressed as

$$WW(G) = \frac{1}{2} \sum_{k \geq 1} (k^2 + k)\, d(G, k)\,. \tag{1}$$

Recall that $d(G, 1) = m$. The maximum value of k for which $d(G, k)$ is non-zero, is the diameter of the graph G.

Mathematical properties of the hyper-Wiener index were much studied, see [4, 5, 18, 19, 23, 37, 40] and the references cited therein. The papers [21, 22] are concerned with relations between the Wiener and hyper-Wiener indices.

In [24, 25], the multiplicative version of the Wiener index of G was put forward as

$$\pi = \pi(G) = \prod_{\{v_i,v_j\} \subseteq V(G)} d_G(v_i, v_j)\,,$$

which can be written also as

$$\pi(G) = \prod_{k \geq 2} k^{d_G(G,k)}\,.$$

Recently, Hua et al. [27, 28] studied the mathematical properties of π. In [8], the present authors reported results on comparing W and π.

In 1993, Plavšić et al. [36] and Ivanciuc et al. [31] independently introduced the Harary index, named in honor of Frank Harary on the occasion of his 70th birthday. The Harary index is defined as:

$$H = H(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{1}{d_G(u,v)}\,.$$

For its basic mathematical properties, including various lower and upper bounds, see [14, 15, 40] and the references cited therein.

In 2000, Ivanciuc [30] introduced the reciprocal complementary Wiener index, defined as:

$$RCW = RCW(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{1}{d+1-d_G(u,v)}\,,$$

where d is the diameter of the graph G. Recently, several mathematical investigations of RCW were communicated [3, 40, 41].

Topological indices are graph invariants and are used for quantitative structure-activity relationship ($QSAR$) and quantitative structure-property relationship ($QSPR$) studies. Many topological indices have been defined in the literature and several of them have found applications as means to model physical, chemical, pharmaceutical, and other properties of molecules. Comparison between various topological graph invariants have received much attention over the past few years, see e.g., [7, 10–13, 35]. Moreover, several relations have been obtained between distance-based and degree-based topological indices of graphs, see [1, 2, 9, 29, 39] and the references cited therein.

This paper is organized as follows. In the next section, we give a lower bound on Harary index for starlike trees. In Section 3, we compare the Harary and reciprocal complementary Wiener indices. In Section 4, we compare the hyper-Wiener and the multiplicative Wiener indices. In Section 5, we present some additional relations between distance–based topological indices W, WW, RCW, and H.

2 Lower bound on Harary index for starlike trees

Let P_n denote the path on n vertices. By $S(n_1, n_2, \ldots, n_k)$ we denote the starlike tree which has a vertex v_0 of degree $k \geq 3$ and which has the property

$$S(n_1, n_2, \ldots, n_k) - v_0 = P_{n_1} \cup P_{n_2} \cup \ldots \cup P_{n_k}.$$

This tree has $n_1 + n_2 + \cdots + n_k + 1 = n$ vertices. Clearly, the parameters $n_1, n_2, \ldots, n_k$ determine the starlike tree up to isomorphism. In what follows, it will be assumed that $n_1 \geq n_2 \geq \ldots \geq n_k \geq 1$. We say that the starlike tree $S(n_1, n_2, \ldots, n_k)$ has k branches, the lengths of which are $n_1, n_2, \ldots, n_k$.

We now calculate $H(S)$ and $RCW(S)$ for any starlike tree. For this we define

$$HR = HR(G) = \sum_{\{u,v\} \subseteq V(G)} \Upsilon_G(u,v)\,,$$

where

$$\Upsilon_G(u,v) = \frac{1}{a\, d_G(u,v) + b} \quad \text{for } \{u,v\} \subseteq V(G)\,,$$

and a, b are any real numbers. Thus we have

$$HR(G) = \begin{cases} H(G) & \text{if } (a,b) = (1,0), \\ RCW(G) & \text{if } (a,b) = (-1, d+1)\,. \end{cases} \tag{2}$$

Theorem 1. *Let $S(n_1, n_2, \ldots, n_k)$ be a starlike tree of order $n = n_1 + n_2 + \cdots + n_k + 1$ $(n_1 \geq n_2 \geq \cdots \geq n_k)$. Then*

$$HR(S) = \sum_{i=1}^{k} \sum_{j=1}^{n_i} \frac{n_i + 1 - j}{aj + b} + \sum_{i=1}^{k-1} \sum_{j=i+1}^{k} \sum_{r=1}^{n_i} \sum_{s=1}^{n_j} \frac{1}{(r+s)a + b}\,. \tag{3}$$

Proof. We obtain

$$\begin{aligned}
HR(S) &= \sum_{\{u,v\} \subseteq V(G)} \frac{1}{a\, d_G(u,v) + b} \\
&= \sum_{i=1}^{k} \left[\sum_{v \in V(P_{n_i})} \frac{1}{a\, d_G(v_0, v) + b} + \sum_{\substack{u,v \in V(P_{n_i}),\\ u \neq v}} \frac{1}{a\, d_G(u,v) + b} \right] \\
&+ \sum_{i=1}^{k-1} \sum_{j=i+1}^{k} \sum_{\substack{u \in V(P_{n_i})\\ v \in V(P_{n_j})}} \frac{1}{a\, d_G(u,v) + b} \\
&= \sum_{i=1}^{k} \left[\frac{n_i}{a+b} + \frac{n_i - 1}{2a+b} + \frac{n_i - 2}{3a+b} + \cdots + \frac{2}{a(n_i - 1) + b} + \frac{1}{a\, n_i + b} \right] \\
&+ \sum_{i=1}^{k-1} \sum_{j=i+1}^{k} \left[\left(\frac{1}{2a+b} + \frac{1}{3a+b} + \cdots + \frac{1}{(n_j+1)a + b} \right) \right. \\
&+ \left(\frac{1}{3a+b} + \frac{1}{4a+b} + \cdots + \frac{1}{(n_j+2)a + b} \right)
\end{aligned}$$

$$+ \quad \cdots + \Big(\frac{1}{(n_i+1)a+b} + \frac{1}{(n_i+2)a+b} + \cdots + \frac{1}{(n_i+n_j)a+b} \Big) \Big]$$

$$= \sum_{i=1}^{k} \sum_{j=1}^{n_i} \frac{n_i+1-j}{aj+b} + \sum_{i=1}^{k-1} \sum_{j=i+1}^{k} \sum_{r=1}^{n_i} \sum_{s=1}^{n_j} \frac{1}{(r+s)a+b} .$$

■

Corollary 1. *Let $S(n_1, n_2, \ldots, n_k)$ be a starlike tree of order $n = n_1 + n_2 + \cdots + n_k + 1$ $(n_1 \geq n_2 \geq \cdots \geq n_k)$. Then*

$$H(S) = \sum_{i=1}^{k} \sum_{j=1}^{n_i} \frac{n_i+1-j}{j} + \sum_{i=1}^{k-1} \sum_{j=i+1}^{k} \sum_{r=1}^{n_i} \sum_{s=1}^{n_j} \frac{1}{r+s} . \tag{4}$$

Proof. Setting $(a, b) = (1, 0)$ in Theorem 1 and using (2), we get the required result in (4). ■

Corollary 2. *Let $S(n_1, n_2, \ldots, n_k)$ be a starlike tree of order $n = n_1 + n_2 + \cdots + n_k + 1$ $(n_1 \geq n_2 \geq \cdots \geq n_k)$. Then*

$$RCW(S) = \sum_{i=1}^{k} \sum_{j=1}^{n_i} \frac{n_i+1-j}{n_1+n_2+1-j} + \sum_{i=1}^{k-1} \sum_{j=i+1}^{k} \sum_{r=1}^{n_i} \sum_{s=1}^{n_j} \frac{1}{n_1+n_2+1-r-s} . \tag{5}$$

Proof. The diameter of $S(n_1, n_2, \ldots, n_k)$ is equal to $d = n_1 + n_2$. Setting $(a, b) = (-1, d+1)$ in Theorem 1 and using (2), we get the required result in (5). ■

We now give a lower bound on $H(S)$.

Theorem 2. *Let $S(n_1, n_2, \ldots, n_k)$ be a starlike tree of order $n = n_1 + n_2 + \cdots + n_k + 1$ $(n_1 \geq n_2 \geq \cdots \geq n_k \geq 6)$. Then*

$$\begin{aligned} H(S) \quad &\geq \quad 5.78\,(n-1) - 34.21\,k + \frac{408\,k}{n_1+12} - 2\,n_1 + (k-1)\,(k-2)\,n_k \\ &+ \quad \frac{k\,(k-1)}{8} \left[\frac{6}{n_1+1} - 5 - \frac{4\,n_1^2}{n_k} \right] . \end{aligned} \tag{6}$$

Proof. Since $n_i \geq 6$ $(i = 1, 2, \ldots, k)$ and

$$\sum_{s=1}^{n_i-5} s(n_i - s + 1) = (n_i+1) \sum_{s=1}^{n_i-5} s - \sum_{s=1}^{n_i-5} s^2 = \frac{(n_i-5)(n_i-4)(n_i+12)}{6} ,$$

by weighted arithmetic–harmonic–mean inequality, we get

$$\sum_{j=6}^{n_i} \frac{n_i+1-j}{j} \quad \geq \quad \frac{\left(\sum\limits_{s=1}^{n_i-5} s \right)^2}{\sum\limits_{s=1}^{n_i-5} s(n_i-s+1)} = \frac{\left[\frac{(n_i-4)(n_i-5)}{2} \right]^2}{\frac{(n_i-5)\,(n_i-4)(n_i+12)}{6}}$$

$$= \frac{3\,(n_i-5)(n_i-4)}{2\,(n_i+12)} = \frac{3}{2}\left[n_i - 21 + \frac{272}{n_i+12}\right]. \tag{7}$$

Again, by the weighted arithmetic–harmonic–mean inequality,

$$\sum_{s=1}^{n_j-1} \frac{s}{s+1} \geq \frac{\left(\sum\limits_{s=1}^{n_j-1} s\right)^2}{\sum\limits_{s=1}^{n_j-1} s(s+1)} = \frac{\left[\frac{(n_j-1)\,n_j}{2}\right]^2}{\frac{(n_j-1)\,n_j\,(n_j+1)}{3}} = \frac{3\,n_j\,(n_j-1)}{4(n_j+1)}.$$

Moreover,

$$\sum_{s=1}^{n_j} \frac{n_j-s+1}{n_j+s} \geq \frac{1}{2n_j}\sum_{s=1}^{n_j} s = \frac{n_j+1}{4}$$

and

$$\sum_{r=1}^{n_i-n_j}\ \sum_{s=r}^{n_j+r-1} \frac{1}{n_j+s+1} \geq \frac{n_j\,(n_i-n_j)}{n_i+n_j} \quad \text{if } n_i \geq n_j+1.$$

Using the above results, one can easily see that

$$\sum_{r=1}^{n_i}\sum_{s=1}^{n_j} \frac{1}{r+s} = \sum_{s=1}^{n_j-1} \frac{s}{s+1} + \sum_{s=1}^{n_j} \frac{n_j-s+1}{n_j+s}$$

if $n_i = n_j$, whereas

$$\sum_{r=1}^{n_i}\sum_{s=1}^{n_j} \frac{1}{r+s} = \sum_{s=1}^{n_j-1} \frac{s}{s+1} + \sum_{s=1}^{n_j} \frac{n_j-s+1}{n_j+s} + \sum_{r=1}^{n_i-n_j}\ \sum_{s=r}^{n_j+r-1} \frac{1}{n_j+s+1}$$

if $n_i \geq n_j + 1$. Thus,

$$\begin{aligned}\sum_{r=1}^{n_i}\sum_{s=1}^{n_j} \frac{1}{r+s} &\geq \frac{3\,n_j\,(n_j-1)}{4\,(n_j+1)} + \frac{n_j+1}{4} + \frac{n_j\,(n_i-n_j)}{n_i+n_j} \\ &= 2n_j + \frac{3}{2\,(n_j+1)} - \frac{5}{4} - \frac{2n_j^2}{n_i+n_j}.\end{aligned}$$

Now,

$$\sum_{i=1}^{k-1}\ \sum_{j=i+1}^{k} 2\,n_j = 2\Big[n_2 + 2\,n_3 + \cdots + (k-1)\,n_k\Big] \geq 2(n-1-n_1) + (k-1)(k-2)n_k,$$

$$\sum_{i=1}^{k-1}\ \sum_{j=i+1}^{k} \frac{3}{2\,(n_j+1)} \geq \frac{3\,k\,(k-1)}{4\,(n_2+1)} \geq \frac{3\,k\,(k-1)}{4\,(n_1+1)},$$

and

$$\sum_{i=1}^{k-1}\ \sum_{j=i+1}^{k} \frac{2n_j^2}{n_i+n_j} \leq \frac{k(k-1)\,n_2^2}{2n_k} \leq \frac{k(k-1)\,n_1^2}{2n_k}.$$

This implies

$$\sum_{i=1}^{k-1}\sum_{j=i+1}^{k}\sum_{r=1}^{n_i}\sum_{s=1}^{n_j}\frac{1}{r+s}\ge\sum_{i=1}^{k-1}\sum_{j=i+1}^{k}\left[2n_j+\frac{3}{2(n_j+1)}-\frac{5}{4}-\frac{2n_j^2}{n_i+n_j}\right]$$

$$\ge\ 2(n-1-n_1)+(k-1)(k-2)n_k+\frac{k(k-1)}{8}\left(\frac{6}{n_1+1}-5-\frac{4n_1^2}{n_k}\right)$$

and

$$\begin{aligned}\sum_{i=1}^{k}\sum_{j=1}^{n_i}\frac{n_i+1-j}{j} &= \sum_{i=1}^{k}\left[n_i+\frac{n_i-1}{2}+\frac{n_i-2}{3}+\frac{n_i-3}{4}+\frac{n_i-4}{5}+\sum_{j=6}^{n_i}\frac{n_i+1-j}{j}\right]\\ &\ge \sum_{i=1}^{k}\left[2.28\,n_i-2.71+\frac{3}{2}\left(n_i-21+\frac{272}{n_i+12}\right)\right] \qquad \text{(by (7))}\\ &\ge 3.78\,(n-1)-34.21\,k+\frac{408\,k}{n_1+12}\,.\end{aligned}$$

The above results with Corollary 1 directly leads to (6). ■

3 Comparing Harary index and reciprocal complementary Wiener index

In this section we compare the Harary and reciprocal complementary Wiener indices of graphs.

Example 3. *Let P_n be the path of order n. Then*

$$H(P_n)=n-1+\frac{n-2}{2}+\frac{n-3}{3}+\cdots+\frac{2}{n-2}+\frac{1}{n-1}$$

and

$$RCW(P_n)=\frac{n-1}{n-1}+\frac{n-2}{n-2}+\frac{n-3}{n-3}+\cdots+\frac{2}{2}+\frac{1}{1}=n-1\,.$$

Thus, $H(P_n)>RCW(P_n)$.

Example 4. *For $T\cong K_{1,n-1}$ $(n>4)$,*

$$H(T)=\frac{1}{4}(n-1)(n+2)<\frac{1}{2}(n-1)^2=RCW(T)\,.$$

Example 5. *For $G\cong K_n-e$,*

$$H(G)=\frac{(n+1)(n-2)+1}{2}>\frac{(n-1)(n-2)}{4}+\frac{n}{2}=RCW(G)\,.$$

Denote by $DS_{p,q}$ $(p \geq q \geq 1,\ n = p+q+2)$, a double star of order n which is constructed by joining the central vertices of two stars $K_{1,p}$ and $K_{1,q}$.

Example 6. *Let $T \cong DS_{p,q}$ $(p+q+2 = n, p \geq q \geq 1)$. Then*

$$H(T) = p+q+1+\frac{p^2+p+q^2+q}{4}+\frac{p\,q}{3}$$

and

$$RCW(T) = p\,q+\frac{p^2+p+q^2+q}{4}+\frac{p+q+1}{3}\,.$$

If $q = 1$ or $p = q = 2$, then $H(T) > RCW(T)$. If $p = 3$, $q = 2$, then $H(T) = RCW(T)$. Otherwise, $H(T) < RCW(T)$.

From the above examples, we conclude that in the general case, H and RCW are incomparable. Recall that a graph $G = (V, E)$ is said to be a difference graph if there exist real numbers $a_1, a_2, \ldots, a_n$ associated with the vertices of G and a positive real number t such that (1) $|a_i| < t$ for $i = 1, 2, \ldots, n$; (2) distinct vertices v_i and v_j are adjacent if and only if $|a_i - a_j| \geq t$. We now compare $H(G)$ and $RCW(G)$ for the difference graph. In order to obtain such results we will need the next lemma.

Lemma 7. [26] *Let G be a bipartite graph with bipartition $V = X \cup Y$. Then G is a difference graph if and only if there exist such a labeling of the vertices of set X that $N_G(v_i) \subseteq N_G(v_{i+1})$ for $i = 1, 2, \ldots, |X|-1$, where $v_i \in X$.*

Theorem 3. *Let G $(\ncong K_{p,q})$ be a connected, bipartite, difference graph with bipartition $V = X \cup Y$, $|X| = p$ and $|Y| = q$ $(p+q = n)$. If the number of edges of G is $m \geq pq/2$, then $H(G) \geq RCW(G)$, otherwise, $H(G) < RCW(G)$. For $G \cong K_{p,q}$, we have $H(G) \geq RCW(G)$ if $pq \geq n(n-1)/4$, and $H(G) < RCW(G)$, otherwise.*

Proof. First we consider the case $G \cong K_{p,q}$. Then

$$H(G) = pq + \frac{1}{2}\left[\frac{n(n-1)}{2} - pq\right] \qquad \text{and} \qquad RCW(G) = \frac{n(n-1)}{2} - pq + \frac{1}{2}\,pq\,.$$

Therefore $H(G) \geq RCW(G)$ if $pq \geq \frac{n(n-1)}{4}$, and $H(G) < RCW(G)$, otherwise.

Next we assume that $G \ncong K_{p,q}$. From the definition of the difference graph G, we can assume that $X = \{v_1, v_2, \ldots, v_p\}$ and $Y = \{v_{p+1}, v_{p+2}, \ldots, v_{p+q}\}$ such that $d_1 \leq d_2 \leq \cdots \leq d_p = q$ and $d_{p+1} \leq d_{p+2} \leq \cdots \leq d_{p+q} = p$ as G is connected. Moreover, the diameter of G is 3 as $G \ncong K_{p,q}$. The number of edges of G is $m = d(G,1) = \sum_{i=1}^{p-1} d_i + q$. In addition,

$$d(G,2) = \frac{p\,(p-1) + q\,(q-1)}{2} \qquad \text{and} \qquad d(G,3) = \sum_{i=1}^{p-1}(q-d_i) = \sum_{i=p+1}^{q-1}(p-d_i)\,.$$

Therefore

$$\begin{aligned} H(G) &= \sum_{i=1}^{p-1} d_i + q + \frac{p(p-1)+q(q-1)}{4} + \frac{1}{3}\sum_{i=1}^{p-1}(q-d_i) \\ &= \frac{p(p-1)+q(q-1)}{4} + \frac{2\sum_{i=1}^{p-1} d_i + pq + 2q}{3} \end{aligned}$$

and

$$\begin{aligned} RCW(G) &= \sum_{i=1}^{p-1}(q-d_i) + \frac{p(p-1)+q(q-1)}{4} + \frac{1}{3}\sum_{i=1}^{p-1} d_i + q \\ &= \frac{p(p-1)+q(q-1)}{4} + \frac{-2\sum_{i=1}^{p-1} d_i + 3pq - 2q}{3}\,. \end{aligned}$$

Thus,

$$H(G) \geq RCW(G) \Longleftrightarrow m = q + \sum_{i=1}^{p-1} d_i \geq \frac{pq}{2}.$$

This completes the proof. ■

Theorem 4. *Let G be a connected graph obtained by deleting p $(p \leq n-1)$ edges from the complete graph K_n. Then $H(G) > RCW(G)$.*

Proof. Since $p \leq n-1$, then the diameter of G is at most 3. The number of edges of G is $m = n(n-1)/2 - p$. If $d = 2$, then

$$H(G) = \frac{n(n-1)}{2} - p + \frac{p}{2} > p + \frac{1}{2}\left[\frac{n(n-1)}{2} - p\right] = RCW(G) \ \text{ as } p \leq n-1\,.$$

Otherwise, $d = 3$. In this case p must be equal to $n-1$ and only one pair of vertices has distance three. Again since $p \leq n-1$, we have

$$H(G) = \frac{n(n-1)}{2} - p + \frac{p-1}{2} + \frac{1}{3} > 1 + \frac{p-1}{2} + \frac{1}{3}\left[\frac{n(n-1)}{2} - p\right] = RCW(G)\,.$$

■

Let T be a tree of order n with diameter $d = 4$. Then there exists a vertex v in T (the center of T), such that

$$T - \{v\} = K_{1,a_1} \cup K_{1,a_2} \cup \cdots \cup K_{1,a_q} \cup p\,K_1 \,(p \geq 0, q \geq 2, a_i \geq 1, i = 1, 2, \ldots, q)\,.$$

Note that the degree of the vertex v is equal to $p + q$ and thus the order of T is $n = 1 + p + q + \sum_{i=1}^{q} a_i$.

Theorem 5. *If T is a tree as specified above, and if*

$$\sum_{1 \leq i < j \leq q} a_i\, a_j < \frac{1}{11}\Big[(n-1)(n+11) - 4(p+q)(n-p-q)\Big]\,,$$

then $H(T) > RCW(T)$. Otherwise, $H(T) \leq RCW(T)$.

Proof. The number of edges of T is $n - 1$. We have

$$\begin{aligned}
d(T,2) &= \frac{1}{2}\sum_{i=1}^{q} a_i(a_i+1) + \frac{(p+q)(p+q-1)}{2} \\
d(T,3) &= (p+q-1)\sum_{i=1}^{q} a_i \\
d(T,4) &= \sum_{1 \leq i < j \leq q} a_i\, a_j\,.
\end{aligned}$$

Then

$$\begin{aligned}
H(T) &= n - 1 + \frac{1}{4}\sum_{i=1}^{q} a_i(a_i+1) + \frac{(p+q)(p+q-1)}{4} + \frac{(p+q-1)}{3}\sum_{i=1}^{q} a_i \\
&+ \frac{1}{4}\sum_{1 \leq i < j \leq q} a_i\, a_j
\end{aligned}$$

and

$$\begin{aligned}
RCW(T) &= \frac{n-1}{4} + \frac{1}{6}\sum_{i=1}^{q} a_i(a_i+1) + \frac{(p+q)(p+q-1)}{6} + \frac{(p+q-1)}{2}\sum_{i=1}^{q} a_i \\
&+ \sum_{1 \leq i < j \leq q} a_i\, a_j\,.
\end{aligned}$$

Thus we have $H(T) > RCW(T) \iff$

$$n - 1 + \frac{1}{4}\sum_{i=1}^{q} a_i(a_i+1) + \frac{(p+q)(p+q-1)}{4} + \frac{(p+q-1)}{3}\sum_{i=1}^{q} a_i + \frac{1}{4}\sum_{1 \leq i < j \leq q} a_i\, a_j$$

$$> \frac{n-1}{4} + \frac{1}{6}\sum_{i=1}^{q} a_i(a_i+1) + \frac{(p+q)(p+q-1)}{6} + \frac{(p+q-1)}{2}\sum_{i=1}^{q} a_i + \sum_{1\le i<j\le q} a_i\, a_j$$

$\iff$

$$9\,(n-1) + (p+q)\,(p+q-1) + \sum_{i=1}^{q} a_i^2 > (2p+2q-3)\sum_{i=1}^{q} a_i + 9\sum_{1\le i<j\le q} a_i\, a_j\,.$$

Since

$$(n-1-p-q)^2 = \left(\sum_{i=1}^{q} a_i\right)^2 = \sum_{i=1}^{q} a_i^2 + 2\sum_{1\le i<j\le q} a_i\, a_j\,,$$

from which we get

$$H(T) > RCW(T) \iff \sum_{1\le i<j\le q} a_i\, a_j < \frac{1}{11}\Big[(n-1)(n+11) - 4(p+q)(n-p-q)\Big]\,.$$

This completes the proof of the theorem. ■

4 Comparing hyper-Wiener index and multiplicative Wiener index

From the definition of the indices WW and π, we see that both depend on the distances between pairs of vertices. Therefore, it may be of some interest to compare them. This indeed was done by extensive numerical testing [24, 25], but no mathematical relation between WW and π was found until now.

By direct checking it can be seen that $\pi(G) < 2\,WW(G)$ for $G \cong K_{3,2}$. On the other hand, we have the following result:

Theorem 6. *Let G be a connected bipartite graph of order $n > 5$. Then $\pi(G) > 2\,WW(G)$.*

Proof. Since G is bipartite, we have $m \le \lceil \frac{n}{2} \rceil \lfloor \frac{n}{2} \rfloor$. We consider the following two cases:

Case 1. $d(G,4) = 0$. In this case G has diameter at most 3.

Subcase 1.1. $d = 2$. Since G is bipartite, $G \cong K_{p,q}$ $(p \ge q \ge 1, p+q = n)$. Then

$$\pi(G) = 2^{n(n-1)/2-pq} \qquad \text{and} \qquad WW(G) = \frac{3}{2}n(n-1) - 2pq\,.$$

For $n = 6$, we have $G \cong K_{3,3}$, $G \cong K_{4,2}$, and $G \cong K_{5,1}$. One can easily check that $\pi(G) > 2\,WW(G)$ holds. Otherwise, $n \ge 7$. We have to show that $\pi(G) > 2\,WW(G)$, that is, $2^{\frac{n(n-1)}{2}-pq} > 3n(n-1) - 4pq$, that is, $16\left(\frac{n(n-1)}{2} - pq - 3\right) > 3n(n-1) - 4pq$, that is, $5n(n-1) > 12pq + 48$, which is true for $pq \le \left\lceil \frac{n}{2} \right\rceil \left\lfloor \frac{n}{2} \right\rfloor$ and $n \ge 7$.

Subcase 1.2. $d = 3$. We have $d(G,1) = m$. Let $d(G,2) = p$ and $d(G,3) = q$. Then $p + q + m = n(n-1)/2$, implying

$$\pi(G) = 2^p\,3^q \qquad \text{and} \qquad WW(G) = m + 3p + 6q = \frac{1}{2}n(n-1) + 2p + 5q\,.$$

For $n = 6$, $p + q = d(G,2) + d(G,3) \ge 7$ and $d(G,3) \ge 1$. One can easily check that $\pi(G) > 2\,WW(G)$. For $n = 7$, $p + q = d(G,2) + d(G,3) \ge 10$ and $d(G,3) \ge 1$, again one can easily check that $\pi(G) > 2\,WW(G)$. Otherwise, $n \ge 8$. We have to show that $\pi(G) > 2\,WW(G)$, that is, $2^p\,3^q > 2m + 6p + 12q$, that is, $6\,(2p + 3q - 5) > 2m + 6p + 12q$, that is, $6p + 6q > 2m + 30$, that is, $n^2 - 3n - 30 > 0$, which is true as $n \ge 8$.

Case 2. $d(G,4) \ge 1$. For any non-negative real numbers k and x, we have $k^x \ge kx$. Using this we have

$$\begin{aligned}
\prod_{k\ge 2} k^{d(G,k)} &= 2^{d(G,2)}\,3^{d(G,3)}\,4^{d(G,4)} \prod_{k\ge 5} k^{d(G,k)} \\
&= 24 \times 2^{d(G,2)-1}\,3^{d(G,3)-1}\,4^{d(G,4)-1} \prod_{k\ge 5} k^{d(G,k)} \\
&\ge 24\left[2^{d(G,2)-1} + 3^{d(G,3)-1} + 4^{d(G,4)-1} + \sum_{k\ge 5} k^{d(G,k)}\right] \\
&= 24\left[(2^2)^{\frac{d(G,2)-1}{2}} + (3^2)^{\frac{d(G,3)-1}{2}} + (4^2)^{\frac{d(G,4)-1}{2}} + \sum_{k\ge 5} (k^2)^{\frac{d(G,k)}{2}}\right] \\
&\ge 24\left[2^2\,\frac{d(G,2)-1}{2} + 3^2\,\frac{d(G,3)-1}{2} + 4^2\,\frac{d(G,4)-1}{2} + \sum_{k\ge 5} k^2\,\frac{d(G,k)}{2}\right] \\
&\ge 12\left[\sum_{k\ge 2} k^2\,d(G,k) - 29\right] \\
&= 2\sum_{k\ge 1} k^2\,d(G,k) + 10\sum_{k\ge 2} k^2\,d(G,k) - 2m - 348\,.
\end{aligned} \tag{8}$$

Since $d(G,4) \ge 1$ and $m \le \lceil n/2 \rceil \lfloor n/2 \rfloor$, one can easily see that

$$\sum_{k\ge 2} k^2\,d(G,k) \ge 4\left[\frac{n(n-1)}{2} - m - 3\right] + 18 + 16 \ge (n-1)^2 + 21\,.$$

Together with (8), we get

$$\begin{aligned}\prod_{k\geq 2} k^{d(G,k)} &\geq \sum_{k\geq 1}(k+k^2)d(G,k) + 10\,(n-1)^2 - 2\left\lceil\frac{n}{2}\right\rceil\left\lfloor\frac{n}{2}\right\rfloor - 138 \\ &> \sum_{k\geq 1}(k+k^2)d(G,k) \quad \text{as} \;\; n>5\,.\end{aligned}$$

Thus $\pi(G) > 2\,WW(G)$. ■

For $G \cong K_n$, $K_n - e$ (e is any edge of K_n), we have $\pi(G) < 2\,WW(G)$. On the other hand, the following holds:

Theorem 7. *Let G be a connected graph or order n with m edges and diameter d. If $d \geq 4$ and*

$$m \leq \frac{285\,W(G) - 6624}{287}\,,$$

then $\pi(G) \geq 2\,WW(G)$.

Proof. For any non-negative real numbers k and x, we have $k^x \geq kx$. Since $d \geq 4$,

$$\begin{aligned}\pi(G) &= \prod_{k\geq 2} k^{d(G,k)} = 2^{d(G,2)}\,3^{d(G,3)}\,4^{d(G,4)} \prod_{k\geq 5} k^{d(G,k)} \\ &= 288 \times 2^{d(G,2)-3}\,3^{d(G,3)-2}\,4^{d(G,4)-1} \prod_{k\geq 5} k^{d(G,k)} \\ &\geq 288\left[2^{d(G,2)-3} + 3^{d(G,3)-2} + 4^{d(G,4)-1} + \sum_{k\geq 5} k^{d(G,k)}\right] \\ &= 288\left[(2^2)^{\frac{d(G,2)-3}{2}} + (3^2)^{\frac{d(G,3)-2}{2}} + (4^2)^{\frac{d(G,4)-1}{2}} + \sum_{k\geq 5}(k^2)^{\frac{d(G,k)}{2}}\right] \\ &\geq 288\left[2^2\,\frac{d(G,2)-3}{2} + 3^2\,\frac{d(G,3)-2}{2} + 4^2\,\frac{d(G,4)-1}{2} + \sum_{k\geq 5} k^2\,\frac{d(G,k)}{2}\right] \\ &= 144\left[\sum_{k\geq 2} k^2\,d(G,k) - 46\right].\end{aligned}$$

In view of Eq. (1), since if $m \leq (285\,W(G) - 6624)/287$, then

$$2m \leq 285 \sum_{k\geq 2} k\,d(G,k) - 6624 \leq \sum_{k\geq 2}(143\,k^2 - k)\,d(G,k) - 6624 \;\; \text{as } k \geq 2,$$

that is,

$$144\left[\sum_{k\geq 2} k^2\,d(G,k) - 46\right] \geq \sum_{k\geq 1}(k^2+k)\,d(G,k)\,,$$

which yields the required result $\pi(G) \geq 2\,WW(G)$. ■

5 More relations between distance-based topological indices

We first state a relation between $W(G)$, $WW(G)$, and $RCW(G)$.

Theorem 8. *Let G be a connected graph of order $n > 1$ with m edges and diameter d. Then*

$$RCW(G) > \frac{m}{d} + \frac{1}{d+1}\left[\binom{n}{2} - m + \frac{[W(G)-m]d + 2[WW(G)-m]}{(d+1)^2}\right].$$

Proof. Since G is connected, we have $d_G(v_i, v_j) > 0$ for any vertex pair (v_i, v_j). Then

$$\left[1 - \frac{d_G(v_i,v_j)}{d+1}\right]^{-1} > 1 + \frac{d_G(v_i,v_j)}{d+1} + \frac{d_G(v_i,v_j)^2}{(d+1)^2}.$$

Combining the above result with the definitions of the Wiener and hyper-Wiener indices, we get

$$\begin{aligned}
RCW(G) &= \sum_{1\le i<j\le n} \frac{1}{d+1-d_G(v_i,v_j)} \\
&= \sum_{\substack{1\le i<j\le n \\ v_iv_j\in E(G)}} \frac{1}{d+1-d_G(v_i,v_j)} + \sum_{\substack{1\le i<j\le n \\ v_iv_j\notin E(G)}} \frac{1}{d+1-d_G(v_i,v_j)} \\
&= \frac{m}{d} + \frac{1}{d+1} \sum_{\substack{1\le i<j\le n \\ v_iv_j\notin E(G)}} \left[1 - \frac{d_G(v_i,v_j)}{d+1}\right]^{-1} \\
&> \frac{m}{d} + \frac{1}{d+1} \sum_{\substack{1\le i<j\le n \\ v_iv_j\notin E(G)}} \left[1 + \frac{d_G(v_i,v_j)}{d+1} + \frac{d_G(v_i,v_j)^2}{(d+1)^2}\right] \\
&= \frac{m}{d} + \frac{1}{d+1}\left[\binom{n}{2} - m + \sum_{\substack{1\le i<j\le n \\ v_iv_j\notin E(G)}} \frac{(d+1)\,d_G(v_i,v_j) + d_G(v_i,v_j)^2}{(d+1)^2}\right] \\
&= \frac{m}{d} + \frac{1}{d+1}\left[\binom{n}{2} - m + \frac{(W(G)-m)d + 2(WW(G)-m)}{(d+1)^2}\right].
\end{aligned}$$

This completes the proof of the theorem. ■

In [38], Radon discovered the following inequality:

Lemma 8. (Radon's inequality) *If $a_k, x_k > 0$, $k \in \{1,2,\ldots,r\}$, and $p > 0$, then the following inequality holds:*

$$\sum_{k=1}^{r} \frac{x_k^{p+1}}{a_k^p} \geq \frac{\left(\sum\limits_{k=1}^{r} x_k\right)^{p+1}}{\left(\sum\limits_{k=1}^{r} a_k\right)^{p}}$$

with equality holding if $\dfrac{x_1}{a_1} = \dfrac{x_2}{a_2} = \cdots = \dfrac{x_r}{a_r}$.

Lemma 9. [16] *Let $a_1, a_2, \ldots, a_N$ and $b_1, b_2, \ldots, b_N$ be real numbers for which there exist real constants r and R such that $r\,a_i \leq b_i \leq R\,a_i$ hold for each i, $i = 1,2,\ldots,N$. Then*

$$\sum_{i=1}^{N} b_i^2 + r\,R \sum_{i=1}^{N} a_i^2 \leq (r+R) \sum_{i=1}^{N} a_i\, b_i \tag{9}$$

with equality holding if and only if for at least one i, $1 \leq i \leq N$ holds $r\,a_i = b_i = R\,a_i$.

Theorem 9. *Let G be a graph of order n with m edges and diameter d. Then*

$$4d^2\left(W(G)-m\right)^2 < 2(WW(G)-m)\Big[\frac{n(n-1)(5\,d^2+4)}{2}$$

$$-\quad 4d^2\,H(G) - m\,(d^2+3) - 2\,WW(G) + W(G)\Big].$$

Proof. Suppose that each i in Lemma 9 corresponds to a vertex pair (v_i, v_j) for which $d_G(v_i,v_j) \geq 2$ such that $N = n(n-1)/2 - m$. Setting $r = 4$, $R = d^2$ and replacing each b_i by $d_G(v_i,v_j)$ and each a_i by $\frac{1}{d_G(v_i,v_j)}$, then from (9), we get

$$\sum_{\substack{1\leq i<j\leq n\\ d_G(v_i,v_j)\geq 2}} d_G(v_i,v_j)^2 + 4d^2 \sum_{\substack{1\leq i<j\leq n\\ d_G(v_i,v_j)\geq 2}} \frac{1}{d_G(v_i,v_j)^2} \leq (d^2+4)\left[\frac{n(n-1)}{2} - m\right],$$

that is,

$$\sum_{\substack{1\leq i<j\leq n\\ d_G(v_i,v_j)\geq 2}} \left[d_G(v_i,v_j)^2 + d_G(v_i,v_j) + \frac{4d^2}{d_G(v_i,v_j)^2}\right] - \Big[W(G) - m\Big] \leq (d^2+4)\left[\frac{n(n-1)}{2} - m\right],$$

that is,

$$2\,WW(G) - W(G) - m + 4d^2 \sum_{\substack{1\leq i<j\leq n\\ d_G(v_i,v_j)\geq 2}} \frac{1}{d_G(v_i,v_j)^2} \leq (d^2+4)\left[\frac{n(n-1)}{2} - m\right],$$

that is,

$$\sum_{\substack{1\leq i<j\leq n\\ d_G(v_i,v_j)\geq 2}} \frac{1}{d_G(v_i,v_j)^2} \leq \frac{(d^2+4)\left(\frac{n(n-1)}{2} - m\right) - 2\,WW(G) + W(G) + m}{4d^2}. \tag{10}$$

Suppose that each k in Lemma 8 corresponds to a vertex pair (v_i, v_j) with $d_G(v_i, v_j) \geq 2$ such that $r = \frac{n(n-1)}{2} - m$. Setting $p = 1$, and replacing each x_k by $d_G(v_i, v_j)$ and each a_k by $d_G(v_i, v_j)^2 + d_G(v_i, v_j)$, we get

$$\frac{\left(\sum\limits_{\substack{1\leq i<j\leq n\\ d_G(v_i,v_j)\geq 2}} d_G(v_i, v_j)\right)^2}{\sum\limits_{\substack{1\leq i<j\leq n\\ d_G(v_i,v_j)\geq 2}} \left[d_G(v_i, v_j)^2 + d_G(v_i, v_j)\right]} \leq \sum_{\substack{1\leq i<j\leq n\\ d_G(v_i,v_j)\geq 2}} \frac{d_G(v_i, v_j)^2}{d_G(v_i, v_j)^2 + d_G(v_i, v_j)}\,,$$

that is,

$$\frac{\Big(W(G) - m\Big)^2}{2\Big(WW(G) - m\Big)} \leq \sum_{\substack{1\leq i<j\leq n\\ d_G(v_i,v_j)\geq 2}} \left[1 + \frac{1}{d_G(v_i, v_j)}\right]^{-1}.$$

One can easily see that

$$\left[1 + \frac{1}{d_G(v_i, v_j)}\right]^{-1} < 1 - \frac{1}{d_G(v_i, v_j)} + \frac{1}{d_G(v_i, v_j)^2}\,.$$

Using the above two results, we have

$$\begin{aligned}\frac{\Big(W(G) - m\Big)^2}{2\Big(WW(G) - m\Big)} &< \sum_{\substack{1\leq i<j\leq n\\ d_G(v_i,v_j)\geq 2}} \left[1 - \frac{1}{d_G(v_i, v_j)} + \frac{1}{d_G(v_i, v_j)^2}\right] \\ &= \frac{n(n-1)}{2} - H(G) + \sum_{\substack{1\leq i<j\leq n\\ d_G(v_i,v_j)\geq 2}} \frac{1}{d_G(v_i, v_j)^2}\,.\end{aligned}$$

Combining this with (10), we get

$$\frac{\Big(W(G)-m\Big)^2}{2\Big(WW(G)-m\Big)} < \frac{n(n-1)}{2} - H(G) + \frac{(d^2+4)\left(\frac{n(n-1)}{2} - m\right) - 2\,WW(G) + W(G) + m}{4d^2}\,,$$

which gives the required result. ■

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