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Relationships between Some Distance–Based Topological Indices

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Abstract. The Harary index (HI), the average distance (AD), the Wiener polarity index (WPI) and the connective eccentricity index (CEI) are distance–based graph invariants, some of which found applications in chemistry. We investigate the relationship between HI, AD, and CEI, and between WPI, AD, and CEI. First, we prove that $HI > AD$ for any connected graph and that $HI > CEI$ for trees, with only three exceptions. We compare WPI with CEI for trees, and give a classification of trees for which $CEI \geq WPI$ or $CEI < WPI$. Furthermore, we prove that for trees, $WPI > AD$, with only three exceptions.

1. Introduction

Throughout this paper we consider only simple connected graphs. For a graph $G = (V, E)$ with vertex set $V = V(G)$ and edge set $E = E(G)$, the *degree* of a vertex v, denoted by $d_G(v)$, is the number of edges incident with v. Denote by $d_G(u, v)$ the distance between vertices u and v in G. The *eccentricity* of a vertex v in a graph G is defined to be $\varepsilon_G(v) = \max\{d_G(u, v)|u \in V(G)\}$. The *diameter* of a connected graph G is equal to $\max\{\varepsilon_G(v)|v \in V(G)\}$, whereas its *radius* is equal to $\min\{\varepsilon_G(v)|v \in V(G)\}$.

A connected graph is said to be a *tree* if it contains no cycles. Let P_n, S_n, C_n, and K_n be the path, star, cycle, and complete graph of order n, respectively. For other notation and terminology not defined here, the readers are referred to [3].

One of the oldest and best studied distance–based graph invariants is the Wiener index, defined as [26]

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

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In some applications, it is more convenient to study the *average distance* (AD) of G,

$$\overline{W}(G) = \frac{1}{\binom{n}{2}} \sum_{\{u,v\}\subseteq V(G)} d_G(u,v) = \frac{2}{n(n-1)} W(G)\,.$$

Results on Wiener index can be found in the reviews [12, 16, 27]. For results on average distance see [4–6, 11] and the references cited therein.

Another distance-based graph invariant, put forward independently in [22] and [25], is the reciprocal–analogue of the Wiener index, named *Harary index* (HI), and defined as

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

The *Wiener polarity index* (WPI), introduced also by Wiener in 1947 [26], is

$$W_p(G) = |\{(u,v)\,|\,d_G(u,v) = 3, u,v \in V(G)\}|\,.$$

It also found applications in chemistry [18, 24]. For recent mathematical results on WPI see [13–15, 21, 23, 30].

In 2000, the *connective eccentricity index* (CEI) of a connected graph G, denoted by $C^{\xi}(G)$, was introduced by Gupta et al. [17] as

$$C^{\xi}(G) = \sum_{u\in V(G)} \frac{d_G(u)}{\varepsilon_G(u)}\,.$$

For recent results on the CEI see [1, 28, 29] and the references cited therein.

Relationships between various graph invariants have received much attention over the past few decades, see e.g., [7–10, 19, 20].

In this paper, we investigate various relationships between the above listed distance–based graph invariants. We prove that the Harary index is greater than the average distance for any connected graph. Also, we prove that for trees, the Harary index is greater than the connective eccentricity index, with only three exceptions. Moreover, we compare the Wiener polarity index with the connective eccentricity index for trees, and give an explicit classification of all trees for which CEI is greater or smaller than WPI. We prove that for trees, the Wiener polarity index is greater than the average distance, with only three exceptions. Finally, we compare the Harary index with connective eccentricity index in terms of a radius-dependent condition.

2. Main Results

In this section, we investigate the relationship between the Harary index and average distance and connective eccentricity index, and the relationship between the Wiener polarity index and average distance and connective eccentricity index. We will proceed by dividing our discussions into four subsections.

2.1. Harary index and average distance

For a connected graph G, the *remoteness* of G is defined as $\rho = \rho(G) = \max_{v\in V(G)} \frac{1}{n-1} D_G(v)$. We need a result on remoteness due to Aouchiche and Hansen, which reads as follows:

Lemma 2.1 ([2]). *Let G be a connected graph of order n with remoteness ρ. Then $\rho \le n/2$ with equality if and only if $G \cong P_n$.*

Next, we will show that the Harary index is greater than the average distance for any connected graph. First, we prove a somewhat stronger result:

Theorem 2.2. *Let G be a connected graph with average distance $\overline{W}(G)$ and average degree $\overline{d}(G)$. Then*

$$H(G) > \overline{d}(G) \cdot \overline{W}(G)\,.$$

Proof. Suppose that the order and size of G are n and m, respectively. Then $\overline{d}(G) = \frac{2m}{n}$. By Lemma 2.1,

$$\overline{d}(G) \cdot \overline{W}(G) = \frac{2m}{n} \cdot \frac{\sum_{v\in V(G)} D_G(v)}{n(n-1)} = \frac{2m}{n^2} \cdot \sum_{v\in V(G)} \frac{D_G(v)}{n-1} \le \frac{2m}{n^2} \cdot n\rho \le \frac{2m}{n^2} \cdot n \cdot \frac{n}{2} = m\,.$$

Obviously,

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

with equality if and only if $G \cong K_n$.

Therefore, $H(G) \ge \overline{d}(G) \cdot \overline{W}(G)$. It is not difficult to see that the equality in the above inequality cannot be attained. Thus, $H(G) > \overline{d}(G) \cdot \overline{W}(G)$. □

Since $\overline{d}(G) \ge 1$ for any connected graph G, we have:

Corollary 2.3. *Let G be a connected graph with average distance $\overline{W}(G)$ and Harary index $H(G)$. Then*

$$H(G) > \overline{W}(G)\,.$$

2.2. Harary index and connective eccentricity index

In order to find the relationship between the Harary index and the connective eccentricity index, we first consider the following three special graphs.

For the complete graph K_n, $C^{\xi}(K_n) = n(n-1) > \frac{n(n-1)}{2} = H(K_n)$ for $n \ge 2$.

For $a \ge 1, b \ge 1$, let S_{a+1} and S_{b+1} be stars on $a+1$ and $b+1$ vertices, respectively. Then the *double star $S_{a,b}$* is the tree obtained by connecting an edge between two centers of S_{a+1} and S_{b+1}.

For the double star $S_{a,b}$ $(a+b = n-2)$, $C^{\xi}(S_{a,b}) = \frac{5n-4}{6}$, $H(S_{a,b}) = \frac{ab}{3} + \frac{3(a+b)}{2} + 1 \ge \frac{n-3}{3} + \frac{3(n-2)}{2} + 1 = \frac{11n-18}{6}$. Therefore, $H(S_{a,b}) > C^{\xi}(S_{a,b})$ for $n \ge 4$.

For the complete bipartite graph $K_{\frac{n}{2},\frac{n}{2}}$, where $n \ge 4$ and n is an even integer, $C^{\xi}(K_{\frac{n}{2},\frac{n}{2}}) = \frac{n^2}{4}$, $H(K_{\frac{n}{2},\frac{n}{2}}) = \frac{3n^2}{8} - \frac{n}{4}$. Therefore, $C^{\xi}(K_{\frac{n}{2},\frac{n}{2}}) < H(K_{\frac{n}{2},\frac{n}{2}})$ for $n \ge 4$.

From the above examples, one concludes that in the general case, HI and CEI are incomparable. Bearing this in mind, we shall restrict our considerations to to trees.

Theorem 2.4. *Let T be a tree of order n. If $T \in \{P_2, P_3\}$, then $H(T) < C^{\xi}(T)$. Otherwise,*

$$H(T) \ge C^{\xi}(T)$$

with equality if and only if $T \cong S_4$.

Proof. For $T \in \{P_2, P_3\}$, it can be easily checked that $H(T) < C^{\xi}(T)$. Assume therefore that $T \notin \{P_2, P_3\}$. Then, $n \ge 4$.

Let $A = \{v | d_T(v) = n-1\}$. Since T is a tree, we have $|A| \le 1$.

If $|A| = 0$, then $\varepsilon_T(v) \ge 2$ for each vertex v in T, and thus, $\frac{d_T(v)}{\varepsilon_T(v)} \le \frac{d_T(v)}{2}$. For any vertex v in T, write $\widehat{D}_T(v) = \sum_{u\in V(G)\setminus\{v\}} \frac{1}{d_T(u,v)}$. Note that if $\varepsilon_T(v) \ge 2$, then $\widehat{D}_T(v) > d_T(v)$. Therefore,

$$H(T) = \frac{1}{2} \sum_{v\in V(T)} \widehat{D}_T(v) > \frac{1}{2} \sum_{v\in V(T)} d_T(v) \ge \sum_{v\in V(T)} \frac{d_T(v)}{\varepsilon_T(v)} = C^{\xi}(T)\,.$$

Thus, in this case, $H(T) > C^{\xi}(T)$.

Now, let $|A| = 1$. Then $T \cong S_n$, and thus, $H(T) = H(S_n) = (n-1) + \binom{n-1}{2} \cdot \frac{1}{2} = \frac{(n-1)(n+2)}{4}$, $C^{\xi}(T) = \frac{n-1}{2} + (n-1) = \frac{3(n-1)}{2}$. Note that $n \geq 4$. Thus, $H(T) \geq C^{\xi}(T)$, with equality only if $n = 4$, that is, if $T \cong S_4$. Conversely, if $T \cong S_4$, then $H(T) = C^{\xi}(T)$.

This completes the proof. □

Next, we compare the Harary and connective eccentricity indices for connected graphs under given restricted condition.

Theorem 2.5. *Let G be a connected graph of order $n \geq 4$ with m edges and $p \geq 0$ vertices of degree $n-1$. If $m \geq \frac{(n-1)(n-2p)}{2}$ and $p < \frac{n}{2}$, then $H(G) \leq C^{\xi}(G)$.*

Proof. Let Δ be the maximum degree of graph G. First, we claim that $\Delta = n-1$.

If $\Delta \leq n-2$, then $p = 0$. By our assumption that $m \geq \frac{(n-1)(n-2p)}{2} = \frac{n(n-1)}{2}$, we must have $G \cong K_n$, a contradiction.

Thus, we may assume that $\Delta = n-1$. Then $d \leq 2$. If $d = 1$, then $G \cong K_n$ and hence $H(G) = \frac{n(n-1)}{2} < n(n-1) = C^{\xi}(G)$. Suppose therefore that $d = 2$. Since $m \geq \frac{(n-1)(n-2p)}{2}$, we have

$$H(G) = m + \frac{1}{2}\left[\frac{n(n-1)}{2} - m\right] \leq p(n-1) + \frac{2m - p(n-1)}{2} = C^{\xi}(G)\,.$$

□

2.3. Wiener polarity index and connective eccentricity index

In order to find a relationship between the Wiener polarity index and the connective eccentricity index, we first consider the following two special graphs.

For the complete graph K_n, $C^{\xi}(K_n) = n(n-1) > 0 = W_p(K_n)$ for $n \geq 2$.

For the path P_n, $C^{\xi}(P_n) < n \cdot \frac{2}{\frac{n}{2}} = 4 < n-3 = W_p(P_n)$ for $n \geq 8$.

These examples imply that in the general case, WPI and CEI are incomparable. In view of this, we restrict our considerations to trees.

We first introduce a special class of trees.

Suppose that $P_{d+1} = v_0 v_1 \cdots v_{d-1} v_d$ is a path of length d. For $d \geq 3$, let $T_n(r,t)$ be a tree of order n with diameter d obtained from P_{d+1} by attaching r and t pendent vertices to v_1 and v_{d-1}, respectively. Here, $r \geq 0$, $t \geq 0$, and $r + t = n - d - 1$, See Fig. 1.

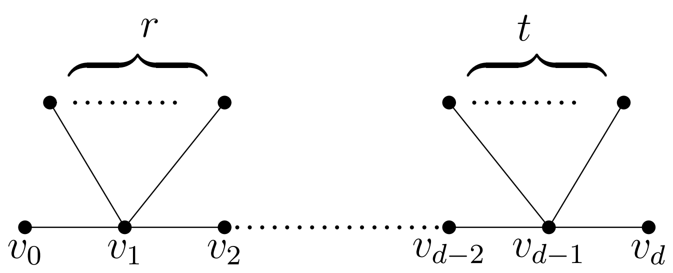

Fig. 1. The tree $T_n(r,t)$, where $r \geq 0$, $t \geq 0$, and $r + t = n - d - 1$.

We first state a result due to Deng et al.

Lemma 2.6 ([14]). *Let T be a tree of order n and diameter $d \geq 3$. Then $W_p(T) \geq n-3$ with equality if and only if $T \cong T_n(r,t)$ for $d > 4$, and $T \cong T_n(n-4,0)$ for $d = 3$.*

Note that the tree $T_n(n-4,0)$ in Lemma 2.6 is isomorphic to the double star $S_{1,n-3}$.

In 2009, Du et al. gave the following remarkable formula for computing the Wiener polarity index of trees.

Lemma 2.7 ([15]). *Let T be a tree. Then*

$$W_p(T) = \sum_{uv \in V(T)} [d_T(u)-1][d_T(v)-1]\,. \tag{1}$$

Theorem 2.8. *Let T be a tree of order n. If $T \in \{S_n, P_5, S_{2,2}, T_6(1,0), T_7(2,0)\}$ or $T \cong S_{1,n-3}$ for $4 \leq n \leq 14$, then $C^\xi(T) \geq W_p(T)$ with equality if and only if $T \cong T_7(2,0)$ or $T = congS_{1,11}$. Otherwise,*

$$W_p(T) > C^\xi(T)\,.$$

Proof. We have to separately consider the following three cases:

Case $d = 2$: Then $T \cong S_n$ and thus $C^\xi(T) = 3(n-1)/2 > 0 = W_p(T)$.

Case $d = 3$: Then $T \cong S_{a,b}$ ($a+b+2 = n$, $1 \leq a \leq b$) and thus

$$W_p(T) - C^\xi(T) = ab - \frac{5a+5b+6}{6} = \frac{5b(a-1)+a(b-5)-6}{6}\,.$$

First we assume that $a = 1$. Then $T \cong S_{1,n-3}$ and then $W_p(T) - C^\xi(T) = \frac{n-14}{6}$. For $4 \leq n \leq 13$, $W_p(T) < C^\xi(T)$, for $n = 14$, $W_p(T) = C^\xi(T)$, whereas for $n \geq 15$, $W_p(T) > C^\xi(T)$. Assume next that $a \geq 2$. If $b = 2$, then $(a,b) = (2,2)$ and therefore $W_p(T) < C^\xi(T)$. Otherwise, $b \geq 3$. Then $5b(a-1)+a(b-5)-6 \geq 5b-2a-6 > 0$. Thus we have $W_p(T) > C^\xi(T)$.

Case $d \geq 4$: Assume first that $T \cong T_n(r,t)$. Then $W_p(T) \geq n-3$, $C^\xi(G) \leq \frac{r+s+2}{4} + \frac{2n-6-r-s}{3} + \frac{2}{2}$, and

$$W_p(T) - C^\xi(T) \geq \frac{n}{3} - \frac{5}{2} + \frac{r+s}{12}\,.$$

If $n \geq 8$, then from the above it follows $W_p(T) > C^\xi(T)$. Otherwise, in this case $n = 5$ or 6 or 7. Since $T \cong T_n(r,t)$, we have $T \cong P_5$ ($n = 5$) or $T \cong P_6$ ($n = 6$) or $T \cong T_6(1,0)$ ($n = 6$) or $T \cong P_7$ ($n = 7$) or $T \cong T_7(1,0)$ ($n = 7$) or $T \cong T_7(2,0)$ ($n = 7$) or $T \cong T_7(1,1)$ ($n = 7$).

For $T \cong P_5$, $C^\xi(T) = 17/6 > 2 = W_p(T)$. For $T \cong P_6$, $C^\xi(T) = 41/15 < 3 = W_p(T)$. For $T \cong T_6(1,0)$, $C^\xi(T) = 41/12 > 3 = W_p(T)$. For $T \cong P_7$, $C^\xi(T) = 14/5 < 4 = W_p(T)$. For $T \cong T_7(1,0)$, $C^\xi(T) = 119/60 > 4 = W_p(T)$. For $T \cong T_7(2,0)$, $C^\xi(T) = 4 = W_p(T)$. For $T \cong T_7(1,1)$, $C^\xi(T) = 4 = W_p(T)$.

Assume next that $T \ncong T_n(r,t)$. Then by Lemma 2.7, $W_p(T) \geq n-2$. Let $P_{d+1} : v_1v_2\ldots v_dv_{d+1}$ be a diametral path in T. Then

$$C^\xi(G) \leq \frac{2}{4} + \frac{d_2+d_d}{3} + \frac{2n-4-d_2-d_d}{2} = n-2-\frac{d_2+d_d-3}{6}$$

where d_2 and d_d are the degrees of the vertices v_2 and v_d, respectively. Thus we have $W_p(T) - C^\xi(T) \geq \frac{d_2+d_d-3}{6} > 0$ as $d_2 \geq 2$ and $d_d \geq 2$.

This completes the proof. □

2.4. Wiener polarity index and average distance

In order to find the relationship between the Wiener polarity index and the average distance, we first consider the following special graphs.

For the complete graph K_n, $\overline{W}(K_n) = 1 > 0 = W_p(K_n)$ for $n \geq 2$.

For the six-membered cycle C_6, $\overline{W}(C_6) = \frac{9}{5} < 3 = W_p(C_6)$.

For the path P_n, $\overline{W}(P_n) < \frac{n}{2} \leq n-3 = W_p(P_n)$ for $n \geq 6$.

These examples show that in the general case, WPI and AD are incomparable. Bearing this in mind, we restrict our considerations to trees.

Theorem 2.9. *Let T be a tree of order n. If $T \in \{S_n, P_4, P_5\}$, then $\overline{W}(T) \geq W_p(T)$ with equality if and only if $T \cong P_5$. Otherwise,*

$$W_p(T) > \overline{W}(T).$$

Proof. We first show that the statement of theorem is true for each tree in the set $\{S_n, P_4, P_5\}$.

If $T \cong S_n$, then $\overline{W}(T) = 2(n-1)/n > 0 = W_p(T)$.

If $T \cong P_4$, then $\overline{W}(T) = 5/3 > 1 = W_p(T)$.

If $T \cong P_5$, then $\overline{W}(T) = 2 = W_p(T)$.

Assume now that $T \notin \{S_n, P_4, P_5\}$. Let d be the diameter of T. Then $d \geq 3$. We consider the following three cases.

Case 1. $3 \leq d \leq n-3$.

By Lemma 2.6, $W_p(T) \geq n-3 \geq d > \overline{W}(T)$.

Case 2. $d = n-2$.

If $T \cong T_n(1,0)$, then by Lemma 2.6, $W_p(T) = n-3$. As $d \geq 3$, we have $n \geq 5$. If $n = 5$, then $T \cong T_5(1,0) = S_{1,2}$. Then $W_p(T) = n-3 = 2 > 9/5 = \overline{W}(T)$. So, we may suppose that $n \geq 6$. Then by Lemma 2.1, $\overline{W}(T) \leq \rho < \frac{n}{2}$, and thus,

$$W_p(T) - \overline{W}(T) > n - 3 - \frac{n}{2} = \frac{1}{2}(n-6) \geq 0,$$

that is, $W_p(T) > \overline{W}(T)$.

Now, we assume that $T \ncong T_n(1,0)$. Then by Lemma 2.6, $W_p(T) \geq n-2 = d > \overline{W}(T)$.

Case 3. $d = n-1$.

Then $T \cong P_n = T_n(0,0)$. By Lemma 2.6, $W_p(T) = n-3$. Note that $n = d+1 \geq 4$. By our assumption that $T \notin \{S_n, P_4, P_5\}$, we have $n \geq 6$. Thus, $\overline{W}(T) < \rho = \frac{n}{2}$. Therefore, $W_p(T) - \overline{W}(T) > n-3-\frac{n}{2} = \frac{1}{2}(n-6) \geq 0$.

This completes the proof. □

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