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ORIGINAL PAPER

On reverse degree distance

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Abstract We report some properties of the reverse degree distance of a connected (molecular) graph, and, in particular, its relationship with the first Zagreb index and Wiener index. We also show that the reverse degree distance satisfies the basic requirement for a branching index.

Keywords Reverse degree distance · Degree distance · Schultz molecular topological index · First Zagreb index · Wiener index · Branching index

1 Introduction

The degree distance was proposed by Dobrynin and Kochetova [1], which also appears to be a part of the molecular topological index (MTI) introduced by Schultz [2]. Properties and applications of MTI may be found in [3–14].

Let G be a simple (molecular) connected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ [15,16]. For $v_i \in V(G)$, $\Gamma(v_i)$ denotes the set of its (first) neighbors in G and the degree of v_i is $\delta_i = |\Gamma(v_i)|$. The adjacency matrix $\mathbf{A}$ of G is an $n \times n$ matrix $(\mathbf{A}_{ij})$ such that $\mathbf{A}_{ij} = 1$ if the vertices v_i and v_j are adjacent and 0 otherwise [17]. The term $\sum_{i=1}^{n} \delta_i^2$ is known as the first Zagreb index [18–21] of G, denoted by $\mathrm{Zg}(G)$. This molecular descriptor found application as a branching index, complexity index and in the structure-property-activity modeling [10,11,19–24].

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Let $\mathbf{M}$ be a (symmetric) distance-based matrix of the graph G. Ivanciuc, Ivanciuc and Balaban [25] introduced molecular graph operators such as the characteristic polynomial operator, spectral operator, Wiener operator, hyper-Wiener operator. For example, the Wiener operator of G is $\mathrm{Wi}(\mathbf{M}, G) = \sum_{i<j} \mathbf{M}_{ij}$. Similarly, the degree distance operator of the graph G is defined as

$$\mathrm{D}'(\mathbf{M}, G) = \vec{\delta}\mathbf{M}\vec{1} = \sum_{i=1}^{n} \delta_i M_i,$$

where $\vec{\delta} = (\delta_1, \delta_2, \ldots, \delta_n)$ for $i = 1, 2, \ldots, n$, $\vec{1}$ is the all 1's $n \times 1$ vector, and $M_i = \sum_{j=1}^{n} \mathbf{M}_{ij}$. Evidently, $\mathrm{D}'(\mathbf{M}, G)$ is a part of the molecular topological operator of the graph G defined as

$$\mathrm{MTI}(\mathbf{M}, G) = \vec{\delta}(\mathbf{A} + \mathbf{M})\vec{1} = \mathrm{Zg}(G) + \mathrm{D}'(\mathbf{M}, G).$$

The distance matrix $\mathbf{D}$ of the graph G is an $n \times n$ matrix $(\mathbf{D}_{ij})$ such that $\mathbf{D}_{ij}$ is just the distance between the vertices v_i and v_j in G [17,26]. Recall that $D_i = \sum_{j=1}^{n} \mathbf{D}_{ij}$. Then the degree distance of G is $\mathrm{D}'(G) = \mathrm{D}'(\mathbf{D}, G) = \sum_{i=1}^{n} \delta_i D_i$, while the molecular topological index of G is $\mathrm{MTI}(G) = \mathrm{MTI}(\mathbf{D}, G) = \mathrm{Zg}(G) + \mathrm{D}'(G)$. The degree distance $\mathrm{D}'(G)$ was called the MTI' index in [3,16], and the true molecular topological index in [8]. Some mathematical properties for the degree distance may be found in [8,27–29].

The diameter of a connected graph is the maximum possible distance between any two vertices in the graph. Let G be a connected graph with n vertices, m edges and diameter d. The reverse Wiener matrix $\mathbf{RW}$ [17,30] of G is an $n \times n$ matrix $(\mathbf{RW}_{ij})$ such that $\mathbf{RW}_{ij} = d - \mathbf{D}_{ij}$ if $i \neq j$ and 0 otherwise. Recall that $RW_i = \sum_{j=1}^{n} \mathbf{RW}_{ij} = (n-1)d - D_i$ and $\sum_{i=1}^{n} \delta_i = 2m$. Then

$$^{\mathrm{r}}\mathrm{D}'(G) = \mathrm{D}'(\mathbf{RW}, G) = \sum_{i=1}^{n} \delta_i RW_i = 2(n-1)md - \mathrm{D}'(G)$$

is called the reverse degree distance of G, which also appears to be a part of the reverse molecular topological index $^{\mathrm{r}}\mathrm{MTI}(G) = \mathrm{MTI}(\mathbf{RW}, G) = \mathrm{Zg}(G) + {}^{\mathrm{r}}\mathrm{D}'(G)$. We point out that Schultz and Schultz [31] introduced and applied the reciprocal MTI, for which some properties may be found in [14].

In this report, we establish properties for the reverse degree distance of a connected graph.

2 Preliminaries

Recall that $\mathrm{W}(G) = \mathrm{Wi}(\mathbf{D}, G)$ is the Wiener index [32], while $\Lambda(G) = \mathrm{Wi}(\mathbf{RW}, G) = \frac{n(n-1)d}{2} - \mathrm{W}(G)$ is the reverse Wiener index [30] of the graph G.

Let P_n, S_n and K_n, be respectively the path, the star and the complete graph on n vertices. Note that a path is a tree with two vertices of degree one and all other vertices of degree two, a star is a tree with one vertex being adjacent to all other vertices with degree one, and a complete graph is a simple graph in which every pair of distinct vertices is adjacent [15].

Lemma 1 [8] *Let G be a tree with n vertices. Then* $D'(G) = 4W(G) - n(n-1)$.

3 Properties of reverse degree distance $^{\mathrm{r}}\mathrm{D}'$

Let G be a connected graph with n vertices. Obviously, $\mathbf{RW} = \mathbf{0}$ if and only if $G = K_n$. Thus $^{\mathrm{r}}\mathrm{D}'(G) \geq 0$ with equality if and only if $G = K_n$. If G is a graph of diameter two, then $\mathbf{RW} = \mathbf{A}$, and thus $^{\mathrm{r}}\mathrm{D}'(G) = Zg(G)$.

Proposition 1 *Let G be a connected graph with* $n \geq 2$ *vertices, m edges and diameter d. Then*

$$(d-1)Zg(G) \leq {}^{\mathrm{r}}\mathrm{D}'(G) \leq 2(d-2)(n-1)m + Zg(G)$$

with either equality if and only if $d \leq 2$.

Proof Let G be a connected graph with n vertices, m edges and diameter d. Then for any $v_i \in V(G)$,

$$D_i \leq \delta_i + d(n - \delta_i - 1) = d(n-1) - (d-1)\delta_i$$

and

$$D_i \geq \delta_i + 2(n - \delta_i - 1) = 2(n-1) - \delta_i$$

with either equality if and only if $d \leq 2$. Since $\sum_{i=1}^{n} \delta_i = 2m$, we have

$$4(n-1)m - \mathrm{Zg}(G) \leq \mathrm{D}'(G) \leq 2d(n-1)m - (d-1)\mathrm{Zg}(G)$$

and then

$$(d-1)\mathrm{Zg}(G) \leq {}^{\mathrm{r}}\mathrm{D}'(\mathrm{G}) \leq 2(\mathrm{d}-2)(n-1)m + \mathrm{Zg}(G)$$

with either equality if and only if $d \leq 2$. □

Note that a Moore graph is a connected graph of diameter d and girth $2d+1$, where the girth of a connected graph G is the length of a shortest cycle in G. A graph in which every vertex has the same degree is called a regular graph. Moore graphs are regular graphs. There are at most four Moore graphs of diameter 2 [33]: pentagon, Petersen graph, Hoffman-Singleton graph, and possibly a 57-regular graph with 3,250 vertices (its existence is still an open problem).

Proposition 2 *Let G be a connected triangle- and quadrangle-free graph with $n \geq 3$ vertices, m edges, diameter d, minimal degree δ and maximal degree Δ. Then*

$$[d-1+\delta(d-2)]\,Zg(G) - 2(d-2)m\delta \leq {}^{\mathrm{r}}\mathrm{D}'(G) \leq (\Delta+2)Zg(G) + 2m\,[(d-3)(n-1)-\Delta]$$

with right equality if and only if G is a Moore graph of diameter 2, *or a regular graph of diameter* 3 *(and girth 5, 6 or 7) and with left equality if and only if $G = S_n$, or G is a Moore graph of diameter* 2, *or a regular graph of diameter* 3 *(and girth 5, 6 or 7).*

Proof Note that the diameter of G is at least 2. Let a_i be the number of vertices that are at distance 2 from vertex v_i. Then $\sum_{i=1}^{n} a_i = \mathrm{Zg}(G) - 2m$. Therefore

$$\begin{aligned}
\mathrm{D}'(G) &\geq \sum_{i=1}^{n} \delta_i\,[\delta_i + 2a_i + 3(n-1-\delta_i-a_i)]\\
&= 3(n-1)\sum_{i=1}^{n}\delta_i - 2\mathrm{Zg}(G) - \sum_{i=1}^{n}\delta_i a_i\\
&\geq 6(n-1)m - 2\mathrm{Zg}(G) - \Delta\left[\mathrm{Zg(G)} - 2m\right]\\
&= 6(n-1)m + 2m\Delta - (\Delta+2)\mathrm{Zg}(G)
\end{aligned}$$

with equality if and only if G is a regular graph with diameter 2 or 3. Similarly,

$$\begin{aligned}
\mathrm{D}'(G) &\leq \sum_{i=1}^{n} \delta_i\,[\delta_i + 2a_i + d(n-1-\delta_i-a_i)]\\
&= d(n-1)\sum_{i=1}^{n}\delta_i - (d-1)\mathrm{Zg}(G) - (d-2)\sum_{i=1}^{n}\delta_i a_i\\
&\leq 2d(n-1)m + 2(d-2)m\delta - [d-1+\delta(d-2)]\,\mathrm{Zg}(G)
\end{aligned}$$

with equality if and only if G is a graph with diameter 2 or a regular graph with diameter 3. By a result of Bondy et al. [34], a quadrangle-free graph with n vertices and diameter 2 is a graph of maximal degree $n-1$, or a Moore graph, or a polarity graph. However, a polarity graph is not triangle-free. Now the result follows easily. □

Let G be a connected triangle- and quadrangle-free graph with $n \geq 3$ vertices, m edges, diameter d and maximal degree Δ. Then $\mathrm{Zg}(G) \leq n(n-1)$ with equality if and only if G is the star or a Moore graph of diameter 2 [35]. By Proposition 2,

$${}^{\mathrm{r}}\mathrm{D}'(G) \leq (\Delta+2)n(n-1) + 2m\,[(d-3)(n-1)-\Delta]$$

with equality if and only if G is a Moore graph of diameter 2.

In the following, we consider the relations between ${}^{\mathrm{r}}\mathrm{D}'(G)$and the Wiener index $\mathrm{W}(G)$.

Proposition 3 *Let G be a connected graph with n vertices, m edges, diameter d, minimal degree δ and maximal degree Δ. Then*

$$2d(n-1)m - 2\Delta W(G) \le {}^{\mathrm{r}}\mathrm{D}'(G) \le 2d(n-1)m - 2\delta W(G)$$

with either equality if and only if G is a regular graph.

Proof Since $2\delta\mathrm{W}(G) \le \mathrm{D}'(G) \le 2\Delta\mathrm{W}(G)$ with either equality if and only if G is a regular graph, the result follows easily. □

Now if we use a modified reverse Wiener index of the graph G [36] with n vertices and diameter d as

$$\Lambda'(G) = \frac{(n-1)^2 d}{2} - \mathrm{W}(G),$$

then

$$\Lambda'(G) = \Lambda(G) - \frac{(n-1)d}{2}.$$

Proposition 4 *Let G be a tree with n vertices and diameter d. Then*

$${}^{\mathrm{r}}\mathrm{D}'(G) = 4 \cdot \Lambda'(G) + n(n-1).$$

Proof Since G is a tree with n vertices, it possesses $n-1$ edges. Then the result follows from Lemma 1. □

Let $P_{n,d,i}$ be the tree obtained from the path $P_{d+1} = v_0 \cdots v_d$ by attaching $n-d-1$ pendant vertices to vertex v_i, where $2 \le d \le n-1$ and $1 \le i \le \lfloor d/2 \rfloor$. In particular, $P_{n,n-1,i} = P_n$. In [36], it is shown that for $3 \le d \le n-2$ and any tree T with n vertices and diameter d that is different from $P_{n,d,\lfloor d/2\rfloor}$, $\mathrm{W}(T) > \mathrm{W}\left(P_{n,d,\lfloor d/2\rfloor}\right)$ and so

$$\Lambda'(T) < \Lambda'\left(P_{n,d,\lfloor d/2\rfloor}\right).$$

Note that, see, e.g. [8], for a tree T with edge set $E(T)$, $\mathrm{W}(T) = \sum_{e \in E(T)} n_{T,1}(e) \cdot n_{T,2}(e)$ where $n_{T,1}(e)$ and $n_{T,2}(e)$ are respectively the number of vertices of T lying on the two sides of the edge e. Thus

$$\begin{aligned}
&\Lambda'\left(P_{n,d+1,\lfloor (d+1)/2\rfloor}\right) - \Lambda'\left(P_{n,d,\lfloor d/2\rfloor}\right)\\
&\quad = \frac{(n-1)^2}{2} - \left[\mathrm{W}\left(P_{n,d+1,\lfloor (d+1)/2\rfloor}\right) - \mathrm{W}\left(P_{n,d,\lfloor d/2\rfloor}\right)\right]\\
&\quad = \frac{(n-1)^2}{2} - \left[\left(\left\lfloor \frac{d}{2}\right\rfloor + 1\right)\left(n - \left\lfloor \frac{d}{2}\right\rfloor - 1\right) - (n-1)\right]\\
&\quad > \frac{(n-1)^2}{2} - \frac{n^2}{4} > 0,
\end{aligned}$$

and then $\Lambda'\left(P_{n,d,\lfloor d/2\rfloor}\right) < \Lambda'\left(P_{n,d+1,\lfloor (d+1)/2\rfloor}\right)$.

By the discussion above and Proposition 4, we have

Proposition 5 *Let T be an n-vertex tree either with p pendant vertices or with maximal degree p, where $3 \le p \le n-2$. Then ${}^{\mathrm{r}}\mathrm{D}'(T) \le {}^{\mathrm{r}}\mathrm{D}'\left(P_{n,n-p+1,\lfloor (n-p+1)/2\rfloor}\right)$ with equality if and only if $T = P_{n,n-p+1,\lfloor (n-p+1)/2\rfloor}$.*

It follows also from the discussion above that among all trees T with n vertices, $\Lambda'(T) \le \Lambda'(P_n)$ with equality if and only if $T = P_n$. On the other hand, among all trees T with $n \ge 3$ vertices,

$$\begin{aligned}
\Lambda'(T) &= \frac{(n-1)^2 d}{2} - \mathrm{W}(T)\\
&\ge \frac{(n-1)^2 d}{2} - (n-1) - d\left[\binom{n}{2} - (n-1)\right]\\
&= (n-1)\left(\frac{d}{2} - 1\right) \ge 0
\end{aligned}$$

with equality if and only if $d = 2$, i.e., $T = S_n$. Now by Proposition 4, we have

Proposition 6 *Let T be a tree with n vertices, different from the path P_n and the star S_n. Then ${}^{\mathrm{r}}\mathrm{D}'(S_n) < {}^{\mathrm{r}}\mathrm{D}'(T) < {}^{\mathrm{r}}\mathrm{D}'(P_n)$.*

By Proposition 6, the reverse true molecular topological index satisfies the basic requirement to be a branching index in that it has the minimum value for a star and the maximum value for a chain (path) [37].

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References

1. A.A. Dobrynin, A.A Kochetova, Degree distance of a graph: a degree analogue of the Wiener index. J. Chem. Inf. Comput. Sci. **34**, 1082–1086 (1994)
2. H.P. Schultz, Topological organic chemistry. 1. Graph theory and topological indices of alkanes. J. Chem. Inf. Comput. Sci. **29**, 227–228 (1989)

3. W.R. Müller, K. Szymanski, J.V. Knop, N. Trinajstić, Molecular topological index. J. Chem. Inf. Comput. Sci. **30**, 160–163 (1990)
4. D.J. Klein, Z. Mihalić, D. Plavšić, N. Trinajstić, Molecular topological index: a relation with Wiener index. J. Chem. Inf. Comput. Sci. **32**, 304–305 (1992)
5. A. Jurić, M. Gagro, S. Nikolić, N. Trinajstić, Molecular topological index: an application in the QSAR study of toxicity of alcohols. J. Math. Chem. **11**, 179–186 (1992)
6. D. Plavšić, S. Nikolić, N. Trinajstić, D.J. Klein, Relation between the Wiener index and the Schultz index for several classes of chemical graphs. Croat. Chem. Acta **66**, 345–353 (1993)
7. S. Nikolić, N. Trinajstić, Z. Mihalić, Molecular topological index: an extension to heterosystems. J. Math. Chem. **12**, 251–264 (1993)
8. I. Gutman, Selected properties of Schultz molecular topological index. J. Chem. Inf. Comput. Sci. **34**, 1087–1089 (1994)
9. S. Klavžar, I. Gutman, A comparison between the Schultz molecular topological index with the Wiener index. J. Chem. Inf. Comput. Sci. **36**, 249–257 (1996)
10. J. Devillers, A.T. Balaban (eds.), *Topological Indices and Related Descriptors in QSAR and QSPR* (Gordon & Breach, Amsterdam, 1999)
11. R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors* (Weinheim, Wiley-VCH, 2000), p. 381
12. D. Vukičević, S. Nikolić, N. Trinajstić, On the Schultz index of thorn graphs. Internet Electron. J. Mol. Des. **4**, 501–514 (2005)
13. B. Zhou, Bounds for the Schultz molecular topological index. MATCH Commun. Math. Comput. Chem. **56**, 189–194 (2006)
14. B. Zhou, N. Trinajstić, On reciprocal molecular topological index. J. Math. Chem. **44**, 235–243 (2008)
15. R.J. Wilson, *Introduction to Graph Theory* (Oliver & Boyd, Edinburgh, 1972)
16. N. Trinajstić, *Chemical Graph Theory, 2nd edn* (CRC Press, Boca Raton, 1992)
17. D. Janežič, A. Miličević, S. Nikolić, N. Trinajstić, *Graph Theoretical Matrices in Chemistry Mathematical Chemistry Monographs No 3* (University of Kragujevac, Kragujevac, 2007), pp. 5–50
18. I. Gutman, N. Trinajstić, Graph theory and molecular orbitals III Total π-electron energy of alternant hydrocarbons. Chem. Phys. Lett. **17**, 535–538 (1972)
19. I. Gutman, B. Rusščić, N. Trinajstić, C.F. Wilcox Jr., Graph theory and molecular orbitals. XII. Acyclic polyenes. J. Phys. Chem. **62**, 3399–3405 (1975)
20. S. Nikolić, G. Kovačević, A. Miličević, N. Trinajstić, The Zagreb indices 30 years after. Croat. Chem. Acta **76**, 113–124 (2003)
21. I. Gutman, K.C. Das, The first Zagreb index 30 years after. MATCH Commun. Math. Comput. Chem. **50**, 83–92 (2004)
22. S. Nikolić, I.M. Tolić, N. Trinajstić, I. Baučić, On the Zagreb indices as complexity indices. Croat. Chem. Acta **73**, 909–921 (2000)
23. D. Bonchev, N. Trinajstić, Overall molecular descriptors 3 overall Zagreb indices. SAR QSAR Environ. Res. **12**, 213–236 (2001)
24. S. Nikolić, N. Trinajstić, I.M. Tolić, G. Rücker, C. Rücker, in *On molecular complexity indices*, ed. by D. Bonchev, D.H. Rouvray, Complexity—Introduction and Fundamentals (Taylor & Francis, London, 2002), pp. 23–76
25. O. Ivanciuc, T. Ivanciuc, A.T. Balaban, Quantitative structure-property relationship evaluation of structure descriptor derived from the distance and reverse Wiener matrices. Internet Electron. J. Mol. Des **1**, 467–487 (2002)
26. Z. Mihalić, D. Veljan, D. Amić, S. Nikolić, D. Plavšić, N. Trinajstić, The distance matrix in chemistry. J. Math. Chem. **11**, 223–258 (1992)
27. I. Tomescu, Some extremal properties of the degree distance of a graph. Discr. Appl. Math. **98**, 159–163 (1999)
28. A.I. Tomescu, Unicyclic and bicyclic graphs having minimum degree distance. Discr. Appl. Math. **156**, 125–130 (2008)
29. O. Bucicovschi, S.M. Cioabă, The minimum degree distance of graphs with given order and size. Discr. Appl. Math. **156**, 3518–3521 (2008)
30. A.T. Balaban, D. Mills, O. Ivanciuc, S.C. Basak, Reverse Wiener indices. Croat. Chem. Acta **73**, 923–941 (2000)

31. H.P. Schultz, T.P. Schultz, Topological organic chemistry. 11. Graph theory and reciprocal Schultz-type molecular topological indices of alkanes and cycloalkanes. J. Chem. Inf. Comput. Sci **38**, 853–857 (1998)
32. H. Wiener, Structural determination of paraffin boiling points. J. Am. Chem. Soc. **69**, 17–20 (1947)
33. A.J. Hoffman, R.R. Singleton, On Moore graphs with diameters 2 and 3. IBM J. Res. Develop. **4**, 497–504 (1960)
34. J.A. Bondy, P. Erdös, S. Fajtlowicz, Graphs of diameter two with no 4-circuits. Discr. Math. **200**, 21–25 (1999)
35. B. Zhou, D. Stevanović, A note on Zagreb indices. MATCH Commun. Math. Comput. Chem. **56**, 571–578 (2006)
36. B. Zhang, B. Zhou, On modified and reverse Wiener indices. Z. Naturforsch. **61a**, 536–540 (2006)
37. O. Ivanciuc, T. Ivanciuc, D. Cabrol-Bass, A.T. Balaban, Investigation of alkane branching (and resulting partial ordering) by topological indices. MATCH Commun. Math. Comput. Chem. **42**, 155–180 (2000)