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On Relations between Distance–Based Topological Indices

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Abstract

Motivated by the recent paper *On topological indices and their reciprocals*, MATCH COMMUN. MATH. COMPUT. CHEM. **91** (2024) 287, we establish additional relations between distance– and degree–and–distance–based molecular structure descriptors: Wiener, hyper–Wiener, Harary, connective eccentricity, eccentric connectivity, degree distance, Gutman, additively weighted Harary, and multiplicatively weighted Harary indices, especially for their products.

1 Introduction

All considered graphs throughout this paper are simple, finite and connected. Let $G = (V, E)$ be such a graph. We denote by $\deg(u)$ the degree of the vertex $u \in V(G)$. The distance $d(u, v)$ between two vertices u and

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v of the graph G is the length of a shortest path connecting them. The eccentricity $\varepsilon(u)$ of a vertex u is the maximum distance from u to other vertices of G . The diameter $\text{diam}(G)$ and radius $\text{rad}(G)$ are, respectively, the maximum and minimum eccentricities of the vertices of G . The transmission $Tr(v)$ of a vertex v is the sum of distances from v to other vertices.

The center of a graph is the set of all vertices with the minimum eccentricity. A graph G is called self-centered if its center consists of all its vertices. For such graphs $\text{diam}(G) = \text{rad}(G)$.

Transmission (also called status or total distance of a vertex) is one of the fundamental concepts in facility problems and local theory [5,12,17,23]. Moreover it plays a significant role in the investigation and constructing of distance-based topological indices in chemical graph theory. Several types of graphs are distinguished with regard to the transmission of their vertices. For instance transmission regular graphs are graphs in which all vertices have the same transmission. A graph is transmission irregular if all its vertices have different transmissions [2].

The reciprocal analogue of transmission, denoted by $h(u)$, is defined as

$$h(u) = \sum_{\substack{v \in V(G) \\ v \neq u}} \frac{1}{d(u, v)}.$$

Relations between distance-based topological indices were investigated in several studies, see [4, 13, 15, 18, 29] and the references cited therein. In this paper, motivated by the researches done in [13] and [14], we establish some additional relations between distance- and degree-and-distance-based topological indices. The following topological indices will be considered:

Wiener index [16, 20, 21, 27]

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u, v) = \frac{1}{2} \sum_{v \in V(G)} Tr(v);$$

hyper-Wiener index [19]

$$WW(G) = \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} [d(u, v)^2 + d(u, v)];$$

Harary index [24, 28]

$$H(G) = \sum_{\substack{\{u,v\} \subseteq V(G) \\ u \neq v}} \frac{1}{d(u,v)} = \frac{1}{2} \sum_{u \in V(G)} h(u);$$

eccentric connectivity index [26]

$$\xi^{ec}(G) = \sum_{v \in V(G)} \deg(v) \varepsilon(v);$$

connective eccentricity index [8]

$$\xi^{ce}(G) = \sum_{v \in V(G)} \frac{\deg(v)}{\varepsilon(v)};$$

degree distance [7, 10, 25]

$$DD(G) = \sum_{\{u,v\} \subseteq V(G)} [\deg(u) + \deg(v)] d(u,v);$$

Gutman index [9–11]

$$ZZ(G) = \sum_{\{u,v\} \subseteq V(G)} [\deg(u) \deg(v)] d(u,v);$$

additively weighted Harary index [1]

$$H_A(G) = \sum_{\substack{\{u,v\} \subseteq V(G) \\ u \neq v}} \frac{\deg(u) + \deg(v)}{d(u,v)}$$

multiplicatively weighted Harary index [3]

$$H_M(G) = \sum_{\substack{\{u,v\} \subseteq V(G) \\ u \neq v}} \frac{\deg(u) \deg(v)}{d(u,v)}.$$

Note that the indices $\xi^{ce}(G)$ and $\xi^{ec}(G)$ can be presented as:

$$\xi^{ce}(G) = \sum_{uv \in E(G)} \left[\frac{1}{\varepsilon(u)} + \frac{1}{\varepsilon(v)} \right]$$

and

$$\xi^{ec}(G) = \sum_{uv \in E(G)} [\varepsilon(u) + \varepsilon(v)].$$

2 Main results

In [4] and [13] estimates for the product of the Wiener and Harary indices were communicated. Here we report some additional results of this kind, for the products $W(G)H(G)$ and $\xi^{ce}(G)\xi^{ec}(G)$. In order to achieve these results, we recall two well known auxiliary lemmas [22].

Lemma 1. (Lagrange identity) *Let $\{a_1, a_2, \dots, a_n\}$ and $\{b_1, b_2, \dots, b_n\}$ be two sets of real numbers. Then*

$$\sum_{i=1}^n a_i^2 \sum_{i=1}^n b_i^2 - \left(\sum_{i=1}^n a_i b_i \right)^2 = \left(\sum_{i < j} [a_i b_j - a_j b_i] \right)^2.$$

Lemma 2. (Cauchy–Schwarz inequality) *Let $\{a_1, a_2, \dots, a_n\}$ and $\{b_1, b_2, \dots, b_n\}$ be two sets of real numbers. Then*

$$\sum_{i=1}^n a_i^2 \sum_{i=1}^n b_i^2 \geq \left(\sum_{i=1}^n a_i b_i \right)^2$$

with equality if and only if $a_1/b_1 = a_2/b_2 = \dots = a_n/b_n$.

A graph G is said to be vertex transitive if for any pair of vertices u and v , there is an automorphism α such that $\alpha(u) = v$. From the fact that distances are preserved by an automorphism, i.e., $d(u, v) = d(\alpha(u), \alpha(v))$ (for each $u, v \in V(G)$ and $\alpha \in \text{Aut}(G)$), a vertex transitive graph is transmission regular and also self-centered. Moreover we have:

Lemma 3. *If G is a vertex transitive graph of order n , then for each vertex u , $\text{Tr}(u) = \frac{2}{n}W(G)$ and $h(u) = \frac{2}{n}H(G)$.*

In what follows, $[n]$ stands for the set $\{1, 2, \dots, n\}$. As usual, the complete graph of order n will be denoted by K_n .

Theorem 1. *Let G be a vertex transitive graph with diameter d . Then*

$$\binom{n}{2}^2 \leq W(G) H(G) \leq \binom{n}{2}^2 + \frac{n^2}{4} \binom{n-1}{2} \frac{(d-1)^2}{d}.$$

Both equalities hold if and only if $G \cong K_n$.

Proof. Let u be a vertex of G . Let $\{d_i \mid i \in [n-1]\}$ be the set of distances between u and the other vertices of G . Considering $a_i = \sqrt{d_i}$ and $b_i = \sqrt{1/d_i}$ for $i \in [n-1]$, the Cauchy–Schwarz inequality yields

$$\text{Tr}(u) h(u) = \sum_{i=1}^{n-1} a_i \sum_{i=1}^{n-1} b_i \geq \left(\sum_{i=1}^{n-1} a_i b_i \right)^2 = (n-1)^2.$$

Since G is vertex transitive, by Lemma 3 we get $W(G) H(G) \geq \binom{n}{2}^2$.

Equality holds if and only if $d_i = d_j$ for all $i, j \in [n-1]$. This implies $\varepsilon(u) = 1$.

By Lemma 2, equality holds if and only if $\varepsilon(u) = 1 = \varepsilon(v)$ for each pair of vertices u and v . Thus $G \cong K_n$.

In order to prove the right inequality, apply Lemma 1. This yields

$$\text{Tr}(u) h(u) - (n-1)^2 = \left[\sum_{i < j} \left(\sqrt{\frac{d_i}{d_j}} - \sqrt{\frac{d_j}{d_i}} \right) \right]^2.$$

The function $f(x) = \sqrt{x} - \frac{1}{\sqrt{x}}$ is ascending on $x \geq 1$. Therefore for $i < j$,

$$\sqrt{\frac{d_i}{d_j}} - \sqrt{\frac{d_j}{d_i}} \leq \sqrt{d} - \frac{1}{\sqrt{d}} \quad (1)$$

where d is the maximal value of d_i/d_j . Thus

$$\text{Tr}(u) h(u) - (n-1)^2 \leq \binom{n-1}{2} \left(d + \frac{1}{d} - 2 \right).$$

Since G is vertex transitive, applying Lemma 3 yields the desired result. Moreover the equality in (1) holds if and only if $d_i = d$ and $d_j = 1$ for $i < j$. Thus the equality

$$\text{Tr}(u)h(u) - (n-1)^2 = \binom{n-1}{2} \frac{(d-1)^2}{d}$$

holds if and only if $d_i = d$ for each $i \in [n-1]$. Consequently $\varepsilon(u) = 1$. Therefore, the right equality holds if and only if $\varepsilon(u) = 1$ for each vertex $u \in V(G)$. Thus $G \cong K_n$. ■

The following results follows by Theorem 1 and the fact that a vertex transitive graph is a regular graph.

Corollary. *Let G be a k -regular and vertex transitive graph of diameter d . Then*

$$\begin{aligned} \binom{n}{2}^2 &\leq \frac{H_A(G)DD(G)}{4k^2} \leq \binom{n}{2}^2 + \frac{n^2}{4} \binom{n-1}{2} \frac{(d-1)^2}{d} \\ \binom{n}{2}^2 &\leq \frac{H_M(G)ZZ(G)}{k^4} \leq \binom{n}{2}^2 + \frac{n^2}{4} \binom{n-1}{2} \frac{(d-1)^2}{d}. \end{aligned}$$

The equalities hold if and only if $G \cong K_n$.

Theorem 2. *Let G be a graph of size m . Then*

$$4m^2 \leq \xi^{ce}(G)\xi^{ec}(G) \leq 4m^2 \frac{\text{diam}(G)}{\text{rad}(G)}.$$

Both equalities hold if and only if G is a self-centered graph.

Proof. Let $V(G) = \{v_i \mid 1 \leq i \leq n\}$. Set $a_i = \sqrt{\deg(v_i)\varepsilon(v_i)}$ and $b_i = \sqrt{\deg(v_i)/\varepsilon(v_i)}$ for $i \in [n]$. Using Lemma 2 we get

$$\xi^{ce}(G)\xi^{ec}(G) = \sum_{i=1}^n \deg(v_i)\varepsilon(v_i) \sum_{i=1}^n \frac{\deg(v_i)}{\varepsilon(v_i)} \geq \left(\sum_{i=1}^n \deg(v_i) \right)^2 = 4m^2.$$

Moreover the equality holds if and only if $a_i/b_i = a_j/b_j$ for $1 \leq i, j \leq n$. This implies that $\varepsilon(v_i) = \varepsilon(v_j)$ for $1 \leq i, j \leq n$. Thus G is a self-centered

graph.

The right inequality is evident from $\varepsilon(v_j) \leq \text{diam}(G)$ and $1/\varepsilon(v_j) \leq 1/\text{rad}(G)$ for each $v_j \in V(G)$. Clearly the equality holds if and only if $\text{rad}(G) = \varepsilon(v_j) = \text{diam}(G)$ for each $v_j \in V(G)$, i.e., if G is self-centered. ■

Lemma 4. [6] *Let $\{a_1, a_2, \dots, a_n\}$ and $\{b_1, b_2, \dots, b_n\}$ be two sets of real numbers for which there exist real constants p and q such that $p a_i \leq b_i \leq q a_i$ holds for each $i \in [n]$. Then*

$$\sum_{i=1}^n b_i^2 + pq \sum_{i=1}^n a_i^2 \leq (p+q) \sum_{i=1}^n a_i b_i$$

with equality if and only if there is an i for which the relation $p a_i = b_i = q a_i$ holds.

Theorem 3. *Let G be a graph of order n and diameter d . Then*

$$W(G) + d H(G) \leq \binom{n}{2} (d+1) \quad (2)$$

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

Proof. For a vertex u , let $\{d_i \mid i \in [n-1]\}$ be same as in the proof of Theorem 1. Set $a_i = \sqrt{1/d_i}$ and $b_i = \sqrt{d_i}$. It is obvious that $1 \leq b_i/a_i = d_i \leq d$. Now by Lemma 4 and considering $p = 1$ and $q = d$, we obtain

$$\sum_{i=1}^{n-1} d_i + d \sum_{i=1}^{n-1} \frac{1}{d_i} \leq (d+1)(n-1)$$

from which it follows

$$\text{Tr}(u) + d h(u) \leq (d+1)(n-1).$$

Summing over all vertices of G , we arrive at inequality (2).

The equality $a_i = b_i = d a_i$ implies that $d = 1$ and thus $G \cong K_n$. ■

Theorem 4. *If G is a graph of order n , size m , and diameter d , then*

$$DD(G) + d H_A(G) \leq 2m(d+1)(n-1). \quad (3)$$

Equality holds if and only if $G \cong K_n$.

Proof. Let u be a vertex of G and $V(G) = \{u = u_0, u_1, u_2, \dots, u_{n-1}\}$. Set $a_i = \sqrt{[\deg(u) + \deg(u_i)]/d(u, u_i)}$ and $b_i = \sqrt{[\deg(u) + \deg(u_i)]d(u, u_i)}$ for $i \in [n-1]$. Clearly $1 \leq b_i/a_i = d(u, u_i) \leq d$. Setting $p = 1, q = d$ in Lemma 4 we get

$$\begin{aligned} & \sum_{i \in [n-1]} [\deg(u) + \deg(u_i)]d(u, u_i) + d \sum_{i \in [n-1]} \frac{\deg(u) + \deg(u_i)}{d(u, u_i)} \\ & \leq (d+1) \sum_{i \in [n-1]} [\deg(u) + \deg(u_i)]. \end{aligned}$$

Summation over all vertices $u \in V(G)$ results in Eq. (3).

Note that the equality $a_i = b_i = d a_i$ holds if and only if $d = 1$, i.e., if $G \cong K_n$. ■

Theorem 5. *Let G be a graph of order n , size m , and diameter d . Then*

$$H_M(G) + d ZZ(G) \leq 2m^2(d+1).$$

Equality holds if and only if $G \cong K_n$.

Proof. Analogously to the the proof of Theorem 4, the result follows by setting

$$a_i = \sqrt{\frac{\deg(u) \deg(u_i)}{d(u, u_i)}} \quad \text{and} \quad b_i = \sqrt{\deg(u) \deg(u_i) d(u, u_i)}$$

for each vertex u . ■

Theorem 6. *Let G be a graph of diameter d . Then*

$$\begin{aligned} & \binom{n}{2}(1 + pq) + \sum_{\substack{\{u,v\} \subseteq V(G) \\ u \neq v}} \left(\frac{1}{d(u,v)} \right)^2 \leq (p+q)[W(G) - H(G)] \\ & + pq[W(G) - 2WW(G)] + 2H(G) \end{aligned} \quad (4)$$

where $p = (1-d)/(d+1)$ and $q = (d-1)/(2d)$. The equality holds if and only if $G \cong K_n$.

Proof. For a vertex u , let $\{d_i \mid i \in [n-1]\}$ be same as in the proof of Theorem 1. Let $a_i = d_i + 1$ and $b_i = (d_i - 1)/d_i$ for $i \in [n-1]$. It is clear that

$$2 \leq a_i \leq d+1 \quad \text{and} \quad 0 \leq b_i \leq \frac{d-1}{d}.$$

Moreover $b_i/a_i \leq (d-1)/(2d)$ and $(a_i - 1)(1 - b_i) = 1$. This implies

$$\frac{b_i}{a_i} = \frac{2}{a_i} + b_i - 1 \geq \frac{2}{d+1} - 1 = \frac{1-d}{d+1}.$$

Therefore,

$$\frac{1-d}{d+1} a_i \leq b_i \leq \frac{d-1}{2d} a_i.$$

Set $p = (1-d)/(1+d)$ and $q = (d-1)/(2d)$ in Lemma 4. It follows that for each vertex u

$$\sum_{i \in [n-1]} \left(\frac{d_i - 1}{d_i} \right)^2 + pq \sum_{i \in [n-1]} (d_i + 1)^2 \leq (p+q) \sum_{i \in [n-1]} \left(d_i - \frac{1}{d_i} \right).$$

Thus by summing over all vertices we get:

$$\begin{aligned} & \binom{n}{2} + \sum_{\substack{\{u,v\} \subseteq V(G) \\ u \neq v}} \frac{1}{d(u,v)^2} - 2H(G) + pq \left[2WW(G) + W(G) + \binom{n}{2} \right] \\ & \leq (p+q)[W(G) - H(G)] \end{aligned}$$

from which Eq. (4) straightforwardly follows.

In view of Lemma 4, the equality $pa_i = b_i = qa_i$ holds if $d = 1$, i.e.,

for $G \cong K_n$. ■

Corollary. *Let G be a graph of diameter d . Then*

$$\binom{n}{2} \left(1 + pq + \frac{1}{d^2} \right) \leq (p + q + pq)W(G) - (p + q - 2)H(G) - 2pq WW(G)$$

where $p = (1 - d)/(d + 1)$ and $q = (d - 1)/(2d)$. Equality is attained if and only if $G \cong K_n$.

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