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DEGREE DISTANCE OF UNICYCLIC GRAPHS

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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 $d_G(u)$ 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

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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.

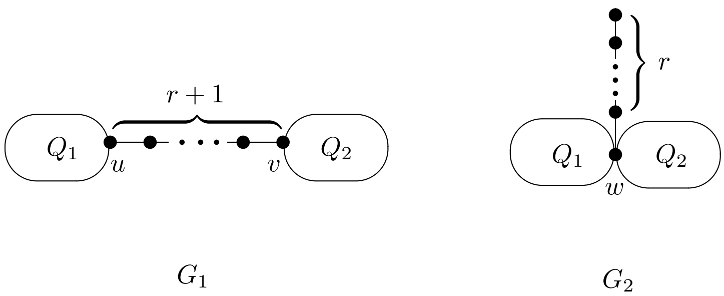

Fig. 1. The graphs G_1 and G_2 in Lemma 1.

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

Lemma 2. *For integers i and j with $2 \leq i < j \leq m$, let $G_{a_i,a_j} = C_m(T_1, T_2, \ldots, T_m)$, 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

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

$$= \sum_{\substack{x\in Z\\ y\in V(G)\setminus(Z\cup W)}} a_i = a_i a_j(n-a_i-a_j-1),$$

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

and then

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

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

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

For $k\ne 1,i,j$ and $a_k\ge 1$, 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

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

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

Thus

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

It follows that

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

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

$$4\sum_{\substack{1\le k\le m \\ k\ne j}} a_k\left[d(v_k,v_j) - d(v_k,v_i)\right] \ge 4a_i(n-a_i-a_j) - 2a_i,$$

and thus

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

Now the result follows. □

For $n \ge m \ge 3$, let $U_{n,m} = C_m(P_{n-m+1}, -, \ldots, -)$, 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 $2 \le i \le \lfloor\frac{m}{2}\rfloor+1$ and $m \ge 3$, let $G_i(a,m) = C_m(T_1, T_2, \ldots, T_m)$, where T_i is the path P_{a+1} with an end vertex v_i, $T_j = P_1$ for $2 \le j \le m$ with $j \ne i$, and T_1 is a fixed tree. Let $G(a,m) = G_{\lfloor\frac{m}{2}\rfloor+1}(a,m)$. For fixed $k = a+m \ge 4$, $D'(G_i(a,m)) < \max\{D'(G(k-3,3)), D'(G(k-4,4))\}$ 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 $a \ge 1$.

We first prove that $D'(G_i(a,m)) \le D'(G(a,m))$. If $|V(T_1)| = 1$ or $a = 0$, then $G_i(a,m)$ is (isomorphic to) $G(a,m)$. Suppose that $|V(T_1)| \ge 2$ and $a \ge 1$. Suppose that $G_i(a,m) \ne G(a,m)$, i.e., $i < \lfloor\frac{m}{2}\rfloor+1$. Let $G_1 = G_i(a,m)$. Let $G_2 = G_1 - \{v_iv\} + \left\{v_{\lfloor\frac{m}{2}\rfloor+1}v\right\}$, 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 $V_1(G_2) = (V_1(G_2)\cap V(T_1))\cup\left\{v_{\lfloor\frac{m}{2}\rfloor+1}, v_i^*\right\}$. 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

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

and thus $D'(G(a,m)) > D'(G_i(a,m))$. It follows that $D'(G_i(a,m)) \le D'(G(a,m))$ 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 $a \ge 0$. Note that $U_{m+a,m}$ is a subgraph of $G(a,m)$.

Suppose that $m \ge 5$. 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 $a \ge 1$. For

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

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

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

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

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

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

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

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

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

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. □

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

Proof. Suppose that $G = H(a_1,a_2,\ldots,a_t)$ 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

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

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

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 $G_2 = G_1 - \{u_1 w\} + \{u_1 u_2\}$, $G_3 = G_1 - \{u_1 w\} + \{u_1 v_1\}$ and $G_4 = G_1 - \{u_1 w\} + \{u_1 v_3\}$, 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

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

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. □

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 $U^1_{n,\Delta} = U_{n,3}(n-\Delta, 0)$ if $\Delta \leq n-1$, $U^2_{n,\Delta} = U_{n,4}(1, n-\Delta-2)$ if $\Delta \leq n-2$, and $U^3_{n,\Delta}$ 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

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

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

In $U^1_{n,\Delta}$, 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

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

By similar calculation, we have

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

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

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

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

(*i*) *if $\Delta = 3,4,5$, then $U^1_{n,\Delta}$ is the unique graph with the maximum degree distance,*

(*ii*) *if $\Delta = n-2$, then $U^1_{n,n-2}$ for $n = 5,6,7$, $U^1_{n,n-2}$ and $U^2_{n,n-2}$ for $n = 8$, and $U^2_{n,n-2}$ for $n \ge 9$ are the unique graphs with the maximum degree distance,*

(*iii*) *if $6 \le \Delta \le n-3$, then $U^1_{n,\Delta}$ for $9 \le n \le 14$, $U^1_{n,\Delta}$ with $\Delta < \frac{n+1-\sqrt{n^2-18n+45}}{2}$ or $\frac{n+1+\sqrt{n^2-18n+45}}{2} < \Delta < \frac{11n-16}{12}$, $U^1_{n,\Delta}$ and $U^3_{n,\Delta}$ with $\Delta = \frac{n+1\pm\sqrt{n^2-18n+45}}{2}$, $U^3_{n,\Delta}$ with $\frac{n+1-\sqrt{n^2-18n+45}}{2} < \Delta < \frac{n+1+\sqrt{n^2-18n+45}}{2}$, $U^1_{n,\Delta}$ and $U^2_{n,\Delta}$ with $\Delta = \frac{11n-16}{12}$, and $U^2_{n,\Delta}$ with $\Delta > \frac{11n-16}{12}$ for $15 \le n \le 36$, $U^1_{n,\Delta}$ with $\Delta < \frac{n+1-\sqrt{n^2-18n+45}}{2}$, $U^1_{n,\Delta}$ and $U^3_{n,\Delta}$ with $\Delta = \frac{n+1-\sqrt{n^2-18n+45}}{2}$, $U^3_{n,\Delta}$ with $\frac{n+1-\sqrt{n^2-18n+45}}{2} < \Delta < \frac{n-5+\sqrt{n^2-8n+37}}{2}$, $U^2_{n,\Delta}$ and $U^3_{n,\Delta}$ with $\Delta = \frac{n-5+\sqrt{n^2-8n+37}}{2}$, and $U^2_{n,\Delta}$ with $\Delta > \frac{n-5+\sqrt{n^2-8n+37}}{2}$ for $n \ge 37$ are the unique graphs with the maximum degree distance,*

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

$$D'(U^1_{n,\Delta}) = \frac{2}{3}n^3 - \left(2\Delta^2 - 4\Delta + \frac{2}{3}\right)n + \frac{4}{3}\Delta^3 - \Delta^2 - \frac{7}{3}\Delta - 6,$$

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

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

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 $\Delta \ge 3$, we have $G \ne C_n$.

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 $G = U^1_{n,\Delta}$. 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 $G = U^2_{n,\Delta}$ with $\Delta \ge 5$. Note that

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

Thus, $G = U^1_{n,\Delta}$ if $\Delta = 3, 4$, and $G = U^1_{n,\Delta}$ or $U^2_{n,\Delta}$ if $\Delta \ge 5$.
Case 2. v lies outside C.

In this case $\Delta \le n-3$. 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 $G^* \ne C_3$. 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 $4 \le k \le n-\Delta$. 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

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

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 $n \le 6k - 22$, then $D'(G_1) > D'(G(k,4))$, and if $k \ge 5$ 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 $G \ne U^3_{n,\Delta}$. Denote by w the pendent vertex of the longest pendent path at v, and w_1 the neighbor of w. Then $d_G(v,w) \ge 2$. Let $t = d_G(v,w_1) \ge 1$. Note that $n - \Delta - t \ge 3$. Denote by $x_1, x_2, \ldots, x_{\Delta-2}$ the pendent neighbors of v. Consider $G_3 = G - \{vx_1, \ldots, vx_{\Delta-2}\} + \{w_1x_1, \ldots, w_1x_{\Delta-2}\} \in \mathbb{U}(n,\Delta)$. 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

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

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

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

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

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

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

Now the results for $\Delta = 3, 4, 5, n-2$ follow by direct calculation, proving (i) and (ii). Suppose that $6 \le \Delta \le n-3$. For $9 \le n \le 14$, we have $D'(U^1_{n,\Delta}) > D'(U^3_{n,\Delta})$ 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 $n \ge 15$, we have

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

If $9 \le n \le 14$, then $D'(U^1_{n,\Delta}) > D'(U^3_{n,\Delta})$,

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

and thus $D'(U^1_{n,\Delta}) > \max\left\{D'(U^2_{n,\Delta}), D'(U^3_{n,\Delta})\right\}$. If $15 \le n \le 36$, then

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

and thus

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

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

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

Now (iii) follows. □

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 $P_{n-1} = u_0u_1 \ldots u_{n-2}$ by attaching a pendent vertex to u_s, where $1 \leq s \leq n-2$.

In the following, if the symbol $G = C_m(T_1, T_2, \ldots, T_m)$ 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 $T_2, \ldots, T_m$, let $G(T) = C_m(T, T_2, \ldots, T_m)$ with $|V(T)| = k \geq 1$, and $H = C_m(-, T_2, \ldots, T_m)$. 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

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

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, $D'(G) \leq D'(C_3(T^3_{n-2}))$ with equality if and only if $G = C_3(T^3_{n-2})$. 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 $D'(C_3(T^3_{n-2})) - D'(Q_n) = 8n - 46 > 0$. Then (b) follows. □

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* $C_3(T^1_{n-3}, P_2)$ *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* $C_3(T^1_{n-3}, P_2)$ *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*) $C_3(T^1_{n-3}, P_2)$ *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 $C_3(T^1_3, P_2)$, 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,

$$D'(G) \leq D'(C_3(T^1_{n-3}, P_2)) < D'(C_3(P_{n-3}, P_2))$$

with equality if and only if $G = C_3(T^1_{n-3}, P_2)$. 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 $C_3(T^1_{n-3}, P_2)$ or $C_3(P_{n-4}, P_3)$. It is easily seen that

$$D'(C_3(T^1_{n-3}, P_2)) - D'(C_3(P_{n-4}, P_3)) = 2(n - 13).$$

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 $n = 7$,

$$D'(G) \leq \max\{D'(C_3(P_3, P_2, P_2)), D'(C_3(T^1_3, P_3)), D'(C_3(T^1_4, P_2))\}$$

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

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. □

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. □

Let $H_n = C_{n-1}(P_2, -, \ldots, -)$ 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 $D'(C_n) = 2n \left\lfloor \frac{n^2}{4} \right\rfloor$ and $D'(H_n) = 2(n+1)\left\lfloor \frac{(n-1)^2}{4} \right\rfloor + 3n - 2$, 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, $G = U_{n,r} = C_r(P_{n-r+1}, -, \ldots, -)$. 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. □

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 $n = 6$,

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

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

(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 $n = 6, 7, \ldots, 12$) 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
$C_3(T^1_{n-2})$	$\frac{2}{3}n^3 - \frac{32}{3}n + 24$	104	178	280	414	584	794	1048
$C_3(T^2_{n-2})$	$\frac{2}{3}n^3 - \frac{44}{3}n + 42$	98	168	266	396	562	768	1018
$C_3(T^{n-4}_{n-2})$	$\frac{2}{3}n^3 - \frac{50}{3}n + 54$		166	262	390	554	758	1006
$C_3(T^3_{n-2})$	$\frac{2}{3}n^3 - \frac{56}{3}n + 68$			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
$C_3(T^1_{n-3}, P_2)$	$\frac{2}{3}n^3 - \frac{50}{3}n + 48$		160	256				
$C_4(P_{n-3})$	$\frac{2}{3}n^3 - \frac{35}{3}n + 36$	110	183	284	417	586	795	1048
$C_4(T^1_{n-3})$	$\frac{2}{3}n^3 - \frac{47}{3}n + 46$	96	165	262	391	556	761	1010
$C_4(T^2_{n-3})$	$\frac{2}{3}n^3 - \frac{59}{3}n + 64$		155	248	373	534	735	980
$C^1_4(P_{n-4}, P_2)$	$\frac{2}{3}n^3 - \frac{53}{3}n + 66$	104	171	266	393	556	759	1006
$C^1_4(P_{n-5}, P_3)$	$\frac{2}{3}n^3 - \frac{71}{3}n + 108$			260	381	538	735	
$C^2_4(P_{n-4}, P_2)$	$\frac{2}{3}n^3 - \frac{65}{3}n + 86$	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, $C_3(P_{n-2})$, $C_3(T^1_{n-2})$, $C_3(P_{n-3}, P_2)$, $C_3(T^2_{n-2})$ and $C_3(T^{n-4}_{n-2})$ 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, $C_4(P_{n-3})$, $C_4(T^1_{n-3})$ and $C^1_4(P_{n-4}, P_2)$ 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. □

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