

DEGREE DISTANCE OF UNICYCLIC GRAPHS

Zhibin Du and Bo Zhou*

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 $d_G(u)$ denotes the degree of vertex u and $D_G(u)$ denotes the sum of distances between u and all vertices of G . We determine the maximum degree distance of n -vertex unicyclic graphs with given maximum degree, and the first seven maximum degree distances of n -vertex unicyclic graphs for $n \geq 6$.

1 Introduction

Let G be a simple connected graph with vertex set $V(G)$. For $u, v \in V(G)$, let $d_G(u, v)$ be the distance between u and v in G . For $u \in V(G)$, let $d_G(u)$ be the degree of u in G , and let $D_G(u)$ be the sum of distances between u and all vertices of G , i.e., $D_G(u) = \sum_{v \in V(G)} d_G(u, v)$. The degree distance of G is defined as [1, 2]

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

In 1989, Schultz [3] (see also [4]) put forward a “molecular topological index”, $MTI(G)$, of a connected graph G , which turns out to be [2]

$$MTI(G) = D'(G) + Zg(G),$$

where $Zg(G)$ is equal to the sum of squares of the vertex degrees of G , which is known as the (first) Zagreb index [5–7]. In chemical literature [2], the Schultz’s molecular topological index and the degree distance are also named the Schultz

*Corresponding author

2000 *Mathematics Subject Classifications*. 05C07, 05C12, 05C35, 05C90.

Key words and Phrases. degree, distance, degree distance, Wiener index, unicyclic graph, maximum degree.

Received: May 1, 2010

Communicated by Dragan Stevanović

index and the true Schultz index, respectively. Properties for molecular topological index may be found in, e.g., [8–11].

Recall that the Wiener index of a connected graph G is defined as [12, 13]

$$W(G) = \frac{1}{2} \sum_{u \in V(G)} D_G(u).$$

Gutman [2] showed that if G is an n -vertex tree, then $D'(G) = 4W(G) - n(n-1)$. Thus, the study of the degree distance for trees is equivalent to the study of the Wiener index, which may be found in [12, 14].

An n -vertex connected graph is said to be unicyclic if it possesses n edges for $n \geq 3$ and bicyclic if it possesses $n+1$ edges for $n \geq 4$. I. Tomescu [15] showed that the star is the unique graph with the minimum degree distance in the class of n -vertex connected graphs. A.I. Tomescu [16] characterized the unicyclic and bicyclic graphs with the minimum degree distances. I. Tomescu [17] deduced properties of the graphs with the minimum degree distance in the class of n -vertex connected graphs with $m \geq n-1$ edges, which were determined recently by Bucicovschi and Cioabă [18]. Hou and Chang [19] characterized the unicyclic graphs with the maximum degree distance. The authors [20] determined the bicyclic graphs of exactly two cycles with the maximum degree distance. Dankelmann *et al.* [21] gave asymptotically sharp upper bounds for the degree distance.

In this paper, we determine the maximum degree distance of n -vertex unicyclic graphs with given maximum degree Δ , where $3 \leq \Delta \leq n-2$, the first seven maximum degree distances of n -vertex unicyclic graphs for $n \geq 6$, and the corresponding graphs whose degree distances achieve these values.

2 Preliminaries

Let P_n and S_n be respectively the path and the star on $n \geq 1$ vertices, and C_n the cycle on $n \geq 3$ vertices.

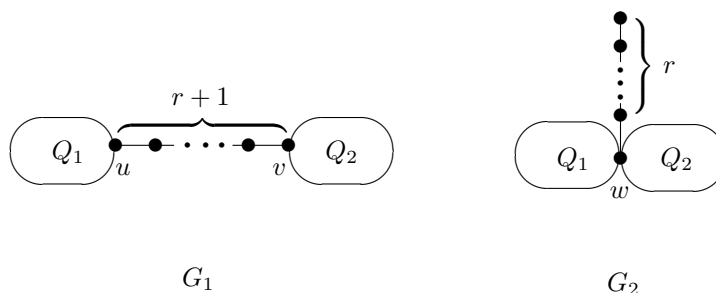


Fig. 1. The graphs G_1 and G_2 in Lemma 1.

Lemma 1. [2] Let Q_1 and Q_2 be vertex-disjoint connected graphs with at least two vertices, and $u \in V(Q_1)$ and $v \in V(Q_2)$. Let G_1 be the graph obtained from Q_1 and

Q_2 by joining u and v by a path of length $r \geq 1$, and G_2 the graph obtained from Q_1 and Q_2 by identifying u and v , which is denoted by w , and attaching a path P_r to w ; see Fig. 1. Then $D'(G_1) > D'(G_2)$.

For a connected graph G , let $V_1(G) = \{x \in V(G) : d_G(x) \neq 2\}$. Then

$$\begin{aligned} D'(G) &= \sum_{x \in V(G)} 2D_G(x) + \sum_{x \in V_1(G)} (d_G(x) - 2)D_G(x) \\ &= 4W(G) + \sum_{x \in V_1(G)} (d_G(x) - 2)D_G(x). \end{aligned}$$

Thus, if G and H are connected graphs, then

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

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

For a subset M of the edge set of the graph G , $G - M$ denotes the graph obtained from G by deleting the edges in M , and for a subset M^* of the edge set of the complement of G , $G + M^*$ denotes the graph obtained from G by adding the edges in M^* .

Let $C_m(T_1, T_2, \dots, T_m)$ be the unicyclic graph with cycle $C_m = v_1v_2 \dots v_mv_1$ such that the deletion of all edges on C_m results in m vertex-disjoint trees T_1, T_2, \dots, T_m with $v_i \in V(T_i)$ for $i = 1, 2, \dots, m$. If T_i with $1 \leq i \leq m$ is trivial, then we write $C_m(T_1, \dots, T_{i-1}, T_i, T_{i+1}, \dots, T_m)$ as $C_m(T_1, \dots, \overline{T_{i-1}}, -, T_{i+1}, \dots, T_m)$.

Lemma 2. For integers i and j with $2 \leq i < j \leq m$, let $G_{a_i, a_j} = C_m(T_1, T_2, \dots, T_m)$, where T_r is the path P_{a_r+1} with an end vertex v_r for $2 \leq r \leq m$, and all trees T_l with $l \neq i, j$ and $1 \leq l \leq m$ are fixed. If $a_i, a_j \geq 1$, then

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

Proof. Let $G = G_{a_i, a_j}$ and $G_1 = G_{a_i+a_j, 0}$. Denote by v the neighbor of v_j outside C_m in G . Let v_k^* be the pendent vertex of G of the path attached to v_k if $a_k \geq 1$, where $2 \leq k \leq m$. Obviously, $G_1 = G - \{vv_j\} + \{vv_i^*\}$. Let Z be the set of vertices in the path from v to v_j^* in G . Let W be the set of vertices in the path from v_i to v_i^* in G . Let $n = |V(G)|$. Let $G_2 = G - \{vv_j\} + \{vv_i\}$, $a_1 = |V(T_1)| - 1$ and $d(x, y) = d_G(x, y)$ for $x, y \in V(G)$. We have

$$\begin{aligned} &W(G_1) - W(G_2) \\ &= \sum_{\substack{x \in Z \\ y \in W}} [d_{G_1}(x, y) - d_{G_2}(x, y)] + \sum_{\substack{x \in Z \\ y \in V(G) \setminus (Z \cup W)}} [d_{G_1}(x, y) - d_{G_2}(x, y)] \\ &= 0 + \sum_{\substack{x \in Z \\ y \in V(G) \setminus (Z \cup W)}} [d_{G_1}(x, y) - d_{G_2}(x, y)] \end{aligned}$$

$$\begin{aligned}
&= \sum_{\substack{x \in Z \\ y \in V(G) \setminus (Z \cup W)}} a_i = a_i a_j (n - a_i - a_j - 1), \\
&W(G_2) - W(G) \\
&= \sum_{\substack{x \in Z \\ y \in V(C_m)}} [d_{G_2}(x, y) - d(x, y)] + \sum_{\substack{x \in Z \\ y \in V(G) \setminus (Z \cup V(C_m))}} [d_{G_2}(x, y) - d(x, y)] \\
&= 0 + \sum_{\substack{x \in Z \\ y \in V(G) \setminus (Z \cup V(C_m))}} [d_{G_2}(x, y) - d(x, y)] \\
&= \sum_{x \in Z} \sum_{\substack{1 \leq k \leq m \\ k \neq j}} a_k [d(v_k, v_i) - d(v_k, v_j)] \\
&= a_j \sum_{\substack{1 \leq k \leq m \\ k \neq j}} a_k [d(v_k, v_i) - d(v_k, v_j)],
\end{aligned}$$

and then

$$\begin{aligned}
W(G_1) - W(G) &= [W(G_1) - W(G_2)] + [W(G_2) - W(G)] \\
&= a_i a_j (n - a_i - a_j - 1) + a_j \sum_{\substack{1 \leq k \leq m \\ k \neq j}} a_k [d(v_k, v_i) - d(v_k, v_j)].
\end{aligned}$$

Note that $V_1(G_1) = (V_1(G_1) \cap V(T_1)) \cup \left(\bigcup_{\substack{2 \leq k \leq m \\ a_k \geq 1, k \neq i, j}} \{v_k, v_k^*\} \right) \cup \{v_i, v_j^*\}$ and $V_1(G) = (V_1(G) \cap V(T_1)) \cup \left(\bigcup_{\substack{2 \leq k \leq m \\ a_k \geq 1}} \{v_k, v_k^*\} \right)$. For $x \in V(T_k)$ with $1 \leq k \leq m$ and $k \neq i, j$, we have $D_{G_1}(x) - D_G(x) = D_{G_1}(v_k) - D_G(v_k)$. Setting $k = 1$, we have

$$\begin{aligned}
&\sum_{x \in V_1(G_1) \cap V(T_1)} (d_{G_1}(x) - 2)D_{G_1}(x) - \sum_{x \in V_1(G) \cap V(T_1)} (d_G(x) - 2)D_G(x) \\
&= \sum_{x \in V(T_1)} (d_G(x) - 2) [D_{G_1}(x) - D_G(x)] \\
&= [D_{G_1}(v_1) - D_G(v_1)] \left[\sum_{x \in V(T_1)} (d_{T_1}(x) - 2) + 2 \right] = 0.
\end{aligned}$$

For $k \neq 1, i, j$ and $a_k \geq 1$, we have

$$\begin{aligned}
&\sum_{x \in \{v_k, v_k^*\}} (d_{G_1}(x) - 2)D_{G_1}(x) - \sum_{x \in \{v_k, v_k^*\}} (d_G(x) - 2)D_G(x) \\
&= (3 - 2)[D_{G_1}(v_k) - D_G(v_k)] + (1 - 2)[D_{G_1}(v_k^*) - D_G(v_k^*)] = 0.
\end{aligned}$$

Note that

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

$$\begin{aligned}
&= (3-2)[D_{G_1}(v_i) - D_G(v_i)] + (1-2)[D_{G_1}(v_j^*) - D_G(v_j^*)] \\
&\quad - (1-2)D_G(v_i^*) - (3-2)D_G(v_j) \\
&= [D_{G_1}(v_i) - D_{G_1}(v_j^*)] + [D_G(v_i^*) - D_G(v_i)] + [D_G(v_j^*) - D_G(v_j)] \\
&= -(a_i + a_j)(n - a_i - a_j - 1) + a_i(n - a_i - 1) + a_j(n - a_j - 1) = 2a_i a_j.
\end{aligned}$$

Thus

$$\sum_{x \in V_1(G_1)} (d_{G_1}(x) - 2)D_{G_1}(x) - \sum_{x \in V_1(G)} (d_G(x) - 2)D_G(x) = 2a_i a_j.$$

It follows that

$$\begin{aligned}
&D'(G_{a_i+a_j,0}) - D'(G_{a_i,a_j}) \\
&= 4a_i a_j(n - a_i - a_j) - 2a_i a_j + 4a_j \sum_{\substack{1 \leq k \leq m \\ k \neq j}} a_k [d(v_k, v_i) - d(v_k, v_j)].
\end{aligned}$$

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

$$4 \sum_{\substack{1 \leq k \leq m \\ k \neq j}} a_k [d(v_k, v_j) - d(v_k, v_i)] \geq 4a_i(n - a_i - a_j) - 2a_i,$$

and thus

$$\begin{aligned}
&D'(G_{0,a_i+a_j}) - D'(G_{a_i,a_j}) \\
&= 4a_i a_j(n - a_i - a_j) - 2a_i a_j + 4a_i \sum_{\substack{1 \leq k \leq m \\ k \neq i}} a_k [d(v_k, v_j) - d(v_k, v_i)] \\
&= 4a_i a_j(n - a_i - a_j) - 2a_i a_j - 4a_i(a_i + a_j)d(v_i, v_j) \\
&\quad + a_i \cdot 4 \sum_{\substack{1 \leq k \leq m \\ k \neq j}} a_k [d(v_k, v_j) - d(v_k, v_i)] \\
&\geq 4a_i a_j(n - a_i - a_j) - 2a_i a_j - 4a_i(a_i + a_j)d(v_i, v_j) \\
&\quad + a_i[4a_i(n - a_i - a_j) - 2a_i] \\
&= 2a_i(a_i + a_j)[2(n - a_i - a_j) - 2d(v_i, v_j) - 1] \\
&\geq 2a_i(a_i + a_j) \left(2m - 2 \cdot \frac{m}{2} - 1 \right) \\
&= 2a_i(a_i + a_j)(m - 1) > 0.
\end{aligned}$$

Now the result follows. \square

For $n \geq m \geq 3$, let $U_{n,m} = C_m(P_{n-m+1}, -, \dots, -)$, where v_1 is an end vertex of the path P_{n-m+1} . 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

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

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

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

Lemma 3. For integers i and m with $2 \leq i \leq \lfloor \frac{m}{2} \rfloor + 1$ and $m \geq 3$, let $G_i(a, m) = C_m(T_1, T_2, \dots, T_m)$, where T_i is the path P_{a+1} with an end vertex v_i , $T_j = P_1$ for $2 \leq j \leq m$ with $j \neq i$, and T_1 is a fixed tree. Let $G(a, m) = G_{\lfloor \frac{m}{2} \rfloor + 1}(a, m)$. For fixed $k = a + m \geq 4$, $D'(G_i(a, m)) < \max\{D'(G(k-3, 3)), D'(G(k-4, 4))\}$ if $m > 4$, or $m = 4$ and $i = 2$.

Proof. Let v_i^* be the pendent vertex of the path attached to v_i in $G_i(a, m)$ if $a \geq 1$.

We first prove that $D'(G_i(a, m)) \leq D'(G(a, m))$. If $|V(T_1)| = 1$ or $a = 0$, then $G_i(a, m)$ is (isomorphic to) $G(a, m)$. Suppose that $|V(T_1)| \geq 2$ and $a \geq 1$. Suppose that $G_i(a, m) \neq G(a, m)$, i.e., $i < \lfloor \frac{m}{2} \rfloor + 1$. Let $G_1 = G_i(a, m)$. Let $G_2 = G_1 - \{v_i v\} + \{v_{\lfloor \frac{m}{2} \rfloor + 1} v\}$, where v is the neighbor of v_i outside C_m in G_1 . Obviously, $G_2 = G(a, m)$. It is easily seen that $V_1(G_1) = (V_1(G_1) \cap V(T_1)) \cup \{v_i, v_i^*\}$ and $V_1(G_2) = (V_1(G_2) \cap V(T_1)) \cup \{v_{\lfloor \frac{m}{2} \rfloor + 1}, v_i^*\}$. Note that for $x \in V(T_1)$, $D_{G_2}(x) - D_{G_1}(x) = D_{G_2}(v_1) - D_{G_1}(v_1)$, and thus

$$\sum_{x \in V_1(G_2) \cap V(T_1)} (d_{G_2}(x) - 2)D_{G_2}(x) - \sum_{x \in V_1(G_1) \cap V(T_1)} (d_{G_1}(x) - 2)D_{G_1}(x) = 0.$$

We have

$$\begin{aligned} & D'(G(a, m)) - D'(G_i(a, m)) \\ &= 4[W(G_2) - W(G_1)] + (1-2)[D_{G_2}(v_i^*) - D_{G_1}(v_i^*)] \\ & \quad + (3-2)D_{G_2}(v_{\lfloor \frac{m}{2} \rfloor + 1}) - (3-2)D_{G_1}(v_i) \\ &= 4[W(G_2) - W(G_1)] + [D_{G_1}(v_i^*) - D_{G_1}(v_i)] + [D_{G_2}(v_{\lfloor \frac{m}{2} \rfloor + 1}) - D_{G_2}(v_i^*)] \\ &= 4 \left(\left\lfloor \frac{m}{2} \right\rfloor + 1 - i \right) a(|V(T_1)| - 1) + a(n-a-1) - a(n-a-1) \\ &= 4 \left(\left\lfloor \frac{m}{2} \right\rfloor + 1 - i \right) a(|V(T_1)| - 1) > 0, \end{aligned}$$

and thus $D'(G(a, m)) > D'(G_i(a, m))$. It follows that $D'(G_i(a, m)) \leq D'(G(a, m))$ with equality if and only if $G_i(a, m) = G(a, m)$. Thus, the result for $m = 4$ and $i = 2$ follows.

To prove the result for $m > 4$, we need only to show that

$$D'(G(a, m)) < \max\{D'(G(k-3, 3)), D'(G(k-4, 4))\}$$

for $a \geq 0$. Note that $U_{m+a,m}$ is a subgraph of $G(a, m)$.

Suppose that $m \geq 5$. Let $G_3 = G(a+2, m-2)$. Let $A_1 = V(U_{m+a,m-2}) \setminus \{v_1\}$, $A_2 = V(U_{m+a,m}) \setminus \{v_1\}$ and $A_3 = V(T_1) \setminus \{v_1\}$. First suppose that $a \geq 1$. For

$y \in V(T_1)$, $d_{G_3}(v_1, y) = d_{G_2}(v_1, y)$, and then

$$\begin{aligned}
& \sum_{x \in A_1, y \in A_3} d_{G_3}(x, y) - \sum_{x \in A_2, y \in A_3} d_{G_2}(x, y) \\
&= \sum_{x \in A_1, y \in A_3} [d_{G_3}(x, v_1) + d_{G_3}(v_1, y)] - \sum_{x \in A_2, y \in A_3} [d_{G_2}(x, v_1) + d_{G_2}(v_1, y)] \\
&= \left[\sum_{x \in A_1, y \in A_3} d_{G_3}(x, v_1) - \sum_{x \in A_2, y \in A_3} d_{G_2}(x, v_1) \right] \\
&\quad + \left[\sum_{x \in A_1, y \in A_3} d_{G_3}(v_1, y) - \sum_{x \in A_2, y \in A_3} d_{G_2}(v_1, y) \right] \\
&= (|V(T_1)| - 1) \left[\sum_{x \in A_1} d_{G_3}(x, v_1) - \sum_{x \in A_2} d_{G_2}(x, v_1) \right] \\
&\quad + (m + a - 1) \sum_{y \in A_3} [d_{G_3}(v_1, y) - d_{G_2}(v_1, y)] \\
&= (|V(T_1)| - 1) [D_{U_{m+a, m-2}}(v_1) - D_{U_{m+a, m}}(v_1)].
\end{aligned}$$

Let $n = a + m + |V(T_1)| - 1$. Using Eqs. (1) and (2),

$$\begin{aligned}
& W(G_3) - W(G_2) \\
&= \left[W(U_{m+a, m-2}) + W(T_1) + \sum_{x \in A_1, y \in A_3} d_{G_3}(x, y) \right] \\
&\quad - \left[W(U_{m+a, m}) + W(T_1) + \sum_{x \in A_2, y \in A_3} d_{G_2}(x, y) \right] \\
&= [W(U_{m+a, m-2}) - W(U_{m+a, m})] + (|V(T_1)| - 1) [D_{U_{m+a, m-2}}(v_1) - D_{U_{m+a, m}}(v_1)] \\
&= \frac{m^2}{2} + \left(a - 2 \left\lfloor \frac{m}{2} \right\rfloor - n + \frac{1}{2} \right) m + \left\lfloor \frac{m^2}{4} \right\rfloor + 2 \left\lfloor \frac{m}{2} \right\rfloor (n - a) + (a + 2)(n - a - 2).
\end{aligned}$$

Note that $V_1(G_3) = (V_1(G_3) \cap V(T_1)) \cup \{v_{\lfloor \frac{m}{2} \rfloor}, v_{\lfloor \frac{m}{2} \rfloor}^*\}$. Then

$$\begin{aligned}
& D'(G(a + 2, m - 2)) - D'(G(a, m)) \\
&= 4[W(G_3) - W(G_2)] + (3 - 2) \left[D_{G_3} \left(v_{\lfloor \frac{m}{2} \rfloor} \right) - D_{G_2} \left(v_{\lfloor \frac{m}{2} \rfloor + 1} \right) \right] \\
&\quad + (1 - 2) \left[D_{G_3} \left(v_{\lfloor \frac{m}{2} \rfloor}^* \right) - D_{G_2} \left(v_{\lfloor \frac{m}{2} \rfloor + 1}^* \right) \right] \\
&= 4[W(G_3) - W(G_2)] + \left[D_{G_3} \left(v_{\lfloor \frac{m}{2} \rfloor} \right) - D_{G_3} \left(v_{\lfloor \frac{m}{2} \rfloor}^* \right) \right] \\
&\quad + \left[D_{G_2} \left(v_{\lfloor \frac{m}{2} \rfloor + 1}^* \right) - D_{G_2} \left(v_{\lfloor \frac{m}{2} \rfloor + 1} \right) \right] \\
&= 4[W(G_3) - W(G_2)] - (a + 2)(n - a - 3) + a(n - a - 1)
\end{aligned}$$

$$= \begin{cases} -m^2 + 2m - 4a^2 + 4(n-3)a + 6n - 10 & \text{if } m \text{ is even,} \\ -m^2 + 6m - 4a^2 + 4(n-2)a + 2n - 11 & \text{if } m \text{ is odd.} \end{cases}$$

If $a = 0$, then by similar calculation, the last expressions for $D'(G(a+2, m-2)) - D'(G(a, m))$ also hold.

Suppose that m is even. Let $f(m) = -m^2 + 2m - 4a^2 + 4(n-3)a + 6n - 10$. Then

$$\begin{aligned} f(6) &= (4a+6)n - 4a^2 - 12a - 34 \\ &\geq (4a+6)(a+6) - 4a^2 - 12a - 34 = 18a + 2 > 0. \end{aligned}$$

Let r_1 and r_2 be the two roots of $f(m) = 0$, where $r_1 \leq r_2$. It is easily seen that $r_1 < 6 < r_2$. Thus, when $6 \leq m \leq r_2$, $f(m) \geq 0$, and when $m > r_2$, $f(m) < 0$. Suppose that k is even. Then $m \leq k$. If $r_2 \geq k$, then $D'(G(k-4, 4))$ is maximum, while if $r_2 < k$, then $D'(G(k-4, 4))$ or $D'(G(0, k))$ is maximum. Let $G_4 = G(k-4, 4)$ and $G_5 = G(0, k)$. By similar calculation of $D'(G(a+2, m-2)) - D'(G(a, m))$, we have

$$\begin{aligned} &D'(G(k-4, 4)) - D'(G(0, k)) \\ &= 4[W(G_4) - W(G_5)] + [(3-2)D_{G_4}(v_3) + (1-2)D_{G_4}(v_3^*)] \\ &= 4 \left[-\frac{5}{24}k^3 + \left(\frac{n}{4} + \frac{3}{2}\right)k^2 - \left(\frac{3}{2}n + \frac{25}{6}\right)k + 2n + 6 \right] \\ &\quad - (k-4)(n-k+3) \\ &= n(k^2 - 7k + 12) - \frac{5}{6}k^3 + 7k^2 - \frac{71}{3}k + 36 \\ &\geq k(k^2 - 7k + 12) - \frac{5}{6}k^3 + 7k^2 - \frac{71}{3}k + 36 \\ &= \frac{k^3}{6} - \frac{35}{3}k + 36 > 0, \end{aligned}$$

and thus $D'(G(k-4, 4)) > D'(G(0, k))$. Suppose that k is odd. Then $m \leq k-1$. Similarly, we have $D'(G(k-4, 4))$ or $D'(G(1, k-1))$ is maximum. By similar calculation, $D'(G(k-4, 4)) > D'(G(1, k-1))$. Thus, whether k is even or odd, we have $D'(G(a, m)) < D'(G(k-4, 4))$ for $m > 4$.

If m is odd, then by similar arguments as above, $D'(G(a, m)) < D'(G(k-3, 3))$ for $m > 4$. The result follows easily. \square

Lemma 4. For any unicyclic graph H with $u \in V(H)$, let $H(a_1, a_2, \dots, a_t)$ be the graph obtained from H by attaching $t \geq 2$ paths $P_{a_1}, P_{a_2}, \dots, P_{a_t}$ to u , where $a_1 \geq a_2 \geq \dots \geq a_t \geq 1$. For fixed $k = a_1 + a_2 + \dots + a_t$, $D'(H(a_1, a_2, \dots, a_t)) \leq D'(H(k-t+1, 1, \dots, 1))$ with equality if and only if $a_1 = k-t+1$ and $a_i = 1$ for $i = 2, \dots, t$.

Proof. Suppose that $G = H(a_1, a_2, \dots, a_t)$ is a graph with the maximum degree distance satisfying the given condition. Suppose that there is some i such that $a_i \geq 2$ for $2 \leq i \leq t$ in G . For fixed a_s with $s \neq i-1, i$, and fixed unicyclic graph H , we

write $G = H(a_{i-1}, a_i)$. Denote by v_1 and v_2 the pendent vertices of the path $P_{a_{i-1}}$ and P_{a_i} , respectively, and v_3 the neighbor of v_2 in G . Let $G_1 = G - \{v_2v_3\} + \{v_1v_2\}$. Obviously $G_1 = H(a_{i-1} + 1, a_i - 1)$. Let $G_2 = G - \{v_2v_3\} + \{uv_2\}$ and $n = |V(G)|$. Then

$$\begin{aligned} W(G_1) - W(G) &= [D_{G_1}(v_2) - D_{G_2}(v_2)] + [D_{G_2}(v_2) - D_G(v_2)] \\ &= a_{i-1}(n - a_{i-1} - 2) - (a_i - 1)(n - a_i - 1) \\ &= (a_{i-1} - a_i + 1)(n - a_{i-1} - a_i - 1). \end{aligned}$$

Let Q be the (unicyclic) graph obtained from G by deleting the vertices of the paths $P_{a_{i-1}}$ and P_{a_i} . For $x \in V(Q)$, $D_{G_1}(x) - D_G(x) = D_{G_1}(u) - D_G(u)$, we have

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

It follows that

$$\begin{aligned} &D'(H(a_{i-1} + 1, a_i - 1)) - D'(G) \\ &= 4[W(G_1) - W(G)] + 2[D_{G_1}(u) - D_G(u)] \\ &\quad + (1 - 2)[D_{G_1}(v_2) - D_G(v_2)] + (1 - 2)D_{G_1}(v_3) - (1 - 2)D_G(v_1) \\ &= 4[W(G_1) - W(G)] + [D_{G_1}(u) - D_G(u)] + [D_{G_1}(u) - D_{G_1}(v_3)] \\ &\quad + [D_G(v_2) - D_G(u)] + [D_G(v_1) - D_G(u)] \\ &= 4[W(G_1) - W(G)] - (a_{i-1} + 1)(n - a_{i-1} - 2) - (a_i - 1)(n - a_i) \\ &\quad + a_i(n - a_i - 1) + a_{i-1}(n - a_{i-1} - 1) \\ &= 4(a_{i-1} - a_i + 1)(n - a_{i-1} - a_i - 1) + 2(a_{i-1} - a_i + 1) > 0, \end{aligned}$$

and thus $D'(H(a_{i-1} + 1, a_i - 1)) > D'(G)$, a contradiction. Hence $a_i = 1$ for $i = 2, \dots, t$, and the result follows. \square

For $a \geq 1$, $b \geq 0$ and $m = 3, 4$, let $U_{n,m}(a, b)$ be the graph obtained by attaching $n - a - b - m$ pendent vertices and a path P_a to $v_1 \in V(H)$, where $H = C_3(-, -, P_{b+1})$ for $m = 3$, $H = C_4(-, -, P_{b+1}, -)$ for $m = 4$, and v_3 is an end vertex of P_{b+1} .

Lemma 5. For $a \geq 1$, $b \geq 0$ and $m = 3, 4$, let $s = a + b \geq 2$ and $k = n - s - m$. Then for $m = 3$, or $m = 4$ and $k = 0, 1$,

$$D'(U_{n,m}(a, b)) \leq D'(U_{n,m}(s, 0))$$

with equality if and only if $U_{n,m}(a, b) = U_{n,m}(s, 0)$, and for $m = 4$ and $k \geq 2$,

$$D'(U_{n,m}(a, b)) \leq D'(U_{n,m}(1, s - 1))$$

with equality if and only if $U_{n,m}(a, b) = U_{n,m}(1, s - 1)$.

Proof. For $U_{n,m}(a,b)$, let u_1 be the pendent vertex of the path attached to v_1 , let u_2 be the pendent vertex of the path attached to v_3 if $b \geq 1$, and let u be a pendent vertex adjacent to v_1 if $k \geq 1$. Let $G_1 = U_{n,m}(a,b)$. For $a \geq 2$, let $G_2 = G_1 - \{u_1w\} + \{u_1u_2\}$, $G_3 = G_1 - \{u_1w\} + \{u_1v_1\}$ and $G_4 = G_1 - \{u_1w\} + \{u_1v_3\}$, where w is the neighbor of u_1 in G_1 . Obviously $G_2 = U_{n,m}(a-1, b+1)$. Then

$$\begin{aligned} & W(G_2) - W(G_1) \\ &= [D_{G_2}(u_1) - D_{G_4}(u_1)] + [D_{G_4}(u_1) - D_{G_3}(u_1)] + [D_{G_3}(u_1) - D_{G_1}(u_1)] \\ &= b(a+k+m-2) + \left\lfloor \frac{m}{2} \right\rfloor (k+a-1-b) - (a-1)(k+m-1+b) \\ &= (1-a+b) \left(k + \left\lfloor \frac{m-1}{2} \right\rfloor \right) + k \left\lfloor \frac{m}{2} \right\rfloor. \end{aligned}$$

Suppose that $a \geq 2$. Note that $D_{G_2}(u) - D_{G_1}(u) = D_{G_2}(v_1) - D_{G_1}(v_1)$. If $b \geq 1$, then

$$\begin{aligned} & D'(U_{n,m}(a-1, b+1)) - D'(U_{n,m}(a, b)) \\ &= 4[W(G_2) - W(G_1)] + (k+3-2)[D_{G_2}(v_1) - D_{G_1}(v_1)] \\ &\quad + k \cdot (1-2)[D_{G_2}(u) - D_{G_1}(u)] + (1-2)[D_{G_2}(u_1) - D_{G_1}(u_1)] \\ &\quad + (3-2)[D_{G_2}(v_3) - D_{G_1}(v_3)] + (1-2)D_{G_2}(w) - (1-2)D_{G_1}(u_2) \\ &= 4[W(G_2) - W(G_1)] + [D_{G_2}(v_1) - D_{G_2}(w)] + [D_{G_2}(v_3) - D_{G_2}(u_1)] \\ &\quad + [D_{G_1}(u_1) - D_{G_1}(v_1)] + [D_{G_1}(u_2) - D_{G_1}(v_3)] \\ &= 4[W(G_2) - W(G_1)] - (a-1)(n-a) - (b+1)(n-b-2) \\ &\quad + a(n-a-1) + b(n-b-1) \\ &= 4 \left[(1-a+b) \left(k + \left\lfloor \frac{m-1}{2} \right\rfloor + \frac{1}{2} \right) + k \left\lfloor \frac{m}{2} \right\rfloor \right] \\ &= \begin{cases} 4 \left[(1-a+b) \left(k + \frac{3}{2} \right) + k \right] & \text{if } m = 3, \\ 4 \left[(1-a+b) \left(k + \frac{3}{2} \right) + 2k \right] & \text{if } m = 4. \end{cases} \end{aligned}$$

If $b = 0$, then by similar calculation, the last expressions for $D'(U_{n,m}(a-1, b+1)) - D'(U_{n,m}(a, b))$ also hold.

Suppose that $m = 3$. Then $D'(U_{n,3}(a-1, b+1)) \geq D'(U_{n,3}(a, b))$ if and only if $a-b \leq \frac{4k+3}{2k+3}$, implying that $D'(U_{n,3}(s, 0))$ or $D'(U_{n,3}(1, s-1))$ is maximum. If $m = 4$, then similarly we have $D'(U_{n,4}(s, 0))$ or $D'(U_{n,4}(1, s-1))$ is maximum. Note that

$$\begin{aligned} & D'(U_{n,m}(1, s-1)) - D'(U_{n,m}(s, 0)) \\ &= \sum_{i=2}^s [D'(U_{n,m}(i-1, s-i+1)) - D'(U_{n,m}(i, s-i))] \\ &= \begin{cases} -6(s-1) & \text{if } m = 3, \\ 4(s-1) \left(k - \frac{3}{2} \right) & \text{if } m = 4. \end{cases} \end{aligned}$$

Then the result follows. \square

3 The maximum degree distance of unicyclic graphs of given maximum degree

Stevanović [14] determined the unique n -vertex tree of given maximum degree with the maximum Wiener index. By the relation between the Wiener index and the degree distance for trees [2], this tree is also the unique n -vertex tree of given maximum degree with the maximum degree distance. In this section, we determine the maximum degree distance of n -vertex unicyclic graphs of given maximum degree, and the corresponding graphs whose degree distances achieve this value.

A pendent path at a vertex v of a graph G is a path in G connecting vertex v and some pendent vertex such that all internal vertices (if exist) in this path have degree two and the degree of v is at least three.

Suppose that $\Delta \geq 3$. Let $U_{n,\Delta}^1 = U_{n,3}(n-\Delta, 0)$ if $\Delta \leq n-1$, $U_{n,\Delta}^2 = U_{n,4}(1, n-\Delta-2)$ if $\Delta \leq n-2$, and $U_{n,\Delta}^3$ the unicyclic graph obtained by joining a triangle and the center of S_Δ by a path of length $n-\Delta-2$ if $\Delta \leq n-3$.

Let $k = n - a - b - m$. It was shown in [22] that

$$\begin{aligned} & W(U_{n,m}(a, b)) \\ &= \left(a + b + \frac{m}{2}\right) \left\lfloor \frac{m^2}{4} \right\rfloor + \binom{a+1}{3} + \binom{b+1}{3} \\ &+ m \left[\binom{a+1}{2} + \binom{b+1}{2} \right] + \frac{1}{2} ab \left(2 \left\lfloor \frac{m}{2} \right\rfloor + a + b + 2 \right) \\ &+ k \left[\left\lfloor \frac{m^2}{4} \right\rfloor + m + \frac{1}{2} a(a+3) + \frac{1}{2} b \left(2 \left\lfloor \frac{m}{2} \right\rfloor + b + 3 \right) \right] + k(k-1), \end{aligned}$$

from which we have the expressions for $W(U_{n,\Delta}^1) = W(U_{n,3}(n-\Delta, 0))$, $W(U_{n,\Delta}^2) = W(U_{n,4}(1, n-\Delta-2))$ and $W(U_{n,\Delta}^3) = W(U_{n,\Delta+1}^1) + (\Delta-2)(n-\Delta-2)$.

In $U_{n,\Delta}^1$, note that v_1 is the vertex with degree Δ , let u be a pendent vertex adjacent to v_1 for $\Delta \geq 4$, and u_1 the pendent vertex of the path attached to v_1 . Then

$$\begin{aligned} D'(U_{n,\Delta}^1) &= 4W(U_{n,\Delta}^1) + (\Delta-2)D_{U_{n,\Delta}^1}(v_1) + (\Delta-3) \cdot (1-2)D_{U_{n,\Delta}^1}(u) \\ &+ (1-2)D_{U_{n,\Delta}^1}(u_1) \\ &= 4W(U_{n,\Delta}^1) + (\Delta-3) \left[D_{U_{n,\Delta}^1}(v_1) - D_{U_{n,\Delta}^1}(u) \right] \\ &+ \left[D_{U_{n,\Delta}^1}(v_1) - D_{U_{n,\Delta}^1}(u_1) \right] \\ &= 4W(U_{n,\Delta}^1) - (\Delta-3) \cdot (n-2) - (n-\Delta)(\Delta-1) \\ &= \frac{2}{3}n^3 - \left(2\Delta^2 - 4\Delta + \frac{2}{3} \right) n + \frac{4}{3}\Delta^3 - \Delta^2 - \frac{7}{3}\Delta - 6. \end{aligned}$$

By similar calculation, we have

$$D'(U_{n,\Delta}^2) = \frac{2}{3}n^3 - \left(2\Delta^2 - 4\Delta + \frac{35}{3} \right) n + \frac{4}{3}\Delta^3 - \Delta^2 + \frac{29}{3}\Delta + 10,$$

$$D'(U_{n,\Delta}^3) = \frac{2}{3}n^3 - \left(2\Delta^2 - 6\Delta + \frac{32}{3}\right)n + \frac{4}{3}\Delta^3 - 3\Delta^2 - \frac{1}{3}\Delta + 16.$$

Let $\mathbb{U}(n, \Delta)$ be the set of n -vertex unicyclic graphs with maximum degree Δ , where $2 \leq \Delta \leq n - 1$. Obviously, $\mathbb{U}(n, 2) = \{C_n\}$ and $\mathbb{U}(n, n - 1) = \{U_{n,n-1}^1\}$.

Theorem 1. *Among the graphs in $\mathbb{U}(n, \Delta)$ with $3 \leq \Delta \leq n - 2$,*

- (i) *if $\Delta = 3, 4, 5$, then $U_{n,\Delta}^1$ is the unique graph with the maximum degree distance,*
- (ii) *if $\Delta = n - 2$, then $U_{n,n-2}^1$ for $n = 5, 6, 7$, $U_{n,n-2}^1$ and $U_{n,n-2}^2$ for $n = 8$, and $U_{n,n-2}^2$ for $n \geq 9$ are the unique graphs with the maximum degree distance,*
- (iii) *if $6 \leq \Delta \leq n - 3$, then $U_{n,\Delta}^1$ for $9 \leq n \leq 14$, $U_{n,\Delta}^1$ with $\Delta < \frac{n+1-\sqrt{n^2-18n+45}}{2}$ or $\frac{n+1+\sqrt{n^2-18n+45}}{2} < \Delta < \frac{11n-16}{12}$, $U_{n,\Delta}^1$ and $U_{n,\Delta}^3$ with $\Delta = \frac{n+1+\sqrt{n^2-18n+45}}{2}$, $U_{n,\Delta}^3$ with $\frac{n+1-\sqrt{n^2-18n+45}}{2} < \Delta < \frac{n+1+\sqrt{n^2-18n+45}}{2}$, $U_{n,\Delta}^1$ and $U_{n,\Delta}^2$ with $\Delta = \frac{11n-16}{12}$, and $U_{n,\Delta}^2$ with $\Delta > \frac{11n-16}{12}$ for $15 \leq n \leq 36$, $U_{n,\Delta}^1$ with $\Delta < \frac{n+1-\sqrt{n^2-18n+45}}{2}$, $U_{n,\Delta}^1$ and $U_{n,\Delta}^3$ with $\Delta = \frac{n+1-\sqrt{n^2-18n+45}}{2}$, $U_{n,\Delta}^3$ with $\frac{n+1-\sqrt{n^2-18n+45}}{2} < \Delta < \frac{n-5+\sqrt{n^2-8n+37}}{2}$, $U_{n,\Delta}^2$ and $U_{n,\Delta}^3$ with $\Delta = \frac{n-5+\sqrt{n^2-8n+37}}{2}$, and $U_{n,\Delta}^2$ with $\Delta > \frac{n-5+\sqrt{n^2-8n+37}}{2}$ for $n \geq 37$ are the unique graphs with the maximum degree distance,*

and the expressions for $D'(U_{n,\Delta}^1)$, $D'(U_{n,\Delta}^2)$ and $D'(U_{n,\Delta}^3)$ are given by

$$\begin{aligned} D'(U_{n,\Delta}^1) &= \frac{2}{3}n^3 - \left(2\Delta^2 - 4\Delta + \frac{2}{3}\right)n + \frac{4}{3}\Delta^3 - \Delta^2 - \frac{7}{3}\Delta - 6, \\ D'(U_{n,\Delta}^2) &= \frac{2}{3}n^3 - \left(2\Delta^2 - 4\Delta + \frac{35}{3}\right)n + \frac{4}{3}\Delta^3 - \Delta^2 + \frac{29}{3}\Delta + 10, \\ D'(U_{n,\Delta}^3) &= \frac{2}{3}n^3 - \left(2\Delta^2 - 6\Delta + \frac{32}{3}\right)n + \frac{4}{3}\Delta^3 - 3\Delta^2 - \frac{1}{3}\Delta + 16. \end{aligned}$$

Proof. Let G be a graph with the maximum degree distance in $\mathbb{U}(n, \Delta)$. Let C be the unique cycle, and v a vertex of degree Δ in G . Since $\Delta \geq 3$, we have $G \neq C_n$.

Case 1. v lies on C .

By Lemma 1, the vertices outside C are of degree one or two, and the vertices on C different from v are of degree two or three. By Lemma 2, there is at most one vertex on C different from v with degree three. Thus, G is a graph obtained by attaching $\Delta - 2$ paths to v and attaching at most one path to a vertex on C different from v . By Lemmas 3 and 4, we know that the cycle length of C is three or four, and among the pendent paths at v in G , there is at most one path with length at least two. If the cycle length of C is three, then by Lemma 5, we have $G = U_{n,\Delta}^1$. If the cycle length of C is four, then by Lemma 5, we have $G = U_{n,4}(n - \Delta - 1, 0)$ with $\Delta = 3, 4$, and $G = U_{n,\Delta}^2$ with $\Delta \geq 5$. Note that

$$D'(U_{n,\Delta}^1) - D'(U_{n,4}(n - \Delta - 1, 0)) = \begin{cases} 5n - 22 > 0 & \text{if } \Delta = 3, \\ 9n - 52 > 0 & \text{if } \Delta = 4. \end{cases}$$

Thus, $G = U_{n,\Delta}^1$ if $\Delta = 3, 4$, and $G = U_{n,\Delta}^1$ or $U_{n,\Delta}^2$ if $\Delta \geq 5$.

Case 2. v lies outside C .

In this case $\Delta \leq n - 3$. Suppose that u is the vertex on C that is nearest to v . By Lemma 1, the vertices outside C different from v are of degree one or two, and the vertices on C are of degree two or three. By Lemma 2, there is at most one vertex on C different from u with degree three. By Lemma 4, among the pendent paths at v in G , there is at most one path with length at least two.

Denote by G^* the graph obtained from G by deleting the vertices of the subtree attached to u . Suppose that $G^* \neq C_3$. By Lemma 3, G^* is either $U_{k,3}$, or $U_{k,4}$ for which the two vertices on C_4 of degree three are non-adjacent, where $4 \leq k \leq n - \Delta$. We write $G = G(k, 3)$ if $G^* = U_{k,3}$, and $G = G(k, 4)$ if $G^* = U_{k,4}$. Denote by u_1 the vertex on C_3 with degree three different from u , u_2 the pendent vertex of the path attached to u_1 , and u_3 the neighbor of u outside C_3 in $G(k, 3)$. Let $G_1 = G(k, 3) - \{uu_3\} + \{u_2u_3\} \in \mathbb{U}(n, \Delta)$. We will show that $D'(G_1) > D'(G)$, i.e., $D'(G_1) > D'(G(k, 3))$ and $D'(G_1) > D'(G(k, 4))$.

First suppose that $G = G(k, 3)$. Let Q be the subtree attached to u . For $x \in V(Q)$, we have $D_{G_1}(x) - D_G(x) = D_{G_1}(u_3) - D_G(u_3)$, and thus

$$\begin{aligned} & \sum_{x \in V_1(G_1) \cap V(Q)} (d_{G_1}(x) - 2)D_{G_1}(x) - \sum_{x \in V_1(G) \cap V(Q)} (d_G(x) - 2)D_G(x) \\ &= [D_{G_1}(u_3) - D_G(u_3)] \left[\sum_{x \in V(Q)} (d_Q(x) - 2) + 1 \right] = -[D_{G_1}(u_3) - D_G(u_3)]. \end{aligned}$$

Let $G_2 = G(k, 3) - \{uu_3\} + \{u_1u_3\}$. Note that

$$\begin{aligned} W(G_1) - W(G) &= [W(G_1) - W(G_2)] + [W(G_2) - W(G)] \\ &= 2(k-3)(n-k) - (k-3)(n-k) = (k-3)(n-k). \end{aligned}$$

Then

$$\begin{aligned} & D'(G_1) - D'(G) \\ &= 4[W(G_1) - W(G)] - [D_{G_1}(u_3) - D_G(u_3)] + (3-2)[D_{G_1}(u_1) - D_G(u_1)] \\ &\quad - (1-2)D_G(u_2) - (3-2)D_G(u) \\ &= 4[W(G_1) - W(G)] + [D_{G_1}(u_1) - D_{G_1}(u_3)] + [D_G(u_3) - D_G(u)] \\ &\quad + [D_G(u_2) - D_G(u_1)] \\ &= 4(k-3)(n-k) + (k-2)(n-k-3) + (2k-n) + (k-3)(n-k+2) \\ &= 6(k-3)(n-k) > 0, \end{aligned}$$

and thus $D'(G_1) > D'(G(k, 3))$.

Now we consider $G = G(k, 4)$. Using Eqs. (1) and (2), and by similar calculation of $D'(G(a+2, m-2)) - D'(G(a, m))$ as in the proof of Lemma 3, we have

$$D'(G(k, 3)) - D'(G(k, 4)) = 6k - n - 22,$$

and thus

$$\begin{aligned} D'(G_1) - D'(G(k, 4)) &= [D'(G_1) - D'(G(k, 3))] + [D'(G(k, 3)) - D'(G(k, 4))] \\ &= 6(k-3)(n-k) + 6k - n - 22. \end{aligned}$$

If $k = 4$ or $n \leq 6k - 22$, then $D'(G_1) > D'(G(k, 4))$, and if $k \geq 5$ and $n > 6k - 22$, then

$$\begin{aligned} D'(G_1) - D'(G(k, 4)) &= [6(k-3) - 1]n - 6k(k-4) - 22 \\ &> [6(k-3) - 1](6k-22) - 6k(k-4) - 22 \\ &= 6(k-3)(5k-22) > 0, \end{aligned}$$

and thus $D'(G_1) > D'(G(k, 4))$.

It follows that $D'(G_1) > D'(G)$, a contradiction. Thus $G^* = C_3$.

Suppose that $G \neq U_{n,\Delta}^3$. Denote by w the pendent vertex of the longest pendent path at v , and w_1 the neighbor of w . Then $d_G(v, w) \geq 2$. Let $t = d_G(v, w_1) \geq 1$. Note that $n - \Delta - t \geq 3$. Denote by $x_1, x_2, \dots, x_{\Delta-2}$ the pendent neighbors of v . Consider $G_3 = G - \{vx_1, \dots, vx_{\Delta-2}\} + \{w_1x_1, \dots, w_1x_{\Delta-2}\} \in \mathbb{U}(n, \Delta)$. Note that

$$\begin{aligned} D_{G_3}(w_1) - D_G(v) &= [D_{G_3}(w_1) - D_G(w_1)] + [D_G(w_1) - D_G(v)] \\ &= -t(\Delta-2) + t(n-t-3) = t(n-\Delta-t-1). \end{aligned}$$

Then

$$\begin{aligned} &D'(G_3) - D'(G) \\ &= 4[W(G_3) - W(G)] + (3-2)[D_{G_3}(u) - D_G(u)] + (1-2)[D_{G_3}(w) - D_G(w)] \\ &\quad + (\Delta-2) \cdot (1-2)[D_{G_3}(x_1) - D_G(x_1)] + (\Delta-2)[D_{G_3}(w_1) - D_G(v)] \\ &= 4 \cdot t(\Delta-2)(n-\Delta-t-1) + t(\Delta-2) + t(\Delta-2) \\ &\quad - (\Delta-2) \cdot t(n-\Delta-t-1) + (\Delta-2) \cdot t(n-\Delta-t-1) \\ &= 2t(\Delta-2)[2(n-\Delta-t-1) + 1] > 0, \end{aligned}$$

and thus $D'(G_3) > D'(G)$, a contradiction. It follows that $G = U_{n,\Delta}^3$ with $\Delta \leq n-3$.

Combining Cases 1 and 2, we have $G = U_{n,\Delta}^1$ or $U_{n,\Delta}^3$ if $\Delta = 3, 4$, $G = U_{n,\Delta}^1$ or $U_{n,\Delta}^2$ if $\Delta = n-2$, and $G = U_{n,\Delta}^1, U_{n,\Delta}^2$, or $U_{n,\Delta}^3$ if $5 \leq \Delta \leq n-3$. Note that

$$D'(U_{n,\Delta}^2) - D'(U_{n,\Delta}^1) = 12 \left(\Delta - \frac{11n-16}{12} \right),$$

$$\begin{aligned} D'(U_{n,\Delta}^2) - D'(U_{n,\Delta}^3) &= 2 \left[\Delta^2 - (n-5)\Delta - \frac{n}{2} - 3 \right] \\ &= 2 \left(\Delta - \frac{n-5-\sqrt{n^2-8n+37}}{2} \right) \\ &\quad \cdot \left(\Delta - \frac{n-5+\sqrt{n^2-8n+37}}{2} \right), \end{aligned}$$

$$D'(U_{n,\Delta}^1) - D'(U_{n,\Delta}^3) = 2[\Delta^2 - (n+1)\Delta + 5n - 11].$$

Now the results for $\Delta = 3, 4, 5, n-2$ follow by direct calculation, proving (i) and (ii). Suppose that $6 \leq \Delta \leq n-3$. For $9 \leq n \leq 14$, we have $D'(U_{n,\Delta}^1) > D'(U_{n,\Delta}^3)$ because the discriminant of the quadratic equation $\Delta^2 - (n+1)\Delta + 5n - 11 = 0$ on Δ is $n^2 - 18n + 45 < 0$, and for $n \geq 15$, we have

$$\begin{aligned} D'(U_{n,\Delta}^1) - D'(U_{n,\Delta}^3) &= 2 \left(\Delta - \frac{n+1 - \sqrt{n^2 - 18n + 45}}{2} \right) \\ &\quad \cdot \left(\Delta - \frac{n+1 + \sqrt{n^2 - 18n + 45}}{2} \right). \end{aligned}$$

If $9 \leq n \leq 14$, then $D'(U_{n,\Delta}^1) > D'(U_{n,\Delta}^3)$,

$$\begin{aligned} D'(U_{n,\Delta}^2) - D'(U_{n,\Delta}^1) &= 12 \left(\Delta - \frac{11n-16}{12} \right) \\ &\leq 12 \left(n-3 - \frac{11n-16}{12} \right) = n-20 < 0, \end{aligned}$$

and thus $D'(U_{n,\Delta}^1) > \max \{D'(U_{n,\Delta}^2), D'(U_{n,\Delta}^3)\}$. If $15 \leq n \leq 36$, then

$$\begin{aligned} &\frac{n-5 - \sqrt{n^2 - 8n + 37}}{2} < \frac{n+1 - \sqrt{n^2 - 18n + 45}}{2} \\ < \frac{n+1 + \sqrt{n^2 - 18n + 45}}{2} < \frac{n-5 + \sqrt{n^2 - 8n + 37}}{2} < \frac{11n-16}{12}, \end{aligned}$$

and thus

$$\begin{aligned} D'(U_{n,\Delta}^1) &> D'(U_{n,\Delta}^2) > D'(U_{n,\Delta}^3) && \text{if } \Delta < \frac{n-5 - \sqrt{n^2 - 8n + 37}}{2}, \\ D'(U_{n,\Delta}^1) &> D'(U_{n,\Delta}^2) = D'(U_{n,\Delta}^3) && \text{if } \Delta = \frac{n-5 - \sqrt{n^2 - 8n + 37}}{2}, \\ D'(U_{n,\Delta}^1) &> D'(U_{n,\Delta}^3) > D'(U_{n,\Delta}^2) && \text{if } \frac{n-5 - \sqrt{n^2 - 8n + 37}}{2} < \Delta < \frac{n+1 - \sqrt{n^2 - 18n + 45}}{2}, \\ D'(U_{n,\Delta}^1) &= D'(U_{n,\Delta}^3) > D'(U_{n,\Delta}^2) && \text{if } \Delta = \frac{n+1 - \sqrt{n^2 - 18n + 45}}{2}, \\ D'(U_{n,\Delta}^3) &> D'(U_{n,\Delta}^1) > D'(U_{n,\Delta}^2) && \text{if } \frac{n+1 - \sqrt{n^2 - 18n + 45}}{2} < \Delta < \frac{n+1 + \sqrt{n^2 - 18n + 45}}{2}, \\ D'(U_{n,\Delta}^1) &= D'(U_{n,\Delta}^3) > D'(U_{n,\Delta}^2) && \text{if } \Delta = \frac{n+1 + \sqrt{n^2 - 18n + 45}}{2}, \\ D'(U_{n,\Delta}^1) &> D'(U_{n,\Delta}^3) > D'(U_{n,\Delta}^2) && \text{if } \frac{n+1 + \sqrt{n^2 - 18n + 45}}{2} < \Delta < \frac{n-5 + \sqrt{n^2 - 8n + 37}}{2}, \\ D'(U_{n,\Delta}^1) &> D'(U_{n,\Delta}^2) = D'(U_{n,\Delta}^3) && \text{if } \Delta = \frac{n-5 + \sqrt{n^2 - 8n + 37}}{2}, \\ D'(U_{n,\Delta}^1) &> D'(U_{n,\Delta}^2) > D'(U_{n,\Delta}^3) && \text{if } \frac{n-5 + \sqrt{n^2 - 8n + 37}}{2} < \Delta < \frac{11n-16}{12}, \\ D'(U_{n,\Delta}^1) &= D'(U_{n,\Delta}^2) > D'(U_{n,\Delta}^3) && \text{if } \Delta = \frac{11n-16}{12}, \\ D'(U_{n,\Delta}^2) &> D'(U_{n,\Delta}^1) > D'(U_{n,\Delta}^3) && \text{if } \Delta > \frac{11n-16}{12}. \end{aligned}$$

If $n \geq 37$, then

$$\begin{aligned} & \frac{n-5-\sqrt{n^2-8n+37}}{2} < \frac{n+1-\sqrt{n^2-18n+45}}{2} \\ < \frac{11n-16}{12} < \frac{n-5+\sqrt{n^2-8n+37}}{2} < \frac{n+1+\sqrt{n^2-18n+45}}{2}, \end{aligned}$$

and thus

$$\begin{aligned} D'(U_{n,\Delta}^1) &> D'(U_{n,\Delta}^2) > D'(U_{n,\Delta}^3) && \text{if } \Delta < \frac{n-5-\sqrt{n^2-8n+37}}{2}, \\ D'(U_{n,\Delta}^1) &> D'(U_{n,\Delta}^2) = D'(U_{n,\Delta}^3) && \text{if } \Delta = \frac{n-5-\sqrt{n^2-8n+37}}{2}, \\ D'(U_{n,\Delta}^1) &> D'(U_{n,\Delta}^3) > D'(U_{n,\Delta}^2) && \text{if } \frac{n-5-\sqrt{n^2-8n+37}}{2} < \Delta < \frac{n+1-\sqrt{n^2-18n+45}}{2}, \\ D'(U_{n,\Delta}^1) &= D'(U_{n,\Delta}^3) > D'(U_{n,\Delta}^2) && \text{if } \Delta = \frac{n+1-\sqrt{n^2-18n+45}}{2}, \\ D'(U_{n,\Delta}^3) &> D'(U_{n,\Delta}^1) > D'(U_{n,\Delta}^2) && \text{if } \frac{n+1-\sqrt{n^2-18n+45}}{2} < \Delta < \frac{11n-16}{12}, \\ D'(U_{n,\Delta}^3) &> D'(U_{n,\Delta}^1) = D'(U_{n,\Delta}^2) && \text{if } \Delta = \frac{11n-16}{12}, \\ D'(U_{n,\Delta}^3) &> D'(U_{n,\Delta}^2) > D'(U_{n,\Delta}^1) && \text{if } \frac{11n-16}{12} < \Delta < \frac{n-5+\sqrt{n^2-8n+37}}{2}, \\ D'(U_{n,\Delta}^2) &= D'(U_{n,\Delta}^3) > D'(U_{n,\Delta}^1) && \text{if } \Delta = \frac{n-5+\sqrt{n^2-8n+37}}{2}, \\ D'(U_{n,\Delta}^2) &> D'(U_{n,\Delta}^1) > D'(U_{n,\Delta}^3) && \text{if } \frac{n-5+\sqrt{n^2-8n+37}}{2} < \Delta < \frac{n+1+\sqrt{n^2-18n+45}}{2}, \\ D'(U_{n,\Delta}^2) &> D'(U_{n,\Delta}^1) = D'(U_{n,\Delta}^3) && \text{if } \Delta = \frac{n+1+\sqrt{n^2-18n+45}}{2}, \\ D'(U_{n,\Delta}^2) &> D'(U_{n,\Delta}^1) > D'(U_{n,\Delta}^3) && \text{if } \Delta > \frac{n+1+\sqrt{n^2-18n+45}}{2}. \end{aligned}$$

Now (iii) follows. \square

4 The first seven maximum degree distances of unicyclic graphs

In this section, we consider the first seven maximum degree distances of n -vertex unicyclic graphs and characterize the graphs whose degree distances achieve these values. First we give some lemmas.

Let T_n^s be the tree obtained from the path $P_{n-1} = u_0u_1 \dots u_{n-2}$ by attaching a pendent vertex to u_s , where $1 \leq s \leq n-2$.

In the following, if the symbol $G = C_m(T_1, T_2, \dots, T_m)$ is used, then we require $d_G(v_i) = 3$ when $T_i = P_r$ with $r \geq 2$, and $v_i = u_{r-2}$ when $T_i = T_r^s$ with $r \geq 3$.

Lemma 6. *For fixed trees T_2, \dots, T_m , let $G(T) = C_m(T, T_2, \dots, T_m)$ with $|V(T)| = k \geq 1$, and $H = C_m(-, T_2, \dots, T_m)$. If $k \geq 4$, then $G(P_k)$, $G(T_k^1)$ and $G(T_k^2)$ are respectively the unique graphs with the first, the second and the third maximum degree distances, and if $k \geq 5$, then $G(T_k^{k-2})$ is the unique graph with the fourth maximum degree distance for $|V(H)| = 3$, while $G(T_k^3)$ is the unique graph with the fourth maximum degree distance for $|V(H)| \geq 4$.*

Proof. Let $G = G(T)$. If $T \neq P_k$, then by Lemma 1, we have $D'(G) < D'(G(P_k))$. Thus, $G(P_k)$ is the unique graph with the maximum degree distance. Suppose that $T \neq P_k$. Then either $d_G(v_1) \geq 4$, or $d_G(v_1) = 3$ and some vertex in T different from v_1 has degree at least three. If $d_G(v_1) \geq 4$, then by Lemmas 1 and 4, $D'(G) \leq D'(G(T_k^{k-2}))$ with equality if and only if $G = G(T_k^{k-2})$.

Suppose that $d_G(v_1) = 3$ and some vertex in T different from v_1 has degree at least three. Let t be the maximum degree of T , and x a maximum degree vertex. Then $t \geq 3$ and $x \neq v_1$.

Suppose first that $t \geq 4$, or $t = 3$ and there are at least two vertices of T with degree three. Let G_0 be a graph with the maximum degree distance. If $t \geq 5$, then by Lemma 1, we may get a graph with $t = 4$ with larger degree distance, a contradiction. Thus, $t = 3, 4$. If $t = 3$, then by Lemmas 1 and 4, $D'(G_0) < D'(G(T_k^{i_1}))$ for some i_1 with $3 \leq i_1 \leq k - 3$. Suppose that $t = 4$. By Lemma 1, all vertices of T different from x are of degree one or two. If there is a pendent path at x of length at least two, then by Lemmas 1 and 4, we have $D'(G_0) < D'(G(T_k^{i_2}))$ for some i_2 with $3 \leq i_2 \leq k - 3$. Suppose that all the three pendent paths at x are of length one in G_0 . Denote by x_1, x_2 and x_3 the pendent neighbors of x in G_0 . Let $G_1 = G_0 - \{xx_1\} + \{x_1x_2\}$. Obviously $G_1 = G(T_k^2)$. For $x \in V(H)$, $D_{G_1}(x) - D_{G_0}(x) = D_{G_1}(v_1) - D_{G_0}(v_1)$, and thus

$$\begin{aligned} & \sum_{x \in V_1(G_1) \cap V(H)} (d_{G_1}(x) - 2)D_{G_1}(x) - \sum_{x \in V_1(G_0) \cap V(H)} (d_{G_0}(x) - 2)D_{G_0}(x) \\ &= [D_{G_1}(v_1) - D_{G_0}(v_1)] \left[\sum_{x \in V(H)} (d_H(x) - 2) + 1 \right] = D_{G_1}(v_1) - D_{G_0}(v_1). \end{aligned}$$

Note that $V_1(G_0) = (V_1(G_0) \cap V(H)) \cup \{x, x_1, x_2, x_3\}$, $V_1(G_1) = (V_1(G_1) \cap V(H)) \cup \{x, x_1, x_3\}$, and thus

$$\begin{aligned} & D'(G(T_k^2)) - D'(G_0) \\ &= 4[W(G_1) - W(G_0)] + [D_{G_1}(v_1) - D_{G_0}(v_1)] + (1 - 2)[D_{G_1}(x_1) - D_{G_0}(x_1)] \\ & \quad + (1 - 2)[D_{G_1}(x_3) - D_{G_0}(x_3)] + (3 - 2)D_{G_1}(x) \\ & \quad - (4 - 2)D_{G_0}(x) - (1 - 2)D_{G_0}(x_2) \\ &= 4[W(G_1) - W(G_0)] + [D_{G_1}(v_1) - D_{G_0}(v_1)] - [D_{G_1}(x_1) - D_{G_0}(x_1)] \\ & \quad - [D_{G_1}(x_3) - D_{G_0}(x_3)] + [D_{G_1}(x) - D_{G_0}(x)] + [D_{G_0}(x_2) - D_{G_0}(x)] \\ &= 4(n - 3) + 1 - (n - 3) - 1 + 1 + (n - 2) = 4n - 10. \end{aligned}$$

On the other hand, by similar calculation of $D'(G_3) - D'(G)$ as in the proof of Theorem 1, we have $D'(G(T_k^3)) - D'(G(T_k^2)) = -4n + 26$. Then

$$D'(G(T_k^3)) - D'(G_0) = [D'(G(T_k^3)) - D'(G(T_k^2))] + [D'(G(T_k^2)) - D'(G_0)] = 16 > 0,$$

and thus $D'(G(T_k^3)) > D'(G_0) \geq D'(G)$.

Next suppose that $t = 3$ and there is exactly one vertex, say y , with maximum degree three in T . Denote by a and b the lengths of the two pendent paths at y ,

where $a \geq b$. If $b \geq 2$, then by Lemma 4, $D'(G) < D'(G(T_k^{i_3}))$ for some i_3 with $3 \leq i_3 \leq k-3$. If $b = 1$, then $G = G(T_k^{i_4})$ for some i_4 with $1 \leq i_4 \leq k-3$.

Now we have shown that $D'(G) < \max\{D'(G(T_k^i)) : 3 \leq i \leq k-2\}$ or $G = G(T_k^i)$ with $1 \leq i \leq k-2$.

Let $n = |V(H)| + k - 1$. By similar calculation of $D'(G_3) - D'(G)$ as in the proof of Theorem 1, $D'(G(T_k^1)) - D'(G(T_k^2)) = 4n - 18 > 0$, and for $3 \leq i \leq k-2$,

$$\begin{aligned} D'(G(T_k^2)) - D'(G(T_k^i)) &= 4(i-2)n - 4i^2 - 6i + 28 \\ &\geq 4(i-2)(i+4) - 4i^2 - 6i + 28 = 2(i-2) > 0. \end{aligned}$$

Thus

$$\max\{D'(G(T_k^i)) : 3 \leq i \leq k-2\} < D'(G(T_k^2)) < D'(G(T_k^1)),$$

implying that $G(T_k^1)$ and $G(T_k^2)$ are respectively the unique graphs with the second and the third maximum degree distances, and the fourth maximum degree distance is only possibly achieved by $G(T_k^i)$ with $3 \leq i \leq k-2$. Note that $D'(G(T_k^2)) - D'(G(T_k^3)) = 4n - 26$. For $3 < i \leq k-3$,

$$\begin{aligned} D'(G(T_k^3)) - D'(G(T_k^i)) &= [D'(G(T_k^2)) - D'(G(T_k^i))] \\ &\quad - [D'(G(T_k^2)) - D'(G(T_k^3))] \\ &= 4(i-3)n - 4i^2 - 6i + 54 \\ &\geq 4(i-3)(i+5) - 4i^2 - 6i + 54 = 2(i-3) > 0, \end{aligned}$$

and thus $D'(G(T_k^3)) > D'(G(T_k^i))$. On the other hand, it is easily seen that

$$D'(G(T_k^3)) - D'(G(T_k^{k-2})) = 2(k-5)(2|V(H)| - 7),$$

which is negative if $|V(H)| = 3$ and positive if $|V(H)| \geq 4$. The result follows. \square

Let $C_3(T) = C_3(T, -, -)$, $C_3(T_1, T_2) = C_3(T_1, T_2, -)$, $C_4(T) = C_4(T, -, -, -)$, $C_4^1(T_1, T_2) = C_4(T_1, -, T_2, -)$ and $C_4^2(T_1, T_2) = C_4(T_1, T_2, -, -)$.

Let $\mathbb{U}_1(n)$ be the set of n -vertex unicyclic graphs of the form $C_3(T)$, and $\mathbb{U}_2(n)$ the set of n -vertex unicyclic graphs of the form $C_3(T_1, T_2, T_3)$, where at least two of T_1, T_2, T_3 are not P_1 .

Lemma 7. *Among the graphs in $\mathbb{U}_1(n)$,*

- (a) $C_3(P_{n-2})$, $C_3(T_{n-2}^1)$, $C_3(T_{n-2}^2)$ for $n \geq 6$, and $C_3(T_{n-2}^{n-4})$ for $n \geq 7$ are respectively the unique graphs with the first, the second, the third, and the fourth maximum degree distances, which are equal to $\frac{2}{3}n^3 - \frac{20}{3}n + 14$, $\frac{2}{3}n^3 - \frac{32}{3}n + 24$, $\frac{2}{3}n^3 - \frac{44}{3}n + 42$, and $\frac{2}{3}n^3 - \frac{50}{3}n + 54$, respectively;
- (b) $C_3(T_{n-2}^3)$ for $n = 8, 12$ is the unique graph with the fifth maximum degree distance, which is equal to $\frac{2}{3}n^3 - \frac{56}{3}n + 68$.

Proof. (a) follows from Lemma 6. We consider (b). Suppose that $n = 8, 12$. Let Q_n be the graph obtained by attaching two paths P_2 and P_{n-5} to a vertex of a triangle. Let G be a graph in $\mathbb{U}_1(n)$ different from the graphs with the first four maximum

degree distances. Note that $d_G(v_1) \geq 3$, and $d_G(v_2), d_G(v_3) = 2$. If $d_G(v_1) = 3$, then by the arguments in the proof of Lemma 6, $D'(G) \leq D'(C_3(T_{n-2}^3))$ with equality if and only if $G = C_3(T_{n-2}^3)$. If $d_G(v_1) \geq 4$, then by Lemma 1 and the inequality $D'(H(a_{i-1} + 1, a_i - 1)) > D'(G)$ in the proof of Lemma 4, $D'(G) \leq D'(Q_n)$. Note that $D'(C_3(T_{n-2}^3)) - D'(Q_n) = 8n - 46 > 0$. Then (b) follows. \square

Lemma 8. *Among the graphs in $\mathbb{U}_2(n)$,*

- (a) $C_3(P_{n-3}, P_2)$ for $n \geq 6$ is the unique graph with the maximum degree distance, which is equal to $\frac{2}{3}n^3 - \frac{38}{3}n + 38$;
- (b) $C_3(P_2, P_2, P_2)$ for $n = 6$ is the unique graph with the second maximum degree distance, which is equal to 96, $C_3(P_{n-4}, P_3)$ for $7 \leq n \leq 12$ is the unique graph with the second maximum degree distance, which is equal to $\frac{2}{3}n^3 - \frac{56}{3}n + 74$, $C_3(P_{n-4}, P_3)$ and $C_3(T_{n-3}^1, P_2)$ for $n = 13$ are the unique graphs with the second maximum degree distance, which is equal to $\frac{2}{3}n^3 - \frac{56}{3}n + 74 = \frac{2}{3}n^3 - \frac{50}{3}n + 48$, and $C_3(T_{n-3}^1, P_2)$ for $n \geq 14$ is the unique graph with the second maximum degree distance, which is equal to $\frac{2}{3}n^3 - \frac{50}{3}n + 48$;
- (c) $C_3(T_{n-3}^1, P_2)$ for $n = 7, 8$ is the unique graph with the third maximum degree distance, which is equal to $\frac{2}{3}n^3 - \frac{50}{3}n + 48$.

Proof. Let $G = C_3(T_1, T_2, T_3) \in \mathbb{U}_2(n)$ with $|V(T_1)| \geq |V(T_2)| \geq |V(T_3)|$. If $n = 6$, then $G = C_3(P_2, P_2, P_2)$, $C_3(P_3, P_2)$, or $C_3(T_3^1, P_2)$, and thus the result for $n = 6$ follows by direct calculation. In the following suppose that $n \geq 7$.

If $|V(T_3)| \geq 2$, then by Lemmas 1, 2 and using the equation on $D'(U_{n,m}(a-1, b+1)) - D'(U_{n,m}(a, b))$ in the proof of Lemma 5 with $k = 0$, $D'(G) < D'(C_3(P_{n-4}, P_3))$.

Suppose that $|V(T_3)| = 1$. If $|V(T_2)| = 2$ and $G \neq C_3(P_{n-3}, P_2)$, then by Lemma 6,

$$D'(G) \leq D'(C_3(T_{n-3}^1, P_2)) < D'(C_3(P_{n-3}, P_2))$$

with equality if and only if $G = C_3(T_{n-3}^1, P_2)$. If $|V(T_2)| \geq 3$, then by Lemma 1 and using the equation on $D'(U_{n,m}(a-1, b+1)) - D'(U_{n,m}(a, b))$ in the proof of Lemma 5 with $k = 0$, $D'(G) \leq D'(C_3(P_{n-4}, P_3))$ with equality if and only if $G = C_3(P_{n-4}, P_3)$.

Using the equation on $D'(U_{n,m}(a-1, b+1)) - D'(U_{n,m}(a, b))$ in the proof of Lemma 5 with $k = 0$, we have $D'(C_3(P_{n-4}, P_3)) < D'(C_3(P_{n-3}, P_2))$. Thus, $C_3(P_{n-3}, P_2)$ is the unique graph with the maximum degree distance, and (a) follows.

Note that the second maximum degree distance is only possibly achieved by $C_3(T_{n-3}^1, P_2)$ or $C_3(P_{n-4}, P_3)$. It is easily seen that

$$D'(C_3(T_{n-3}^1, P_2)) - D'(C_3(P_{n-4}, P_3)) = 2(n - 13).$$

Then (b) follows easily.

Now we consider (c). Suppose that $n = 7, 8$. Let $G \neq C_3(P_{n-3}, P_2), C_3(P_{n-4}, P_3)$. By Lemmas 1 and 6, for $n = 7$,

$$D'(G) \leq \max\{D'(C_3(P_3, P_2, P_2)), D'(C_3(T_3^1, P_3)), D'(C_3(T_4^1, P_2))\}$$

$$= D'(C_3(T_4^1, P_2)) = 160$$

with equality if and only if $G = C_3(T_4^1, P_2)$, and for $n = 8$,

$$\begin{aligned} D'(G) &\leq \max\{D'(C_3(P_3, P_3, P_2)), D'(C_3(P_4, P_2, P_2)), D'(C_3(T_3^1, P_4)), \\ &\quad D'(C_3(T_4^1, P_3)), D'(C_3(T_5^1, P_2))\} \\ &= D'(C_3(T_5^1, P_2)) = 256 \end{aligned}$$

with equality if and only if $G = C_3(T_5^1, P_2)$. Then (c) follows. \square

Let $\mathbb{U}_3(n)$ be the set of n -vertex unicyclic graphs of the form $C_4(T)$, and $\mathbb{U}_4(n)$ the set of n -vertex unicyclic graphs of the form $C_4(T_1, T_2, T_3, T_4)$, where at least two of T_1, T_2, T_3, T_4 are not P_1 . By Lemma 6, we have Lemma 9 directly.

Lemma 9. *Among the graphs in $\mathbb{U}_3(n)$, $C_4(P_{n-3})$, $C_4(T_{n-3}^1)$ for $n \geq 6$, and $C_4(T_{n-3}^2)$ for $n \geq 7$ are respectively the unique graphs with the maximum, the second, and the third maximum degree distances, which are equal to $\frac{2}{3}n^3 - \frac{35}{3}n + 36$, $\frac{2}{3}n^3 - \frac{47}{3}n + 46$, and $\frac{2}{3}n^3 - \frac{59}{3}n + 64$, respectively.*

Lemma 10. *Among the graphs in $\mathbb{U}_4(n)$,*

- (a) $C_4^1(P_{n-4}, P_2)$ for $n \geq 6$ is the unique graph with the maximum degree distance, which is equal to $\frac{2}{3}n^3 - \frac{53}{3}n + 66$;
- (b) $C_4^2(P_{n-4}, P_2)$ for $n = 6, 7$ or $n \geq 12$ is the unique graph with the second maximum degree distance, which is equal to $\frac{2}{3}n^3 - \frac{65}{3}n + 86$, $C_4^1(P_{n-5}, P_3)$ for $8 \leq n \leq 10$ is the unique graph with the second maximum degree distance, which is equal to $\frac{2}{3}n^3 - \frac{71}{3}n + 108$, and $C_4^2(P_{n-4}, P_2)$ and $C_4^1(P_{n-5}, P_3)$ for $n = 11$ are the unique graphs with the second maximum degree distance, which is equal to $\frac{2}{3}n^3 - \frac{65}{3}n + 86 = \frac{2}{3}n^3 - \frac{71}{3}n + 108$.

Proof. Let $G = C_4(T_1, T_2, T_3, T_4) \in \mathbb{U}_4(n)$. If $n = 6$, then $G = C_4^1(P_2, P_2)$ or $C_4^2(P_2, P_2)$. If $n = 7$, then $G = C_4^1(P_3, P_2)$, $C_4^2(P_3, P_2)$, $C_4^1(T_3^1, P_2)$, $C_4^2(T_3^1, P_2)$, or $C_4(P_2, P_2, P_2, -)$. Thus, the results for $n = 6, 7$ follow by direct calculation. In the following suppose that $n \geq 8$.

If there are at least three of T_1, T_2, T_3, T_4 that are not P_1 , then by Lemmas 1, 2, 3 and using the equation on $D'(U_{n,m}(a-1, b+1)) - D'(U_{n,m}(a, b))$ in the proof of Lemma 5 with $k = 0$, we have $D'(G) < D'(C_4^1(P_{n-5}, P_3))$.

Suppose that there are exactly two of T_1, T_2, T_3, T_4 that are not P_1 . Suppose without loss of generality that $d_G(v_1) \geq 3$. Suppose that $d_G(v_2)$ or $d_G(v_4) \geq 3$. By symmetry, we may assume that $d_G(v_2) \geq 3$ and $|V(T_1)| \geq |V(T_2)|$. If $|V(T_2)| = 2$, then by Lemma 1, we have $D'(G) \leq D'(C_4^2(P_{n-4}, P_2))$ with equality if and only if $G = C_4^2(P_{n-4}, P_2)$. If $|V(T_2)| \geq 3$, then by Lemmas 1, 3 and using the equation on $D'(U_{n,m}(a-1, b+1)) - D'(U_{n,m}(a, b))$ in the proof of Lemma 5 with $k = 0$, we have $D'(G) < D'(C_4^1(P_{n-5}, P_3))$. Suppose that $d_G(v_3) \geq 3$. Assume that $|V(T_1)| \geq |V(T_3)|$. If $|V(T_3)| = 2$ and $G \neq C_4^1(P_{n-4}, P_2)$, then by Lemma 6,

$$D'(G) \leq D'(C_4^1(T_{n-4}^1, P_2)) < D'(C_4^1(P_{n-4}, P_2)).$$

If $|V(T_3)| \geq 3$, then by Lemma 1 and using the equation on $D'(U_{n,m}(a-1, b+1)) - D'(U_{n,m}(a, b))$ in the proof of Lemma 5 with $k = 0$, we have $D'(G) \leq D'(C_4^1(P_{n-5}, P_3))$ with equality if and only if $G = C_4^1(P_{n-5}, P_3)$.

By the equation on $D'(U_{n,m}(a-1, b+1)) - D'(U_{n,m}(a, b))$ with $k = 0$ in the proof of Lemma 5, $D'(C_4^1(P_{n-5}, P_3)) < D'(C_4^1(P_{n-4}, P_2))$, and by Lemma 3, $D'(C_4^2(P_{n-4}, P_2)) < D'(C_4^1(P_{n-4}, P_2))$, implying that $C_4^1(P_{n-4}, P_2)$ is the unique graph with the maximum degree distance, and then (a) follows.

Note that $D'(C_4^2(P_{n-4}, P_2)) - D'(C_4^1(T_{n-4}^1, P_2)) = 10 > 0$. Thus the second maximum degree distance is only possibly achieved by $C_4^2(P_{n-4}, P_2)$ or $C_4^1(P_{n-5}, P_3)$. It is easily seen that

$$D'(C_4^2(P_{n-4}, P_2)) - D'(C_4^1(P_{n-5}, P_3)) = 2(n-11).$$

Then (b) follows easily. \square

Let $H_n = C_{n-1}(P_2, -, \dots, -)$ for $n \geq 4$.

Lemma 11. *Suppose that G is an n -vertex unicyclic graph with cycle length $r \geq 5$ and $n \geq 7$. Then $D'(G) < D'(C_3(P_{n-4}, P_3))$.*

Proof. If $r = n-1$, then $G = H_n$, and if $r = n$, then $G = C_n$. It is easily checked that $D'(C_n) = 2n \lfloor \frac{n^2}{4} \rfloor$ and $D'(H_n) = 2(n+1) \lfloor \frac{(n-1)^2}{4} \rfloor + 3n-2$, and thus $\max\{D'(C_n), D'(H_n)\} < D'(C_3(P_{n-4}, P_3))$.

Suppose that $r \leq n-2$. Let G be a graph with the maximum degree distance satisfying the given condition, and C_r its unique cycle. By Lemmas 1 and 2, $G = U_{n,r} = C_r(P_{n-r+1}, -, \dots, -)$. Setting $a = 0$, $m = r$, and $T_1 = P_{n-r+1}$ in Lemma 3, we have $D'(G) < \max\{D'(C_3(P_{n-r+1}, P_{r-2})), D'(C_4^1(P_{n-r+1}, P_{r-3}))\}$. By the equation on $D'(U_{n,m}(a-1, b+1)) - D'(U_{n,m}(a, b))$ with $k = 0$ in the proof of Lemma 5, $D'(C_3(P_{n-r+1}, P_{r-2})) \leq D'(C_3(P_{n-4}, P_3))$ and $D'(C_4^1(P_{n-r+1}, P_{r-3})) \leq D'(C_4^1(P_{n-5}, P_3))$. Now by the equation $D'(G(k, 3)) - D'(G(k, 4)) = 6k - n - 22$ in the proof of Theorem 1 with $k = n-2$, $D'(C_4^1(P_{n-5}, P_3)) < D'(C_3(P_{n-4}, P_3))$. Then $D'(G) < D'(C_3(P_{n-4}, P_3))$, as desired. \square

There are five 5-vertex unicyclic graphs, for which by direct checking, the degree distances are ordered as:

$$D'(C_3(T_3^1)) < D'(C_3(P_2, P_2)) < D'(C_5) < D'(H_5) < D'(C_3(P_3)).$$

Theorem 2. *The degree distances of n -vertex unicyclic graphs with $n \geq 6$ may be ordered by the following inequalities, where G is an n -vertex unicyclic graph different from any other graph in the inequalities:*

(i) for $n = 6$,

$$\begin{aligned} D'(G) &< D'(C_3(T_4^2)) = 98 \\ &< D'(C_4^2(P_2, P_2)) = D'(H_6) = 100 \\ &< D'(C_3(T_4^1)) = D'(C_4^1(P_2, P_2)) = 104 \\ &< D'(C_3(P_3, P_2)) = 106 < D'(C_6) = 108 \end{aligned}$$

$$< D'(C_4(P_3)) = 110 < D'(C_3(P_4)) = 118;$$

(ii) for $n = 7$,

$$\begin{aligned} D'(G) &< D'(C_3(T_5^3)) = 166 \\ &< D'(C_7) = D'(C_3(T_5^2)) = 168 \\ &< D'(C_4^1(P_3, P_2)) = 171 < D'(C_3(P_3, P_3)) = 172 \\ &< D'(C_3(P_4, P_2)) = D'(C_3(T_5^1)) = 178 \\ &< D'(C_4(P_4)) = 183 < D'(C_3(P_5)) = 196; \end{aligned}$$

(iii) for $n = 8$,

$$\begin{aligned} D'(G) &< D'(C_4^1(P_3, P_3)) = D'(C_3(T_6^3)) = 260 \\ &< D'(C_3(T_6^4)) = D'(C_4(T_5^1)) = 262 \\ &< D'(C_3(P_4, P_3)) = D'(C_3(T_6^2)) \\ &= D'(C_4^1(P_4, P_2)) = 266 \\ &< D'(C_3(P_5, P_2)) = 278 < D'(C_3(T_6^1)) = 280 \\ &< D'(C_4(P_5)) = 284 < D'(C_3(P_6)) = 302; \end{aligned}$$

(iv) for $n = 9$,

$$\begin{aligned} D'(G) &< D'(C_3(P_5, P_3)) = 392 < D'(C_4^1(P_5, P_2)) = 393 \\ &< D'(C_3(T_7^2)) = 396 < D'(C_3(P_6, P_2)) = 410 \\ &< D'(C_3(T_7^1)) = 414 < D'(C_4(P_6)) = 417 \\ &< D'(C_3(P_7)) = 440; \end{aligned}$$

(v) for $n = 10$,

$$\begin{aligned} D'(G) &< D'(C_3(T_8^6)) = D'(C_3(P_6, P_3)) = 554 \\ &< D'(C_4(T_7^1)) = D'(C_4^1(P_6, P_2)) = 556 \\ &< D'(C_3(T_8^2)) = 562 < D'(C_3(P_7, P_2)) = 578 \\ &< D'(C_3(T_8^1)) = 584 < D'(C_4(P_7)) = 586 \\ &< D'(C_3(P_8)) = 614; \end{aligned}$$

(vi) for $n = 11$,

$$\begin{aligned} D'(G) &< D'(C_4^1(P_7, P_2)) = 759 < D'(C_4(T_8^1)) = 761 \\ &< D'(C_3(T_9^2)) = 768 < D'(C_3(P_8, P_2)) = 786 \\ &< D'(C_3(T_9^1)) = 794 < D'(C_4(P_8)) = 795 \\ &< D'(C_3(P_9)) = 828; \end{aligned}$$

(vii) for $n = 12$,

$$D'(G) < D'(C_3(P_8, P_3)) = 1002$$

$$\begin{aligned}
&< D'(C_3(T_{10}^8)) = D'(C_4^1(P_8, P_2)) = 1006 \\
&< D'(C_4(T_9^1)) = 1010 < D'(C_3(T_{10}^2)) = 1018 \\
&< D'(C_3(P_9, P_2)) = 1038 \\
&< D'(C_3(T_{10}^1)) = D'(C_4(P_9)) = 1048 \\
&< D'(C_3(P_{10})) = 1086;
\end{aligned}$$

(viii) for $n \geq 13$,

$$\begin{aligned}
D'(G) &< D'(C_3(T_{n-2}^{n-4})) = \frac{2}{3}n^3 - \frac{50}{3}n + 54 \\
&< D'(C_4(T_{n-3}^1)) = \frac{2}{3}n^3 - \frac{47}{3}n + 46 \\
&< D'(C_3(T_{n-2}^2)) = \frac{2}{3}n^3 - \frac{44}{3}n + 42 \\
&< D'(C_3(P_{n-3}, P_2)) = \frac{2}{3}n^3 - \frac{38}{3}n + 38 \\
&< D'(C_4(P_{n-3})) = \frac{2}{3}n^3 - \frac{35}{3}n + 36 \\
&< D'(C_3(T_{n-2}^1)) = \frac{2}{3}n^3 - \frac{32}{3}n + 24 \\
&< D'(C_3(P_{n-2})) = \frac{2}{3}n^3 - \frac{20}{3}n + 14.
\end{aligned}$$

Proof. Let G be an n -vertex unicyclic graph, where $n \geq 6$. If the cycle length of G is three, then $G \in \mathbb{U}_1(n) \cup \mathbb{U}_2(n)$, and if the cycle length of G is four, then $G \in \mathbb{U}_3(n) \cup \mathbb{U}_4(n)$. The graphs with cycle length three or four with the first several large degree distances are determined in Lemmas 7–10, which (especially for $n = 6, 7, \dots, 12$) are shown in Table 1.

Suppose that $n = 6$. Note that $D'(C_6) = 108$ and $D'(H_6) = 100$. If $G \neq C_6, H_6$, then $G \in \bigcup_{i=1}^4 \mathbb{U}_i(6)$. Note that $\mathbb{U}_4(6) = \{C_4^1(P_2, P_2), C_4^2(P_2, P_2)\}$. From Table 1, the first four maximum degree distances of graphs in $\mathbb{U}_1(6) \cup \mathbb{U}_2(6)$ are 118, 106, 104, 98, while the first four maximum degree distances of graphs in $\mathbb{U}_3(6) \cup \mathbb{U}_4(6)$ are 110, 104, 100, 96. Then (i) follows from Table 1.

Suppose that $n = 7$. Note that $D'(C_7) = 168$. If the cycle length of G is at least five and $G \neq C_7$, then by Lemmas 1, 2 and direct calculation, $D'(G) < 166$. From Table 1, the first five maximum degree distances of graphs in $\mathbb{U}_1(7) \cup \mathbb{U}_2(7)$ are 196, 178, 172, 168, 166, while the first four maximum degree distances of graphs in $\mathbb{U}_3(7) \cup \mathbb{U}_4(7)$ are 183, 171, 165, 163. Then (ii) follows from Table 1.

Suppose that $n = 8$. If the cycle length of G is at least five, then by Lemmas 1, 2 and direct calculation, $D'(G) < 260$. From Table 1, the first six maximum degree distances of graphs in $\mathbb{U}_1(8) \cup \mathbb{U}_2(8)$ are 302, 280, 278, 266, 262, 260, while the first four maximum degree distances of graphs in $\mathbb{U}_3(8) \cup \mathbb{U}_4(8)$ are 284, 266, 262, 260. Then (iii) follows from Table 1.

Suppose in the following that $n \geq 9$. If the cycle length of G is at least five, then by Lemma 11, $D'(G) < D'(C_3(P_{n-4}, P_3))$. To prove the results for $n \geq 9$,

Table 1: Graphs and their degree distances in Lemmas 7–10.

| graph | degree distances | | | | | | | |
|-----------------------|--|-----|-----|-----|-----|-----|-----|------|
| | n | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
| $C_3(P_{n-2})$ | $\frac{2}{3}n^3 - \frac{20}{3}n + 14$ | 118 | 196 | 302 | 440 | 614 | 828 | 1086 |
| $C_3(T_{n-2}^1)$ | $\frac{2}{3}n^3 - \frac{32}{3}n + 24$ | 104 | 178 | 280 | 414 | 584 | 794 | 1048 |
| $C_3(T_{n-2}^2)$ | $\frac{2}{3}n^3 - \frac{44}{3}n + 42$ | 98 | 168 | 266 | 396 | 562 | 768 | 1018 |
| $C_3(T_{n-2}^{n-4})$ | $\frac{2}{3}n^3 - \frac{50}{3}n + 54$ | | 166 | 262 | 390 | 554 | 758 | 1006 |
| $C_3(T_{n-2}^3)$ | $\frac{2}{3}n^3 - \frac{56}{3}n + 68$ | | | 260 | | | | 996 |
| $C_3(P_{n-3}, P_2)$ | $\frac{2}{3}n^3 - \frac{38}{3}n + 38$ | 106 | 178 | 278 | 410 | 578 | 786 | 1038 |
| $C_3(P_2, P_2, P_2)$ | | 96 | | | | | | |
| $C_3(P_{n-4}, P_3)$ | $\frac{2}{3}n^3 - \frac{56}{3}n + 74$ | | 172 | 266 | 392 | 554 | 756 | 1002 |
| $C_3(T_{n-3}^1, P_2)$ | $\frac{2}{3}n^3 - \frac{50}{3}n + 48$ | | 160 | 256 | | | | |
| $C_4(P_{n-3})$ | $\frac{2}{3}n^3 - \frac{35}{3}n + 36$ | 110 | 183 | 284 | 417 | 586 | 795 | 1048 |
| $C_4(T_{n-3}^1)$ | $\frac{2}{3}n^3 - \frac{47}{3}n + 46$ | 96 | 165 | 262 | 391 | 556 | 761 | 1010 |
| $C_4(T_{n-3}^2)$ | $\frac{2}{3}n^3 - \frac{59}{3}n + 64$ | | 155 | 248 | 373 | 534 | 735 | 980 |
| $C_4^1(P_{n-4}, P_2)$ | $\frac{2}{3}n^3 - \frac{53}{3}n + 66$ | 104 | 171 | 266 | 393 | 556 | 759 | 1006 |
| $C_4^1(P_{n-5}, P_3)$ | $\frac{2}{3}n^3 - \frac{71}{3}n + 108$ | | | 260 | 381 | 538 | 735 | |
| $C_4^2(P_{n-4}, P_2)$ | $\frac{2}{3}n^3 - \frac{65}{3}n + 86$ | 100 | 163 | | | | 735 | 978 |

we need only to consider the graphs in $\bigcup_{i=1}^4 \mathbb{U}_i(n)$ with the degree distances at least $D'(C_3(P_{n-4}, P_3))$.

Suppose that $n = 9$. From Table 1, the first five maximum degree distances of graphs in $\mathbb{U}_1(9) \cup \mathbb{U}_2(9)$ are 440, 414, 410, 396, 392, while the first four maximum degree distances of graphs in $\mathbb{U}_3(9) \cup \mathbb{U}_4(9)$ are 417, 393, 391, 381. Then (iv) follows from Table 1.

Suppose that $n = 10$. From Table 1, the first five maximum degree distances of graphs in $\mathbb{U}_1(10) \cup \mathbb{U}_2(10)$ are 614, 584, 578, 562, 554, while the first three maximum degree distances of graphs in $\mathbb{U}_3(10) \cup \mathbb{U}_4(10)$ are 586, 556, 538. Then (v) follows from Table 1.

Suppose that $n = 11$. From Table 1, the first five maximum degree distances of graphs in $\mathbb{U}_1(11) \cup \mathbb{U}_2(11)$ are 828, 794, 786, 768, 758, while the first three maximum degree distances of graphs in $\mathbb{U}_3(11) \cup \mathbb{U}_4(11)$ are 795, 761, 759. Then (vi) follows from Table 1.

Suppose that $n = 12$. From Table 1, the first six maximum degree distances of

graphs in $\mathbb{U}_1(12) \cup \mathbb{U}_2(12)$ are 1086, 1048, 1038, 1018, 1006, 1002, while the first four maximum degree distances of graphs in $\mathbb{U}_3(12) \cup \mathbb{U}_4(12)$ are 1048, 1010, 1006, 980. Then (vii) follows from Table 1.

Suppose that $n \geq 13$. By Lemmas 7 and 8, $C_3(P_{n-2})$, $C_3(T_{n-2}^1)$, $C_3(P_{n-3}, P_2)$, $C_3(T_{n-2}^2)$ and $C_3(T_{n-2}^{n-4})$ are respectively the graphs in $\mathbb{U}_1(n) \cup \mathbb{U}_2(n)$ with the first five maximum degree distances, which are equal to $\frac{2}{3}n^3 - \frac{20}{3}n + 14$, $\frac{2}{3}n^3 - \frac{32}{3}n + 24$, $\frac{2}{3}n^3 - \frac{38}{3}n + 38$, $\frac{2}{3}n^3 - \frac{44}{3}n + 42$ and $\frac{2}{3}n^3 - \frac{50}{3}n + 54$, respectively. By Lemmas 9 and 10, $C_4(P_{n-3})$, $C_4(T_{n-3}^1)$ and $C_4^1(P_{n-4}, P_2)$ are respectively the graphs in $\mathbb{U}_3(n) \cup \mathbb{U}_4(n)$ with the first three maximum degree distances, which are equal to $\frac{2}{3}n^3 - \frac{35}{3}n + 36$, $\frac{2}{3}n^3 - \frac{47}{3}n + 46$ and $\frac{2}{3}n^3 - \frac{53}{3}n + 66$, respectively. Note that

$$\begin{aligned} & \frac{2}{3}n^3 - \frac{20}{3}n + 14 > \frac{2}{3}n^3 - \frac{32}{3}n + 24 \\ & > \frac{2}{3}n^3 - \frac{35}{3}n + 36 > \frac{2}{3}n^3 - \frac{38}{3}n + 38 > \frac{2}{3}n^3 - \frac{44}{3}n + 42 \\ & > \frac{2}{3}n^3 - \frac{47}{3}n + 46 > \frac{2}{3}n^3 - \frac{50}{3}n + 54 > \frac{2}{3}n^3 - \frac{53}{3}n + 66. \end{aligned}$$

Then (viii) follows. \square

Acknowledgement. This work was supported by the Guangdong Provincial Natural Science Foundation of China (no. 8151063101000026).

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 (1994), 1082–1086.
- [2] I. Gutman, *Selected properties of the Schultz molecular topological index*, J. Chem. Inf. Comput. Sci. 34 (1994), 1087–1089.
- [3] H.P. Schultz, *Topological organic chemistry. 1. Graph theory and topological indices of alkanes*, J. Chem. Inf. Comput. Sci. 29 (1989), 227–228.
- [4] W.R. Müller, K. Szymanski, J.V. Knop, N. Trinajstić, *Molecular topological index*, J. Chem. Inf. Comput. Sci. 30 (1990), 160–163.
- [5] I. Gutman, N. Trinajstić, *Graph theory and molecular orbitals. III. Total π -electron energy of alternant hydrocarbons*, Chem. Phys. Lett. 17 (1972), 535–538.
- [6] I. Gutman, B. Rušćić, N. Trinajstić, C.F. Wilcox Jr., *Graph theory and molecular orbitals. XII. Acyclic polyenes*, J. Chem. Phys. 62 (1975), 3399–3405.
- [7] I. Gutman, K.C. Das, *The first Zagreb index 30 years after*, MATCH Commun. Math. Comput. Chem. 50 (2004), 83–92.

- [8] Z. Mihalić, S. Nikolić, N. Trinajstić, *Comparative study of molecular descriptors derived from the distance matrix*, J. Chem. Inf. Comput. Sci. 32 (1992), 28–37.
- [9] 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.
- [10] B. Zhou, *Bounds for Schultz molecular topological index*, MATCH Commun. Math. Comput. Chem. 56 (2006), 189–194.
- [11] B. Zhou, N. Trinajstić, *On reverse degree distance*, J. Math. Chem. 47 (2010), 268–275.
- [12] A.A. Dobrynin, R. Entringer, I. Gutman, *Wiener index of trees: Theory and applications*, Acta Appl. Math. 66 (2001), 211–249.
- [13] A.A. Dobrynin, I. Gutman, S. Klavžar, P. Žigert, *Wiener index of hexagonal systems*, Acta Appl. Math. 72 (2002), 247–294.
- [14] D. Stevanović, *Maximizing Wiener index of graphs with fixed maximum degree*, MATCH Commun. Math. Comput. Chem. 60 (2008), 71–83.
- [15] I. Tomescu, *Some extremal properties of the degree distance of a graph*, Discrete Appl. Math. 98 (1999), 159–163.
- [16] A.I. Tomescu, *Unicyclic and bicyclic graphs having minimum degree distance*, Discrete Appl. Math. 156 (2008), 125–130.
- [17] I. Tomescu, *Properties of connected graphs having minimum degree distance*, Discrete Math. 309 (2008), 2745–2748.
- [18] O. Bucicovschi, S.M. Cioabă, *The minimum degree distance of graphs of given order and size*, Discrete Appl. Math. 156 (2008), 3518–3521.
- [19] Y. Hou, A. Chang, *The unicyclic graph with maximum degree distance*, J. Math. Study 39 (2006), 18–24.
- [20] Z. Du, B. Zhou, *Maximum degree distance of graphs with exactly two cycles*, Bull. Math. Soc. Sci. Math. Roumanie, in press.
- [21] P. Dankelmann, I. Gutman, S. Mukwembi, H.C. Swart, *On the degree distance of a graph*, Discrete Appl. Math. 157 (2009), 2773–2777.
- [22] Z. Du, B. Zhou, *On the reverse Wiener indices of unicyclic graphs*, Acta Appl. Math. 106 (2009), 293–306.

Department of Mathematics, South China Normal University, Guangzhou 510631, China

E-mails: zhibindu@126.com (Z. Du), zhoubo@scnu.edu.cn (B. Zhou)