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Maximum Degree Distance of Graphs with Exactly Two Cycles

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Abstract

The degree distance of a connected graph G with vertex set V(G) is defined as $D'(G) = \sum_{u \in V(G)} d_G(u)D_G(u)$, where $d_G(u)$ is the degree of vertex u and $D_G(u)$ is the sum of distances between u and all vertices of G. We determine the maximum degree distances in the class of connected graphs with exactly two vertex-disjoint cycles and in the class of connected graphs with exactly two cycles of a common vertex, respectively, and then the maximum degree distance in the class of connected graphs with exactly two cycles. The extremal graphs are characterized.

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1 Introduction

The topological indices are numbers associated with chemical structures via their hydrogen-depleted graphs. The topological indices especially those based on graph distance are widely used in modeling of structure-property relationships [2, 11].

Let G be a simple connected graph with vertex set V(G) and edge set E(G). For $u, v \in V(G)$, let $d_G(u, v)$ be the distance between the vertices u and v in G, let $D_G(u)$ be the sum of distances between u and all vertices of G, i.e., $D_G(u) = \sum_{v \in V(G)} d_G(u, v)$. For $u \in V(G)$, let $d_G(u)$ be the degree of u in G. The degree

distance of G is defined as [5, 6]

$$D'(G) = \sum_{u \in V(G)} d_G(u) D_G(u).$$

Besides as a topological index itself, the degree distance is also the non-trivial part of the molecular topological index (MTI) introduced by Schultz [10] for characterization of alkanes [9, 6, 8]. Some properties for the degree distance may be found, e.g., in [6, 8, 15] in the text of MTI.

The Wiener index of G is defined as [3, 4] $W(G) = \frac{1}{2} \sum_{u \in V(G)} D_G(u)$. Gutman [6] showed that if T is a tree with n vertices, then D'(T) = 4W(T) - n(n-1). Thus, the study of the degree distance for trees is equivalent to the study of the Wiener index, which was summarized in [3].

A connected graph with n vertices is said to be unicyclic for $n \geq 3$ if it possesses n edges and bicyclic for $n \geq 4$ if it possesses n + 1 edges. I. Tomescu [13] showed that the star is the unique graph with the minimum degree distance in the class of connected graphs with n vertices. A. I. Tomescu [12] characterized the unicyclic and bicyclic graphs with the minimum degree distances. I. Tomescu [14] gave properties of the graphs with the minimum degree distance in the class of connected graphs with n vertices and $m \geq n-1$ edges, which were determined recently by Bucicovschi and Cioabă [1]. Hou and Chang [7] characterized the unicyclic graph(s) with the maximum degree distance.

Let $\mathcal{B}_1(n)$ for $n \geq 6$ be the class of connected graphs on n vertices with exactly two vertex-disjoint cycles. Let $\mathcal{B}_2(n)$ for $n \geq 5$ be the class of connected graphs on n vertices with exactly two cycles of a common vertex. Obviously, the graphs in $\mathcal{B}_1(n)$ or $\mathcal{B}_2(n)$ are bicyclic graphs, and $\mathcal{B}_2(5)$ contains only the graph consisting of two triangles of a common vertex. In this paper, we determine the maximum degree distances in $\mathcal{B}_1(n)$, $\mathcal{B}_2(n)$ and $\mathcal{B}_1(n) \cup \mathcal{B}_2(n)$, respectively, for $n \geq 6$. We also characterize the extremal graphs.

2 Preliminaries

For edge subset E_1 of the graph G (the complement of G, respectively), $G - E_1$ ($G + E_1$, respectively) denotes the graph resulting from G by deleting (adding, respectively) the edges in E_1 . A pendant vertex is a vertex of degree one. Let P_n be the path on n vertices.

For vertex-disjoint connected graphs Q_1 and Q_2 with $|V(Q_1)|, |V(Q_2)| \ge 2$, $x \in V(Q_1), y \in V(Q_2)$ and integer $r \ge 1$, let H be the graph obtained from Q_1 and Q_2 by identifying x and y, and attaching a path P_r (at an end vertex) to this common vertex, and H_1 the graph obtained from Q_1 and Q_2 by joining xand y by a path of length r. Gutman [6] proved that $D'(H_1) > D'(H)$.

Lemma 1. Let G and G^* be the graphs in Fig. 1, where M and N are vertexdisjoint connected graphs, T is a tree with $k \ge 3$ vertices, $V(M) \cap V(T) = \{u\}$, $V(N) \cap V(T) = \{v\}$, G^* is formed from G by setting the tree T to be P_k with end vertices u and v. Suppose that $G \ne G^*$.

- (i) If $V(N) = \{v\}$, then $D'(G) < D'(G^*)$.
- (ii) If |V(M)|, $|V(N)| \ge 2$, then $D'(G) < D'(G^*)$.



Fig. 1. The graphs G and G^* .

Proof: Note that T can not be a path from u to v. By proper choosing of Q_1 and Q_2 , and applying the transformation from H to H_1 repeatedly, the results (i) and (ii) follow from Gutman's result mentioned above.

Let G and H be connected graphs. Let $V_1(G) = \{x \in V(G) : d_G(x) \neq 2\}$. Then

$$D'(H) - D'(G) = 4[W(H) - W(G)] + \sum_{x \in V_1(H)} (d_H(x) - 2)D_H(x)$$
$$- \sum_{x \in V_1(G)} (d_G(x) - 2)D_G(x),$$

which will be used frequently to compare the degree distances of two related graphs.

Let C_n be the cycle on $n \geq 3$ vertices. Let s and t be integers with $s, t \geq 3$. Let $a_1, a_2, \ldots, a_{s-1}$ be nonnegative integers. Let U_1 be the unicyclic graph with cycle $C_s = u_0 u_1 \ldots u_{s-1} u_0$ such that $U_1 - E(C_s)$ consists of vertex-disjoint paths $P_1 (= u_0), P_{a_1+1}, P_{a_2+1}, \ldots, P_{a_{s-1}+1}$ with u_i being an end vertex of the path P_{a_i+1} for $i = 1, 2, \ldots, s - 1$, and U_2 a unicyclic graph with a vertex v_0 on its cycle. Let $G(a_1, \ldots, a_{s-1}; U_2)$ be the bicyclic graph obtained by joining u_0 of U_1 and v_0 of U_2 by a path of length at least one, and $H(a_1, \ldots, a_{s-1}; U_2)$ the bicyclic graph obtained by identifying u_0 of U_1 and v_0 of U_2 .

Lemma 2. For fixed *i* and *j* with $1 \le i < j \le s - 1$ and fixed a_k for $k \ne i, j$, let G_{a_i,a_j} be the graph $G(a_1, \ldots, a_{s-1}; U_2)$. If $a_i, a_j \ge 1$, then

$$D'(G_{a_i,a_j}) < \max \{ D'(G_{a_i+a_j,0}), D'(G_{0,a_i+a_j}) \}.$$

Proof: Let $G = G_{a_i,a_j}$, $G_1 = G_{a_i+a_j,0}$. Then $G - E(C_s)$ consists of a unicyclic graph Q and s-1 paths. Let u_k^* be the pendant vertex of G in the path attached to u_k if $a_k \ge 1$, where $k = 1, 2, \ldots, s-1$. Denote by u the neighbor of u_j outside C_s . Obviously, $G_1 = G - \{uu_j\} + \{uu_i^*\}$. Note that

$$V_1(G_1) = (V_1(G_1) \cap V(Q)) \cup \left(\bigcup_{\substack{1 \le k \le s-1 \\ a_k \ge 1, k \ne i, j}} \{u_k, u_k^*\} \right) \cup \{u_i, u_j^*\}$$

and $V_1(G) = (V_1(G) \cap V(Q)) \cup \left(\bigcup_{\substack{1 \le k \le s-1 \\ a_k \ge 1}} \{u_k, u_k^*\} \right)$. It is easily seen that $D_{G_1}(x) - D_G(x) = D_{G_1}(u_0) - D_G(u_0)$ for $x \in V(Q)$, and thus

$$\sum_{x \in V_1(G_1) \cap V(Q)} (d_{G_1}(x) - 2) D_{G_1}(x) - \sum_{x \in V_1(G) \cap V(Q)} (d_G(x) - 2) D_G(x)$$

=
$$\sum_{x \in V(Q)} (d_G(x) - 2) [D_{G_1}(x) - D_G(x)]$$

=
$$[D_{G_1}(u_0) - D_G(u_0)] \cdot \left[\sum_{x \in V(Q)} (d_Q(x) - 2) + 2\right]$$

=
$$2[D_{G_1}(u_0) - D_G(u_0)].$$

For $k \neq i, j$ with $a_k \ge 1, D_{G_1}(u_k) - D_G(u_k) = D_{G_1}(u_k^*) - D_G(u_k^*)$, and then

$$\sum_{x \in \{u_k, u_k^*\}} (d_{G_1}(x) - 2)D_{G_1}(x) - \sum_{x \in \{u_k, u_k^*\}} (d_G(x) - 2)D_G(x)$$

= $(3-2)[D_{G_1}(u_k) - D_G(u_k)] + (1-2)[D_{G_1}(u_k^*) - D_G(u_k^*)] = 0.$

Also we have

$$\sum_{x \in \{u_i, u_j^*\}} (d_{G_1}(x) - 2)D_{G_1}(x) - \sum_{x \in \{u_i, u_j, u_i^*, u_j^*\}} (d_G(x) - 2)D_G(x)$$

= $(3 - 2) \left[D_{G_1}(u_i) - D_G(u_i) \right] + (1 - 2) \left[D_{G_1}(u_j^*) - D_G(u_j^*) \right]$
 $- (1 - 2)D_G(u_i^*) - (3 - 2)D_G(u_j)$
= $\left[D_{G_1}(u_i) - D_{G_1}(u_j^*) \right] + \left[D_G(u_i^*) - D_G(u_i) \right] + \left[D_G(u_j^*) - D_G(u_j) \right]$

Therefore

$$D' (G_{a_i+a_j,0}) - D' (G_{a_i,a_j})$$

= $4 [W(G_1) - W(G)] + 2 [D_{G_1}(u_0) - D_G(u_0)]$
+ $[D_{G_1}(u_i) - D_{G_1}(u_j^*)] + [D_G(u_i^*) - D_G(u_i)] + [D_G(u_j^*) - D_G(u_j)].$

Let $G_2 = G - \{uu_j\} + \{uu_i\}, a_0 = |V(Q)| - 1, n = |V(G)|$, and $d(x, y) = d_G(x, y)$ for $x, y \in V(G)$.

Let Z be the set of vertices in the path from u to u_j^* in G, and W the set of

vertices in the path from u_i to u_i^* in G. We have

$$\begin{split} & W(G_1) - W(G_2) \\ &= \sum_{\substack{x \in Z \\ y \in W}} \left[d_{G_1}(x, y) - d_{G_2}(x, y) \right] + \sum_{\substack{x \in Z \\ y \in V(G) \setminus (Z \cup W)}} \left[d_{G_1}(x, y) - d_{G_2}(x, y) \right] \\ &= 0 + \sum_{\substack{x \in Z \\ y \in V(G) \setminus (Z \cup W)}} \left[d_{G_1}(x, y) - d_{G_2}(x, y) \right] \\ &= \sum_{\substack{x \in Z \\ y \in V(G) \setminus (Z \cup W)}} a_i = a_i a_j (n - a_i - a_j - 1), \\ & W(G_2) - W(G) \\ &= \sum_{\substack{x \in Z \\ y \in V(G) \setminus (Z \cup W)}} \left[d_{G_2}(x, y) - d(x, y) \right] + \sum_{\substack{x \in Z \\ y \in V(G) \setminus (Z \cup V(C_s))}} \left[d_{G_2}(x, y) - d(x, y) \right] \\ &= 0 + \sum_{\substack{x \in Z \\ y \in V(G) \setminus (Z \cup V(C_s))}} \left[d_{G_2}(x, y) - d(x, y) \right] \\ &= \sum_{x \in Z} \sum_{\substack{0 \le k \le s - 1 \\ k \neq j}} a_k \left[d(u_k, u_i) - d(u_k, u_j) \right], \\ &= a_j \sum_{\substack{0 \le k \le s - 1 \\ k \neq j}} a_k \left[d(u_k, u_i) - d(u_k, u_j) \right], \end{split}$$

and then

$$W(G_1) - W(G)$$

$$= [W(G_1) - W(G_2)] + [W(G_2) - W(G)]$$

$$= a_i a_j (n - a_i - a_j - 1) + a_j \sum_{\substack{0 \le k \le s - 1 \\ k \ne j}} a_k [d(u_k, u_i) - d(u_k, u_j)].$$

Note also that

Then

$$D' (G_{a_i+a_j,0}) - D' (G_{a_i,a_j})$$

= $4a_i a_j (n - a_i - a_j) + 2a_j [d(u_0, u_i) - d(u_0, u_j)]$
 $+ 4a_j \sum_{\substack{0 \le k \le s - 1 \\ k \ne j}} a_k [d(u_k, u_i) - d(u_k, u_j)].$

If $D'(G_{a_i+a_j,0}) \le D'(G_{a_i,a_j})$, then

$$2[d(u_0, u_j) - d(u_0, u_i)] + 4 \sum_{\substack{0 \le k \le s - 1 \\ k \ne j}} a_k \left[d(u_k, u_j) - d(u_k, u_i) \right] \ge 4a_i(n - a_i - a_j),$$

and thus

$$\begin{aligned} D'(G_{0,a_i+a_j}) &- D'(G_{a_i,a_j}) \\ &= 4a_i a_j (n-a_i-a_j) + 2a_i [d(u_0,u_j) - d(u_0,u_i)] \\ &+ 4a_i \sum_{\substack{0 \le k \le s^{-1} \\ k \ne i}} a_k [d(u_k,u_j) - d(u_k,u_i)] \\ &= 4a_i a_j (n-a_i-a_j) - 4a_i (a_i+a_j) d(u_i,u_j) \\ &+ 2a_i [d(u_0,u_j) - d(u_0,u_i)] + 4a_i \sum_{\substack{0 \le k \le s^{-1} \\ k \ne j}} a_k [d(u_k,u_j) - d(u_k,u_i)] \\ &\geq 4a_i a_j (n-a_i-a_j) - 4a_i (a_i+a_j) d(u_i,u_j) \\ &+ a_i \cdot 4a_i (n-a_i-a_j) \\ &= 4a_i (a_i+a_j) [(n-a_i-a_j) - d(u_i,u_j)] \\ &> 4a_i (a_i+a_j) \left(s - \frac{s}{2}\right) = 2a_i (a_i+a_j)s > 0. \end{aligned}$$

Now the result follows.

Similar to Lemma 2, we have

Lemma 3. For fixed i and j with $1 \le i < j \le s - 1$ and fixed a_k with $k \ne i, j$, let H_{a_i,a_j} be the graph $H(a_1, \ldots, a_{s-1}; U_2)$. If $a_i, a_j \ge 1$, then

$$D'(H_{a_i,a_j}) < \max \{ D'(H_{a_i+a_j,0}), D'(H_{0,a_i+a_j}) \}.$$

3 Degree distances of graphs in $\mathcal{B}_1(n)$

In this section, we determine the maximum degree distance in the class of connected graphs with exactly two vertex–disjoint cycles.

Let $U_{n,m}$ be the unicyclic graph obtained by attaching a path P_{n-m} to a vertex u of the cycle C_m , where $3 \le m \le n$. In particular, $U_{n,n} = C_n$. Denote by v the pendant vertex in $U_{n,m}$ if $3 \le m \le n-1$, and w a vertex on C_m with $d_{U_{n,m}}(u,w) = \lfloor \frac{m}{2} \rfloor$. Recall that $W(P_s) = \frac{s^3-s}{6}$ and $W(C_s) = \frac{s}{2} \lfloor \frac{s^2}{4} \rfloor$. By direct

calculation, we have

$$W(U_{n,m}) = \frac{n^3}{6} + \left(\left\lfloor \frac{m^2}{4} \right\rfloor - \frac{m^2}{2} + \frac{m}{2} - \frac{1}{6} \right) n - \frac{m}{2} \left\lfloor \frac{m^2}{4} \right\rfloor + \frac{m^3}{3} - \frac{m^2}{2} + \frac{m}{6},$$
(1)

$$D_{U_{n,m}}(u) = \left\lfloor \frac{m^2}{4} \right\rfloor + \frac{1}{2}(n-m)(n-m+1),$$
(2)

$$D_{U_{n,m}}(v) = \left\lfloor \frac{m^2}{4} \right\rfloor + \frac{1}{2}(n-m)(n+m-1),$$
(3)

$$D_{U_{n,m}}(w) = \left\lfloor \frac{m^2}{4} \right\rfloor + \frac{1}{2}(n-m)\left(n-m+1+2\left\lfloor \frac{m}{2} \right\rfloor\right).$$
(4)

Let $C_{s_1} = u_0 u_1 \dots u_{s_1-1} u_0$ and $C_{s_2} = v_0 v_1 \dots v_{s_2-1} v_0$ be two vertex-disjoint cycles. Let $G_n(s_1, s_2)$ be the bicyclic graph obtained by joining u_0 and v_0 by a path of length $n - s_1 - s_2 + 1$, where $s_1 + s_2 \leq n$.

Lemma 4. For integers n, m_1 and m_2 with $n \ge 6$, $m_1, m_2 \ge 3$ and $m_1 + m_2 \le n$, we have $D'(G_n(m_1, m_2)) \le D'(G_n(3, 3))$ with equality if and only if $(m_1, m_2) = (3, 3)$.

Proof: Suppose that $m_1 \ge 5$. Let $G = G_n(m_1, m_2)$ and $G_1 = G_n(m_1 - 2, m_2)$. Note that $V_1(G) = V_1(G_1) = \{u_0, v_0\}$. Then

$$D' (G_n(m_1 - 2, m_2)) - D' (G_n(m_1, m_2))$$

= $4[W(G_1) - W(G)] + (3 - 2)[D_{G_1}(u_0) - D_G(u_0)]$
+ $(3 - 2)[D_{G_1}(v_0) - D_G(v_0)]$
= $4[W(G_1) - W(G)] + [D_{G_1}(u_0) - D_G(u_0)] + [D_{G_1}(v_0) - D_G(v_0)].$

Denote by u_0^* the vertex outside C_{m_1-2} in G_1 with $d_{G_1}(u_0, u_0^*) = 2$. Let Q be the graph obtained from G by deleting the vertices of C_{m_1} . Then $|V(Q)| = n - m_1$.

Note that for $v \in V(Q)$, $d_{G_1}(u_0^*, v) = d_G(u_0, v)$, and then

$$\begin{split} &\sum_{u \in V(U_{m_1,m_1-2})} \sum_{v \in V(Q)} d_{G_1}(u,v) - \sum_{u \in V(C_{m_1})} \sum_{v \in V(Q)} d_G(u,v) \\ &= \sum_{v \in V(Q)} \left[\sum_{u \in V(U_{m_1,m_1-2})} (d_{G_1}(u,u_0^*) + d_{G_1}(u_0^*,v)) \\ &- \sum_{u \in V(C_{m_1})} (d_G(u,u_0) + d_G(u_0,v)) \right] \\ &= \sum_{v \in V(Q)} \left[\sum_{u \in V(U_{m_1,m_1-2})} d_{G_1}(u,u_0^*) - \sum_{u \in V(C_{m_1})} d_G(u,u_0) \right] \\ &+ \sum_{v \in V(Q)} m_1 \cdot [d_{G_1}(u_0^*,v) - d_G(u_0,v)] \\ &= \sum_{v \in V(Q)} \left[\sum_{u \in V(U_{m_1,m_1-2})} d_{G_1}(u,u_0^*) - \sum_{u \in V(C_{m_1})} d_G(u,u_0) \right] + 0 \\ &= (n - m_1) \left[D_{U_{m_1,m_1-2}}(u_0^*) - D_{C_{m_1}}(u_0) \right], \end{split}$$

from which and Eqs. (1) and (3), we have

$$\begin{split} & W(G_1) - W(G) \\ = & \left[W(U_{m_1,m_1-2}) + W(Q) + \sum_{u \in V(U_{m_1,m_1-2})} \sum_{v \in V(Q)} d_{G_1}(u,v) \right] \\ & - \left[W(C_{m_1}) + W(Q) + \sum_{u \in V(C_{m_1})} \sum_{v \in V(Q)} d_G(u,v) \right] \\ = & W(U_{m_1,m_1-2}) - W(C_{m_1}) + (n-m_1) \left[D_{U_{m_1,m_1-2}}(u_0^*) - D_{C_{m_1}}(u_0) \right] \\ = & \left\lfloor \frac{m_1^2}{4} \right\rfloor - \frac{3}{2}m_1^2 + \left(n + \frac{9}{2} \right) m_1 - 2n - 4. \end{split}$$

For $v \in V(Q)$, $d_{G_1}(u_0, v) - d_G(u_0, v) = 2 + d_{G_1}(u_0^*, v) - d_G(u_0, v) = 2$. Using Eq.

(2),

$$D_{G_{1}}(u_{0}) - D_{G}(u_{0})$$

$$= \left[\sum_{v \in V(U_{m_{1},m_{1}-2})} d_{G_{1}}(u_{0},v) + \sum_{v \in V(Q)} d_{G_{1}}(u_{0},v)\right]$$

$$- \left[\sum_{v \in V(C_{m_{1}})} d_{G}(u_{0},v) + \sum_{v \in V(Q)} d_{G}(u_{0},v)\right]$$

$$= \sum_{v \in V(U_{m_{1},m_{1}-2})} d_{G_{1}}(u_{0},v) - \sum_{v \in V(C_{m_{1}})} d_{G}(u_{0},v) + \sum_{v \in V(Q)} 2$$

$$= D_{U_{m_{1},m_{1}-2}}(u_{0}) - D_{C_{m_{1}}}(u_{0}) + 2(n - m_{1})$$

$$= 2n - 3m_{1} + 4.$$

Using Eq. (3),

$$\begin{array}{ll} & D_{G_1}(v_0) - D_G(v_0) \\ = & \sum_{v \in V(U_{m_1,m_1-2})} d_{G_1}(v_0,v) - \sum_{v \in V(C_{m_1})} d_G(v_0,v) \\ = & \sum_{v \in V(U_{m_1,m_1-2})} \left[d_{G_1}(v_0,u_0^*) + d_{U_{m_1,m_1-2}}(u_0^*,v) \right] \\ & - \sum_{v \in V(C_{m_1})} \left[d_G(v_0,u_0) + d_{C_{m_1}}(u_0,v) \right] \\ = & m_1 \cdot \left[d_{G_1}(v_0,u_0^*) - d_G(v_0,u_0) \right] \\ & + \left[\sum_{v \in V(U_{m_1,m_1-2})} d_{U_{m_1,m_1-2}}(u_0^*,v) - \sum_{v \in V(C_{m_1})} d_{C_{m_1}}(u_0,v) \right] \\ = & 0 + \left[D_{U_{m_1,m_1-2}}(u_0^*) - D_{C_{m_1}}(u_0) \right] = m_1 - 2. \end{array}$$

Hence

$$D' (G_n(m_1 - 2, m_2)) - D' (G_n(m_1, m_2))$$

$$= 4 \left[\left\lfloor \frac{m_1^2}{4} \right\rfloor - \frac{3}{2}m_1^2 + \left(n + \frac{9}{2}\right)m_1 - 2n - 4 \right]$$

$$+ (2n - 3m_1 + 4) + (m_1 - 2)$$

$$= \begin{cases} -5m_1^2 + 4(n + 4)m_1 - 6n - 14 & \text{if } m_1 \text{ is even,} \\ -5m_1^2 + 4(n + 4)m_1 - 6n - 15 & \text{if } m_1 \text{ is odd.} \end{cases}$$

Suppose that m_1 is even. Let $f(m_1) = -5m_1^2 + 4(n+4)m_1 - 6n - 14$ for $m_1 \ge 6$. Let r_1 and r_2 be the two roots of $f(m_1) = 0$ with $r_1 \le r_2$. Since

 $\begin{array}{l} f(6)=18n-98>0, \mbox{ we have } r_1<6< r_2. \mbox{ Thus, } f(m_1)\geq 0 \mbox{ if } 6\leq m_1\leq r_2, \mbox{ and } f(m_1)<0 \mbox{ if } m_1>r_2. \mbox{ If } n-m_2 \mbox{ is even, then } m_1\leq n-m_2, \mbox{ } D'(G_n(m_1,m_2)) \mbox{ is maximum for fixed } m_2 \mbox{ only if } m_1=4 \mbox{ for } r_2\geq n-m_2 \mbox{ or } m_1=4, n-m_2 \mbox{ for } r_2< n-m_2. \mbox{ Similarly, if } n-m_2 \mbox{ is odd, then } m_1\leq n-m_2-1, \mbox{ } D'(G_n(m_1,m_2)) \mbox{ is maximum for fixed } m_2 \mbox{ only if } m_1=4, n-m_2-1. \mbox{ Hence } D'(G_n(m_1,m_2)) \mbox{ is maximum implies that } G_n(m_1,m_2)=G_n(4,m_2), \mbox{ } G_n(n-m_2-i,m_2), \mbox{ where } i=0 \mbox{ if } n-m_2 \mbox{ is even and } i=1 \mbox{ if } n-m_2 \mbox{ is odd. For fixed } m_2, \mbox{ let } s=n-m_2-i\geq 6, \mbox{ } G_2=G_n(4,m_2) \mbox{ and } G_3=G_n(n-m_2-i,m_2), \mbox{ by similar technique as in calculation of } D'(G_n(m_1-2,m_2))-D'(G_n(m_1,m_2)), \mbox{ we have} \end{array}$

$$\begin{aligned} D'\left(G_n(4,m_2)\right) &- D'\left(G_n(n-m_2-i,m_2)\right) \\ &= 4[W(G_2) - W(G_3)] + [D_{G_2}(u_0) - D_{G_3}(u_0)] + [D_{G_2}(v_0) - D_{G_3}(v_0)] \\ &= 4\left[-\frac{5}{24}s^3 + \left(\frac{n}{4} + \frac{1}{2}\right)s^2 - \left(\frac{n}{2} + \frac{1}{6}\right)s - 2n + 6\right] \\ &+ \left[-\frac{3}{4}s^2 + \left(n + \frac{1}{2}\right)s - 4n + 10\right] + \left(\frac{s^2}{4} - \frac{s}{2} - 2\right) \\ &= n(s^2 - s - 12) - \frac{5}{6}s^3 + \frac{3}{2}s^2 - \frac{2}{3}s + 32 \\ &\geq (s+3)(s^2 - s - 12) - \frac{5}{6}s^3 + \frac{3}{2}s^2 - \frac{2}{3}s + 32 \\ &= \frac{s^3}{6} + \frac{7}{2}s^2 - \frac{47}{3}s - 4 > 0, \end{aligned}$$

and thus, if $m_1 > 4$ is even, then $D'(G_n(m_1, m_2)) < D'(G_n(4, m_2))$. If $m_1 > 3$ is odd, then by similar arguments as above, we have $D'(G_n(m_1, m_2)) < D'(G_n(3, m_2))$. Since $D'(G_n(3, m_2)) - D'(G_n(4, m_2)) = 5(n - 4) > 0$, we have $D'(G_n(m_1, m_2)) < D'(G_n(3, m_2))$ if $m_1 > 3$, and if $m_2 > 3$, then

$$D'(G_n(3,m_2)) = D'(G_n(m_2,3)) < D'(G_n(3,3)).$$

The result follows.

Theorem 1. Let $G \in \mathcal{B}_1(n)$, where $n \geq 6$. Then

$$D'(G) \leq \frac{2}{3}n^3 + n^2 - \frac{41}{3}n + 24$$

with equality if and only if $G = G_n(3,3)$.

Proof: Suppose that G is a graph in $\mathcal{B}_1(n)$ with the maximum degree distance. Let $C_{m_1} = u_0 u_1 \dots u_{m_1-1} u_0$ and $C_{m_2} = v_0 v_1 \dots v_{m_2-1} v_0$ be the two vertexdisjoint cycles of G. Let $d_G(u_0, v_0) = \min\{d_G(u, v) : u \in V(C_{m_1}), v \in V(C_{m_2})\}$. By Lemma 1 (i) and (ii), $G - E(C_{m_1}) \cup E(C_{m_2})$ consists of vertex-disjoint paths, for which, by Lemma 2, except the path containing u_0 and v_0 , there is at most

one path containing a vertex in C_{m_1} and at most one path containing a vertex in C_{m_2} with length at least one.

Suppose that there is a path of length $a \ge 1$ containing $u_s, s \ne 0$. Denote by u_s^* the pendant vertex of G in this path, and u the neighbor of u_0 outside C_{m_1} . Let $G_1 = G - \{u_0u\} + \{uu_s^*\} \in \mathcal{B}_1(n)$.

Let Q be the component of $G - \{u_0\}$ containing u. Then Q is a unicyclic graph. Note that $V_1(G) \cap V(Q) = V_1(G_1) \cap V(Q) = \{v_0\}$ if all vertices on C_{m_2} except v_0 are of degree two, or $V_1(G) \cap V(Q) = V_1(G_1) \cap V(Q) = \{v_0, v_t, v_t^*\}$ if there is another vertex v_t on C_{m_2} with degree three, where v_t^* is the pendant vertex of the path attached to v_t . In either case, we have $D_{G_1}(x) - D_G(x) = D_{G_1}(u) - D_G(u)$ for $x \in V(Q)$, and thus

$$\begin{split} & \sum_{x \in V_1(G_1) \cap V(Q)} (d_{G_1}(x) - 2) D_{G_1}(x) - \sum_{x \in V_1(G) \cap V(Q)} (d_G(x) - 2) D_G(x) \\ &= \sum_{x \in V(Q)} (d_G(x) - 2) \left[D_{G_1}(x) - D_G(x) \right] \\ &= \left[D_{G_1}(u) - D_G(u) \right] \cdot \left[\sum_{x \in V(Q)} (d_Q(x) - 2) + 1 \right] \\ &= D_{G_1}(u) - D_G(u). \end{split}$$

It is easily seen that $V_1(G) = \{u_s, u_s^*, u_0\} \cup (V_1(G) \cap V(Q))$ and $V_1(G_1) = \{u_s\} \cup (V_1(G_1) \cap V(Q))$, and thus

$$D'(G_1) - D'(G)$$

$$= 4[W(G_1) - W(G)] + (3 - 2)[D_{G_1}(u_s) - D_G(u_s)]$$

$$-(1 - 2)D_G(u_s^*) - (3 - 2)D_G(u_0) + [D_{G_1}(u) - D_G(u)]$$

$$= 4[W(G_1) - W(G)] + [D_{G_1}(u_s) - D_G(u_s)]$$

$$+[D_G(u_s^*) - D_G(u_0)] + [D_{G_1}(u) - D_G(u)].$$

Let $G_2 = G - \{u_0u\} + \{uu_s\}, d_G(u_0, u_s) = c$ and $n_0 = |V(Q)| = n - m_1 - a$. Note that

$$\begin{split} W(G_1) - W(G) &= [W(G_1) - W(G_2)] + [W(G_2) - W(G)] \\ &= an_0(m_1 - 1) - an_0c = an_0(m_1 - 1 - c), \\ D_{G_1}(u_s) - D_G(u_s) &= [D_{G_1}(u_s) - D_{G_2}(u_s)] + [D_{G_2}(u_s) - D_G(u_s)] \\ &= an_0 - cn_0 = (a - c)n_0, \\ D_G(u_s^*) - D_G(u_0) &= [D_G(u_s^*) - D_G(u_s)] + [D_G(u_s) - D_G(u_0)] \\ &= a(m_1 - 1 + n_0) + c(n_0 - a) \\ &= a(m_1 - 1 - c) + n_0(a + c), \\ D_{G_1}(u) - D_G(u) &= [D_{G_1}(u) - D_{G_2}(u)] + [D_{G_2}(u) - D_G(u)] \\ &= a(m_1 - 1) - ac = a(m_1 - 1 - c). \end{split}$$

Then

$$D'(G_1) - D'(G) = 2a[(2n_0 + 1)(m_1 - 1 - c) + n_0]$$

$$\geq 2a\left[(2n_0 + 1)\left(m_1 - 1 - \frac{m_1}{2}\right) + n_0\right]$$

$$= 2a\left[(2n_0 + 1)\left(\frac{m_1}{2} - 1\right) + n_0\right] > 0,$$

and thus $D'(G_1) > D'(G)$, a contradiction. Thus, there is no such path containing a vertex on the cycle C_{m_1} . Similarly, there is no such path containing a vertex on the cycle C_{m_2} . Then $G = G_n(m_1, m_2)$. By Lemma 4, we have $G = G_n(3, 3)$.

4 Degree distances of graphs in $\mathcal{B}_2(n)$

In this section, we determine the maximum degree distance in the class of connected graphs with exactly two cycles of a common vertex.

Let $C_{s_1} = u_0 u_1 \dots u_{s_1-1} u_0$ and $C_{s_2} = v_0 v_1 \dots v_{s_2-1} v_0$ be two vertex-disjoint cycles. Let $H_n(a, s_1, s_2)$ be the bicyclic graph obtained by identifying u_0 of C_{s_1} and v_0 of C_{s_2} , which is denoted by u_0 , and attaching a path P_a and a path P_b to $u_{\lfloor s_1/2 \rfloor}$ and $v_{\lfloor s_2/2 \rfloor}$, respectively, where $a, b \ge 0$ and $a + b = n + 1 - s_1 - s_2$, and if a = 0 or b = 0, then no path is attached to $u_{\lfloor s_1/2 \rfloor}$ or $v_{\lfloor s_2/2 \rfloor}$. If $a \ge 1$, then let u be the pendant vertex of the path attached to $u_{\lfloor s_1/2 \rfloor}$. If $s_1 = s_2$, then $a \ge b$ is required.

Lemma 5. For integers n, m_1 and m_2 with $n \ge 7, m_1, m_2 \ge 3$ and $m_1 + m_2 \le n+1$, we have $D'(H_n(a, m_1, m_2)) \le D'(H_n(n-5, 3, 3))$ with equality if and only if $(a, m_1, m_2) = (n-5, 3, 3)$.

Proof: Suppose that $m_1 \ge 5$. Let $k = a + m_1$. For $G_1 = H_n(a, m_1, m_2)$ and $G_2 = H_n(a + 2, m_1 - 2, m_2)$, using Eqs. (1) and (4), and by similar arguments

as in the proof of Lemma 4, we have

$$\begin{array}{l} D'\left(H_n(a+2,m_1-2,m_2)\right) - D'\left(H_n(a,m_1,m_2)\right) \\ = & 4[W(G_2) - W(G_1)] + (4-2)[D_{G_2}(u_0) - D_{G_1}(u_0)] \\ & + (3-2)\left[D_{G_2}\left(u_{\lfloor \frac{m_1}{2} \rfloor - 1}\right) - D_{G_1}\left(u_{\lfloor \frac{m_1}{2} \rfloor}\right)\right] + (1-2)[D_{G_2}(u) - D_{G_1}(u)] \\ = & 4[W(G_2) - W(G_1)] + 2[D_{G_2}(u_0) - D_{G_1}(u_0)] \\ & + \left[D_{G_2}\left(u_{\lfloor \frac{m_1}{2} \rfloor - 1}\right) - D_{G_2}(u)\right] + \left[D_{G_1}(u) - D_{G_1}\left(u_{\lfloor \frac{m_1}{2} \rfloor}\right)\right] \\ = & 4\left[-\frac{3m_1^2}{2} - \left(2n - 3k - \frac{9}{2}\right)m_1 + \left\lfloor \frac{m_1^2}{4} \right\rfloor \\ & + 2\left\lfloor \frac{m_1}{2} \right\rfloor(n-k) + (k+2)(n-k-2)\right] + 2\left(2\left\lfloor \frac{m_1}{2} \right\rfloor - 2m_1 + k + 2\right) \\ & -(k-m_1+2)(n-k+m_1-3) + (k-m_1)(n-k+m_1-1) \\ = & \begin{cases} -5m_1^2 - (4n - 8k - 12)m_1 - 4k^2 + (4n - 10)k + 6n - 6 \\ & \text{if } m_1 \text{ is even,} \\ -5m_1^2 - (4n - 8k - 12)m_1 - 4k^2 + (4n - 6)k + 2n - 9 \\ & \text{if } m_1 \text{ is odd.} \end{cases} \end{array}$$

Suppose that m_1 is even. Let $g(m_1) = -5m_1^2 - (4n - 8k - 12)m_1 - 4k^2 + (4n - 10)k + 6n - 6$. Note that $k \ge 6$. It is easily seen that

$$g(6) = n(4k - 18) - 4k^2 + 38k - 114$$

$$\geq (k+2)(4k - 18) - 4k^2 + 38k - 114 = 28k - 150 > 0.$$

Let r_1 and r_2 be the two roots of $g(m_1) = 0$, where $r_1 \leq r_2$. It is easily seen that $r_1 < 6 < r_2$. Thus, $g(m_1) \geq 0$ if $6 \leq m_1 \leq r_2$, and $g(m_1) < 0$ if $m_1 > r_2$. If k is even, then $m_1 \leq k$, $D'(H_n(a, m_1, m_2))$ is maximum for fixed m_2 only if $m_1 = 4$ for $r_2 \geq k$ or $m_1 = 4$, k for $r_2 < k$, and by setting $G_3 = H_n(0, k, m_2)$, $G_4 = H_n(k - 4, 4, m_2)$, and using similar arguments as above, we have

$$D' (H_n(k-4,4,m_2)) - D' (H_n(0,k,m_2))$$

$$= 4[W(G_4) - W(G_3)] + 2[D_{G_4}(u_0) - D_{G_3}(u_0)] + [D_{G_4}(u_2) - D_{G_4}(u)]$$

$$= 4\left[-\frac{5}{24}k^3 + \frac{1}{4}(n+6)k^2 - \frac{1}{6}(9n+25)k + 2n+6\right] + 2\left(\frac{k^2}{4} - \frac{3}{2}k + 2\right)$$

$$-(k-4)(n-k+3)$$

$$= n(k^2 - 7k + 12) - \frac{5}{6}k^3 + \frac{15}{2}k^2 - \frac{80}{3}k + 40$$

$$\ge (k+2)(k^2 - 7k + 12) - \frac{5}{6}k^3 + \frac{15}{2}k^2 - \frac{80}{3}k + 40$$

$$= \frac{k^3}{6} + \frac{5}{2}k^2 - \frac{86}{3}k + 64 > 0,$$

implying that $D'(H_n(k-4,4,m_2)) > D'(H_n(0,k,m_2))$. Similarly, if k is odd, then $m_1 \leq k-1$, $D'(H_n(a,m_1,m_2))$ is maximum for fixed m_2 only if $m_1 = 4$

or $m_1 = k - 1$, and thus $D'(H_n(k - 4, 4, m_2)) > D'(H_n(1, k - 1, m_2))$. Let $b = n + 1 - m_1 - m_2 - a$. We conclude that, if $m_1 > 4$ is even, then

$$D'(H_n(a, m_1, m_2)) < D'(H_n(a + m_1 - 4, 4, m_2)) = D'(H_n(b, m_2, 4)).$$

If $m_1 > 3$ is odd, then by similar arguments as above, we have

$$D'(H_n(a, m_1, m_2)) < D'(H_n(a + m_1 - 3, 3, m_2)) = D'(H_n(b, m_2, 3)).$$

Thus, $D'(H_n(a, m_1, m_2))$ is maximum for fixed n only if $m_1, m_2 = 3, 4$. For $0 \le s \le n-7$, let t = n-7-s. We may check that

$$D'(H_n(n-5,3,3)) - D'(H_n(s,4,4)) = 12st + 16s + 16t + 2 > 0,$$

$$D'(H_n(n-5,3,3)) - D'(H_n(0,3,4)) = 5n - 34 > 0,$$

$$D'(H_n(n-5,3,3)) - D'(H_n(s+1,3,4)) = 12st + 11s + 17t + 7 > 0,$$

$$D'(H_n(n-5,3,3)) - D'(H_n(s+1,3,3)) = 12st + 12s + 12t + 12 > 0.$$

The result follows easily.

Theorem 2. Let $G \in \mathcal{B}_2(n)$, where $n \ge 6$. Then for n = 6, $D'(G) \le 112$ with equality if and only if $G = H_6(0, 3, 4)$, and for $n \ge 7$,

$$D'(G) \le \frac{2}{3}n^3 + n^2 - \frac{83}{3}n + 94$$

with equality if and only if $G = H_n(n-5,3,3)$.

Proof: Obviously, there are only three graphs in $\mathcal{B}_2(6)$. By direct calculation, the result follows easily for n = 6. In the following, suppose that $n \ge 7$.

Suppose that G is a graph in $\mathcal{B}_2(n)$ with the maximum degree distance. Let $C_{m_1} = u_0 u_1 \dots u_{m_1-1} u_0$ and $C_{m_2} = v_0 v_1 \dots v_{m_2-1} v_0$ be the two cycles of G with $u_0 = v_0$. By Lemma 1 (i), we have $G - E(C_{m_1}) \cup E(C_{m_2})$ consists of vertexdisjoint paths, for which, by Lemma 3, at most three paths have length at least one: a path Q with u_0 as an end vertex, a path containing some vertex u_s in C_{m_1} with $s \neq 0$, and a path containing some vertex v_t in C_{m_2} with $t \neq 0$.

If there is such a path containing u_s with length $a \ge 1$, then denote by u_s^* the pendant vertex of G in this path. Otherwise, all vertices on C_{m_1} except u_0 have degree two and we set a = 0, $u_s = u_s^* = u_{\lfloor \frac{m_1}{2} \rfloor}$. If there is such a path containing v_t with length at least one, then denote by b the length of this path. Otherwise, all vertices on C_{m_2} except v_0 have degree two and we set b = 0.

Suppose that there is such a path Q containing u_0 with length at least one in G. Let u be the neighbor of u_0 outside the two cycles, and u^* the pendant vertex of G in Q. Suppose without loss of generality that $a \leq b$. Let $G_1 =$ $G - \{u_0u\} + \{u_s^*u\} \in \mathcal{B}_2(n)$. Let $c = d_G(u_0, u_s)$ and $k = d_G(u^*, u_0)$.

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Let $G^* = G - \{u_0u\} + \{u_su\}$. Suppose first that $a \ge 1$. We have

$$W(G_1) - W(G) = [W(G_1) - W(G^*)] + [W(G^*) - W(G)]$$

= $ka(n - a - k - 1) + kc(b + m_2 - 1 - a).$

Note also that

$$\begin{aligned} D_{G_1}(u_s) - D_{G_1}(u^*) &= -(k+a)(n-k-a-1), \\ D_G(u^*) - D_G(u_0) &= k(n-k-1), \\ D_G(u^*_s) - D_G(u_s) &= a(n-a-1), \\ D_{G_1}(u_0) - D_G(u_0) &= [D_{G_1}(u_0) - D_{G^*}(u_0)] + [D_{G^*}(u_0) - D_G(u_0)] \\ &= ka + kc = k(a+c). \end{aligned}$$

Then

$$\begin{split} D'(G_1) &- D'(G) \\ &= & 4[W(G_1) - W(G)] + (3-2)[D_{G_1}(u_s) - D_G(u_s)] \\ &+ (1-2)[D_{G_1}(u^*) - D_G(u^*)] + (4-2)D_{G_1}(u_0) \\ &- (5-2)D_G(u_0) - (1-2)D_G(u^*_s) \\ &= & 4[W(G_1) - W(G)] + [D_{G_1}(u_s) - D_{G_1}(u^*)] + [D_G(u^*) - D_G(u_0)] \\ &+ [D_G(u^*_s) - D_G(u_s)] + 2[D_{G_1}(u_0) - D_G(u_0)] \\ &= & 4kc\left(b + m_2 - a - \frac{1}{2}\right) + 4ka(b + m_1 + m_2 - 1) > 0, \end{split}$$

and thus, $D'(G_1) > D'(G)$. If a = 0, then

$$D'(G_1) - D'(G)$$

$$= 4[W(G_1) - W(G)] + (1 - 2)[D_{G_1}(u^*) - D_G(u^*)] + (4 - 2)D_{G_1}(u_0)$$

$$-(5 - 2)D_G(u_0) + (3 - 2)D_{G_1}\left(u_{\lfloor \frac{m_1}{2} \rfloor}\right)$$

$$= 4[W(G_1) - W(G)] + \left[D_{G_1}\left(u_{\lfloor \frac{m_1}{2} \rfloor}\right) - D_{G_1}(u^*)\right] + \left[D_G(u^*) - D_G(u_0)\right]$$

$$+ 2[D_{G_1}(u_0) - D_G(u_0)]$$

$$= 4k \left\lfloor \frac{m_1}{2} \right\rfloor \left(b + m_2 - \frac{1}{2}\right) > 0,$$

and thus, $D'(G_1) > D'(G)$. In either case, $D'(G_1) > D'(G)$, a contradiction. Thus, there is no such path Q containing u_0 in G, i.e., $d_G(u_0) = 4$.

Suppose that there is such a path containing u_s with length $a \ge 1$ and $d_G(u_0, u_s) = c < \lfloor \frac{m_1}{2} \rfloor$. Let u_{s_1} be the neighbor of u_s outside C_{m_1} in G. For

$$\begin{split} G_2 &= G - \left\{ u_s u_{s_1} \right\} + \left\{ u_{\lfloor \frac{m_1}{2} \rfloor} u_{s_1} \right\} \in \mathcal{B}_2(n), \\ &= \begin{array}{l} D'(G_2) - D'(G) \\ &= \begin{array}{l} 4 \left[W(G_2) - W(G) \right] + (4 - 2) \left[D_{G_2}(u_0) - D_G(u_0) \right] \\ &+ (1 - 2) \left[D_{G_2}(u_s^*) - D_G(u_s^*) \right] \\ &+ (3 - 2) D_{G_2} \left(u_{\lfloor \frac{m_1}{2} \rfloor} \right) - (3 - 2) D_G(u_s) \\ &= \begin{array}{l} 4 \left[W(G_2) - W(G) \right] + 2 \left[D_{G_2}(u_0) - D_G(u_0) \right] \\ &+ \left[D_{G_2} \left(u_{\lfloor \frac{m_1}{2} \rfloor} \right) - D_{G_2}(u_s^*) \right] + \left[D_G(u_s^*) - D_G(u_s) \right] \\ &= \begin{array}{l} 4 \cdot a \left(\left\lfloor \frac{m_1}{2} \right\rfloor - c \right) (n - a - m_1) + 2 \cdot a \left(\left\lfloor \frac{m_1}{2} \right\rfloor - c \right) \\ &- a(n - a - 1) + a(n - a - 1) \\ &= \begin{array}{l} 2a \left(\left\lfloor \frac{m_1}{2} \right\rfloor - c \right) (2n - 2a - 2m_1 + 1) > 0, \end{array} \end{split}$$

and then $D'(G_2) > D'(G)$, a contradiction. Thus, if there is such a path containing u_s with length at least one, then $d_G(u_0, u_s) = \lfloor \frac{m_1}{2} \rfloor$. Similarly, if there is such a path containing v_t with length at least one, then $d_G(u_0, v_t) = \lfloor \frac{m_2}{2} \rfloor$. It follows that $G = H_n(a, m_1, m_2)$, and by Lemma 5, we have $G = H_n(n - 5, 3, 3)$. \Box

5 Conclusions

It is easily checked that $D'(G_6(3,3)) - D'(H_6(0,3,4)) = 10 > 0$, and for $n \ge 7$, $D'(G_n(3,3)) - D'(H_n(n-5,3,3)) = 14n - 70 > 0$. By Theorems 1 and 2, we have the following conclusions:

(i) for $n \ge 6$, $G_n(3,3)$ is the unique graph in $\mathcal{B}_1(n)$ with the maximum degree distance $\frac{2}{3}n^3 + n^2 - \frac{41}{3}n + 24$; (ii) for n = 6, $H_6(0,3,4)$ is the unique graph in $\mathcal{B}_2(6)$ with the maximum degree

(ii) for n = 6, $H_6(0, 3, 4)$ is the unique graph in $\mathcal{B}_2(6)$ with the maximum degree distance 112, and for $n \ge 7$, $H_n(n-5, 3, 3)$ is the unique graph in $\mathcal{B}_2(n)$ with the maximum degree distance $\frac{2}{3}n^3 + n^2 - \frac{83}{3}n + 94$;

(iii) for $n \ge 6$, $G_n(3,3)$ is the unique graph in $\mathcal{B}_1(n) \cup \mathcal{B}_2(n)$ with the maximum degree distance $\frac{2}{3}n^3 + n^2 - \frac{41}{3}n + 24$.

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References

- O. BUCICOVSCHI, S. M. CIOABĂ, The minimum degree distance of graphs of given order and size, Discrete Appl. Math. 156 (2008) 3518–3521.
- [2] J. DEVILLERS, A. T. BALABAN (EDS.), Topological Indices and Related Descriptors in QSAR and QSPR, Gordon and Breach, Amsterdam, 1999.
- [3] A. A. DOBRYNIN, R. ENTRINGER, I. GUTMAN, Wiener index of trees: Theory and applications, Acta Appl. Math. 66 (2001) 211–249.
- [4] A. A. DOBRYNIN, I. GUTMAN, S. KLAVŽAR, P. ŽIGERT, Wiener index of hexagonal systems, Acta Appl. Math. 72 (2002) 247–294.
- [5] 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.
- [6] I. GUTMAN, Selected properties of the Schultz molecular topological index, J. Chem. Inf. Comput. Sci. 34 (1994) 1087–1089.
- [7] Y. HOU, A. CHANG, The unicyclic graph with maximum degree distance, J. Math. Study 39 (2006) 18–24.
- [8] S. KLAVŽAR, I. GUTMAN, A comparison of the Schultz molecular topological index with the Wiener index, J. Chem. Inf. Comput. Sci. 36 (1996) 1001– 1003.
- [9] D. J. KLEIN, Z. MIHALIĆ, D. PLAVŠIĆ, N. TRINAJSTIĆ, Molecular topological index: A relation with Wiener index, J. Chem. Inf. Comput. Sci. 32 (1992) 304–305.
- [10] H. P. SCHULTZ, Topological organic chemistry. 1. Graph theory and topological indices of alkanes, J. Chem. Inf. Comput. Sci. 29 (1989) 227–228.
- [11] R. TODESCHINI, V. CONSONNI, Handbook of Molecular Descriptors, Wiley– VCH, Weinheim, 2000.
- [12] A. I. TOMESCU, Unicyclic and bicyclic graphs having minimum degree distance, Discrete Appl. Math. 156 (2008) 125–130.
- [13] I. TOMESCU, Some extremal properties of the degree distance of a graph, Discrete Appl. Math. 98 (1999) 159–163.
- [14] I. TOMESCU, Properties of connected graphs having minimum degree distance, Discrete Math. 309 (2009) 2745–2748.
- [15] B. ZHOU, Bounds for Schultz molecular topological index, MATCH Commun. Math. Comput. Chem. 56 (2006) 189–194.

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