MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **93** (2025) 509–520
ISSN: 0340–6253
doi: 10.46793/match.93-2.509A

On Relations between Distance–Based Topological Indices

Yaser Alizadeh[a], **Ivan Gutman**[b,*], **Shima Nosratollahi**[c], **Zaryab Hussain**[d]

[a] *Department of Mathematics, Hakim Sabzevari University, Sabzevar, Iran*
[b] *Faculty of Science, University of Kragujevac, Kragujevac, Serbia*
[c] *Ministry of Education, Mashhad, Iran*
[d] *School of Mathematics and Statistics, Northwestern Polytechnical University, Xian, China*

y.alizadeh@hsu.ac.ir, gutman@kg.ac.rs, sh.nosratollahi@gmail.com, zaryabhussain2139@gmail.com

(Received September 18, 2024)

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

*Corresponding author

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 $\mathrm{diam}(G)$ and radius $\mathrm{rad}(G)$ 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 $\mathrm{diam}(G) = \mathrm{rad}(G)$.

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]

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

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]

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

Gutman index [9–11]

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

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

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

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* $\{a_1, a_2, \ldots, a_n\}$ *and* $\{b_1, b_2, \ldots, b_n\}$ *be two sets of real numbers. Then*

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

Lemma 2. (Cauchy–Schwarz inequality) *Let* $\{a_1, a_2, \ldots, a_n\}$ *and* $\{b_1, b_2, \ldots, b_n\}$ *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 $a_1/b_1 = a_2/b_2 = \cdots = a_n/b_n$.

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 $\alpha \in \mathrm{Aut(G)}$), 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*,* $Tr(u) = \frac{2}{n} W(G)$ *and* $h(u) = \frac{2}{n} H(G)$*.*

In what follows, $[n]$ stands for the set $\{1, 2, \ldots, n\}$. 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 $\{d_i \,|\, i \in [n-1]\}$ 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

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

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

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

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

$$\sqrt{\frac{d_i}{d_j}} - \sqrt{\frac{d_j}{d_i}} \leq \sqrt{d} - \frac{1}{\sqrt{d}} \tag{1}$$

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

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

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

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

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*

$$\binom{n}{2}^2 \leq \frac{H_A(G)\,DD(G)}{4k^2} \leq \binom{n}{2}^2 + \frac{n^2}{4}\binom{n-1}{2}\frac{(d-1)^2}{d}$$

$$\binom{n}{2}^2 \leq \frac{H_M(G)\,ZZ(G)}{k^4} \leq \binom{n}{2}^2 + \frac{n^2}{4}\binom{n-1}{2}\frac{(d-1)^2}{d}\,.$$

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

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

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

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

Proof. Let $V(G) = \{v_i \,|\, 1 \leq i \leq n\}$. 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 $\varepsilon(v_j) \leq \mathrm{diam}(G)$ and $1/\varepsilon(v_j) \leq 1/\mathrm{rad}(G)$ for each $v_j \in V(G)$. Clearly the equality holds if and only if $\mathrm{rad}(G) = \varepsilon(v_j) = \mathrm{diam}(G)$ 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*

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

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

Proof. For a vertex u, let $\{d_i \,|\, i \in [n-1]\}$ 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

$$Tr(u) + d\, h(u) \leq (d+1)(n-1)\,.$$

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*

$$DD(G) + d\,H_A(G) \leq 2m(d+1)(n-1)\,. \tag{3}$$

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

Proof. Let u be a vertex of G and $V(G) = \{u = u_0, u_1, u_2, \ldots, u_{n-1}\}$. Set $a_i = \sqrt{\big[\deg(u) + \deg(v_i)\big]/d(u,u_i)}$ and $b_i = \sqrt{\big[\deg(u) + \deg(v_i)\big]d(u,u_i)}$ 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

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

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

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

for each vertex u. ∎

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

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

$$+\ pq\big[W(G)-2\,WW(G)\big]+2H(G) \tag{4}$$

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 $\{d_i\,|\,i\in[n-1]\}$ 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:

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

from which Eq. (4) straightforwardly follows.

In view of Lemma 4, the equality $p\,a_i=b_i=q\,a_i$ 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 $G \cong K_n$.

References

[1] Y. Alizadeh, A. Iranmanesh, T. Došlić, Additively weighted Harary index of some composite graphs, *Discr. Math.* **313** (2013) 26–34.

[2] Y. Alizadeh, S. Klavžar, On graphs whose Wiener complexity equals their order and on Wiener index of asymmetric graphs, *Appl. Math. Comput.* **328** (2018) 113–118.

[3] M. An, L. Xiong, Multiplicatively weighted Harary index of some composite graphs, *Filomat* **29** (2015) 795–805.

[4] E. Azjargal, B. Horoldagva, I. Gutman, Minimum of product of Wiener and Harary indices, *MATCH Commun. Math. Comput. Chem.* **92** (2024) 65–71.

[5] F. Buckley, F. Harary, *Distance in Graphs*, Addison–Wesley, Redwood, 1990.

[6] J. B. Diaz, F. T. Metcalf, Stronger forms of a class of inequalities of G. Pólya–G. Szegő, and L. V. Kantorovich, *Bull. Am. Math. Soc.* **69** (1963) 415–419.

[7] A. A. Dobrynin, A. A. Kochetova, Degree distance of a graph: A degree analogue of the Wiener index, *J. Chem. Inf. Comput. Sci.* **34** (1994) 1082–1086.

[8] S. Gupta, M. Singh, A. K. Madan, Connective eccentricity index: A novel topological descriptor for predicting biological activity, *J. Mol. Graph. Model.* **18** (2000) 18–25.

[9] I. Gutman, Selected properties of the Schultz molecular topological index, *J. Chem. Inf. Comput. Sci.* **34** (1994) 1087–1089.

[10] I. Gutman, On two degree-and-distance-based graph invariants, *Bull. Acad. Serbe Sci. Arts (Cl. Sci. Math. Natur.)* **149** (2016) 21–31.

[11] I. Gutman, Gutman index – a critical personal account, *Bull. Acad. Serbe Sci. Arts (Cl. Sci. Math. Natur.)* **154** (2021) 183–193.

[12] I. Gutman, B. Furtula (Eds.), *Distance in Molecular Graphs – Theory*, Univ. Kragujevac, Kragujevac, 2012.

[13] I. Gutman, B. Furtula, I. Redžepović, On topological indices and their reciprocals, *MATCH Commun. Math. Comput. Chem.* **91** (2024) 287–297.

[14] I. Gutman, I. Redžepović, B. Furtula, On the product of Sombor and modified Sombor indices, *Open J. Appl. Discr. Math.* **6** (2023) 1–6.

[15] I. Gutman, Ž. Tomović, Relation between distance-based topological indices, *J. Chem. Inf. Comput. Sci.* **40** (2000) 1333–1336.

[16] I. Gutman, Y. N. Yeh, S. L. Lee, Y. L. Luo, Some recent results in the theory of the Wiener number, *Indian J. Chem/* **32A** (1993) 651–661.

[17] F. Harary, Status and contrastatus, *Sociometry* **22** (1959) 23–43.

[18] H. Hua, I. Gutman, H. Wang, K. C. Das, Relationships between some distance-based topological indices, *Filomat* **32** (2018) 5809–5815.

[19] 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.

[20] M. Knor, R. Škrekovski, A. Tepeh, Mathematical aspects of Wiener index, *Ars Math. Contemp.* **11** (2016) 327–352.

[21] H. Lin, A survey of recent extremal results on the Wiener index of trees, *MATCH Commun. Math. Comput. Chem.* **92** (2024) 253–270.

[22] D. S. Mitrinović, P. M. Vasić, *Analytic Inequalities*, Springer, Berlin, 1970.

[23] O. R. Oellermann, Distance in graphs, in: M. Dehmer (Ed.), *Structural Analysis of Complex Networks*, Springer, Dordrecht, 2011, pp. 49–72.

[24] 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.

[25] H. P. Schultz, Topological organic chemistry. 1. Graph theory and topological indices of alkanes, *J. Chem. Inf. Compur. Sei.* **29** (1989) 227–228.

[26] V. Sharma, R. Goswami, A. K. Madan, Eccentric connectivity index: A novel highly discriminating topological descriptor for structure property and structure activity studies, *J. Chem. Inf. Model.* bf 37 (1997) 273–282.

[27] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20.

[28] K. Xu, K. C. Das, N. Trinajstić, *The Harary Index of a Graph*, Springer, Heidelberg, 2015.

[29] K. Xu, M. Liu, K. C. Das, I. Gutman, B. Furtula, A survey on graphs extremal with respect to distance–based topological indices, *MATCH Commun. Math. Comput. Chem.* **71** (2014) 461–508.