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ON REVERSE DEGREE DISTANCE OF UNICYCLIC GRAPHS

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Abstract. The reverse degree distance of a connected graph G is defined in discrete mathematical chemistry as

$$^{r}D'(G) = 2(n-1)md - \sum_{u \in V(G)} d_G(u)D_G(u),$$

where n, m and d are the number of vertices, the number of edges and the diameter of G, respectively, $d_G(u)$ is the degree of vertex u, $D_G(u)$ is the sum of distances between vertex u and all other vertices of G, and $V(G)$ is the vertex set of G. We determine the unicyclic graphs of given girth, number of pendant vertices and maximum degree, respectively, with maximum reverse degree distances. We also determine the unicyclic graphs of given number of vertices, girth and diameter with minimum degree distance.

1. Introduction

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

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vertices u and v in G for $u, v \in V(G)$. The degree distance of G is defined as [6, 10, 11]

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

It is a useful molecular descriptor [21]. Earlier as noted in [15, 19], this graph invariant appeared to be part of the molecular topological index (or Schultz index) [18], which may be expressed as $D'(G) + \sum_{u \in V(G)} d_G(u)^2$, see [11, 14, 16, 26], where the latter part $\sum_{u \in V(G)} d_G(u)^2$ is known as the first Zagreb index [12, 13, 17]. Thus the degree distance is also called the true Schultz index in chemical literature [4].

I. Tomescu [23] showed that the star is the unique graph with minimum degree distance in the class of connected graphs with n vertices. Further work on the minimum degree distance (especially for unicyclic and bicyclic graphs) may be found in A.I. Tomescu [22], I. Tomescu [24] and Bucicovschi and Cioabă [2]. Dankelmann et al. [3] gave asymptotically sharp upper bounds for the degree distance. Among others, the authors [8] studied the ordering of unicyclic graphs with large degree distances, and bicyclic graphs were also considered in [9].

Recall that the Wiener index [25] of the graph G is defined as

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

Gutman [11] showed that if G is a tree with n vertices, then

$$D'(G) = 4W(G) - n(n-1).$$

Thus there is no need to study the degree distance for trees because this is equivalent to the study of the Wiener index, see, e.g., [5, 20].

The reverse degree distance of the graph G is defined as [27]

$${}^{r}D'(G) = 2(n-1)md - D'(G)$$

where n, m and d are the number of vertices, the number of edges and the diameter of G, respectively. Some basic properties of the reverse degree distance have been established by Zhou and Trinajstić [27], and in particular, it was shown that the reverse degree distance satisfies the basic requirement to be a branching index usable in chemistry.

Recall that, earlier, Balaban et al. [1] introduced the concept of reverse Wiener index, which is defined to be $\Lambda(G) = \frac{n(n-1)d}{2} - W(G)$. Let

$\Lambda'(G) = \frac{(n-1)^2 d}{2} - W(G)$, which is a revised version of the reverse Wiener index of G [27]. If G is a tree, then from the result of Gutman [11] mentioned above, we have

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

Thus for trees the study of the reverse degree distance is equivalent to the study of the revised reverse Wiener index, see [27].

In continuation to the study of the reverse degree distance, a natural starting point is the reverse degree distances of unicyclic graphs. In this paper, we determine the graphs with maximum reverse degrees distance in the class of unicyclic graphs (connected graphs with a unique cycle) with given girth (cycle length), number of pendant vertices (vertices of degree one), and maximum degree, respectively. Additionally, we also determine the graphs with minimum degree distance in the class of unicyclic graphs with given number of vertices, girth and diameter.

2. **Preliminaries**

In this section we give some lemmas that will be used in the next sections.

Lemma 2.1. *Let G be a graph of the form in Fig. 1, where M and N are vertex-disjoint connected graphs, T is a tree on $k \geq 2$ vertices such that M and T have only one common vertex u, and T and N have only one common vertex v. Let G^* be the graph obtained from M and N by identifying vertices u and v which is denoted by u, and attaching $k-1$ pendant vertices to u.*

(*i*) *If $V(N) = \{v\}$ and $G \ncong G^*$, then $D'(G) > D'(G^*)$.*
(*ii*) *If $|V(M)|,\ |V(N)| \geq 3$, then $D'(G) > D'(G^*)$.*

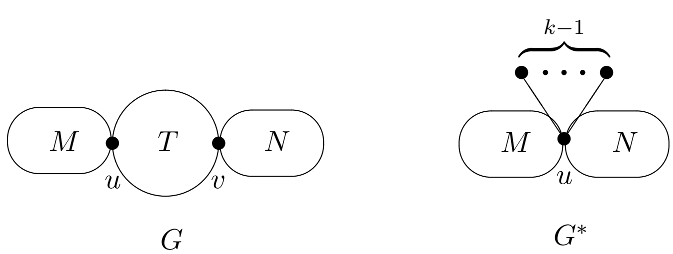

Fig. 1. The graphs G and G^* in Lemma 2.1.

Proof. For vertex–disjoint connected graphs Q_1 and Q_2 with $|V(Q_1)|$, $|V(Q_2)| \geq 2$, and $s \in V(Q_1)$, $t \in V(Q_2)$, let H be the graph obtained from Q_1 and Q_2 by joining s and t by an edge, and H_1 be the graph obtained by identifying vertices s and t which is denoted by s, and attaching a pendant vertex w to s.

Let $d_x = d_H(x)$ for $x \in V(H)$. It is easily seen that

$$\begin{aligned} & (d_s + d_t - 1)D_{H_1}(s) + 1 \cdot D_{H_1}(w) - d_s D_H(s) - d_t D_H(t) \\ = \;& d_s[D_{H_1}(s) - D_H(s)] + d_t[D_{H_1}(s) - D_H(t)] + [D_{H_1}(w) - D_{H_1}(s)] \\ = \;& -d_s(|V(Q_2)| - 1) - d_t(|V(Q_1)| - 1) + (|V(Q_1)| + |V(Q_2)| - 2) \\ = \;& -(d_s - 1)(|V(Q_2)| - 1) - (d_t - 1)(|V(Q_1)| - 1). \end{aligned}$$

Then

$$\begin{aligned} & D'(H_1) - D'(H) \\ = \;& -(|V(Q_2)| - 1) \sum_{x \in V(Q_1) \setminus \{s\}} d_x - (|V(Q_1)| - 1) \sum_{x \in V(Q_2) \setminus \{t\}} d_x \\ & +(d_s + d_t - 1)D_{H_1}(s) + 1 \cdot D_{H_1}(w) - d_s D_H(s) - d_t D_H(t) \\ = \;& -(|V(Q_2)| - 1) \sum_{x \in V(Q_1) \setminus \{s\}} d_x - (|V(Q_1)| - 1) \sum_{x \in V(Q_2) \setminus \{t\}} d_x \\ & -(d_s - 1)(|V(Q_2)| - 1) - (d_t - 1)(|V(Q_1)| - 1) < 0, \end{aligned}$$

and thus $D'(H_1) < D'(H)$.

Now (i) and (ii) follow by applying to G the transformation from H to H_1 repeatedly. □

Lemma 2.2. *Let G_0 be a connected graph with at least three vertices and let u and v be two distinct vertices of G_0. Let $G_{s,t}$ be the graph obtained from G_0 by attaching s and t pendant vertices to u and v, respectively. If $s, t \geq 1$, then $D'(G_{s,t}) > \min\{D'(G_{s+t,0}), D'(G_{0,s+t})\}$.*

Proof. Let $d_x = d_{G_0}(x)$ and $d(x, y) = d_{G_0}(x, y)$ for $x, y \in V(G_0)$. It is easily seen that

$$\begin{aligned} & \left[(d_u + s + t)D_{G_{s+t,0}}(u) - (d_u + s)D_{G_{s,t}}(u)\right] \\ & + \left[d_v D_{G_{s+t,0}}(v) - (d_v + t)D_{G_{s,t}}(v)\right] \\ = \;& (d_u + s)[D_{G_{s+t,0}}(u) - D_{G_{s,t}}(u)] + t[D_{G_{s+t,0}}(u) - D_{G_{s,t}}(v)] \\ & +d_v[D_{G_{s+t,0}}(v) - D_{G_{s,t}}(v)] \\ = \;& -t \cdot d(u, v) \cdot (d_u + s) \end{aligned}$$

$$\begin{aligned}
& +t\left[-s\cdot d(u,v)+\sum_{x\in V(G_0)\setminus\{u,v\}}(d(x,u)-d(x,v))\right]\\
& +t\cdot d(u,v)\cdot d_v\\
= \;& t\left[(d_v-d_u-2s)d(u,v)+\sum_{x\in V(G_0)\setminus\{u,v\}}(d(x,u)-d(x,v))\right]
\end{aligned}$$

and thus

$$\begin{aligned}
& D'(G_{s+t,0})-D'(G_{s,t})\\
= \;& t\sum_{x\in V(G_0)\setminus\{u,v\}} d_x\left(d(x,u)-d(x,v)\right)\\
& -st\cdot d(u,v)+t\Bigg[-s\cdot d(u,v)+\sum_{x\in V(G_0)\setminus\{u,v\}}(d(x,u)-d(x,v))\Bigg]\\
& +\big[(d_u+s+t)D_{G_{s+t,0}}(u)-(d_u+s)D_{G_{s,t}}(u)\big]\\
& +\big[d_vD_{G_{s+t,0}}(v)-(d_v+t)D_{G_{s,t}}(v)\big]\\
= \;& t\sum_{x\in V(G_0)\setminus\{u,v\}}(d_x+1)(d(x,u)-d(x,v))-2st\cdot d(u,v)\\
& +t\left[(d_v-d_u-2s)d(u,v)+\sum_{x\in V(G_0)\setminus\{u,v\}}(d(x,u)-d(x,v))\right]\\
= \;& t\Bigg[(d_v-d_u-4s)d(u,v)+\sum_{x\in V(G_0)\setminus\{u,v\}}(d_x+2)(d(x,u)-d(x,v))\Bigg].
\end{aligned}$$

Similarly, we have

$$\begin{aligned}
& D'(G_{0,s+t})-D'(G_{s,t})\\
= \;& s\Bigg[(d_u-d_v-4t)d(u,v)+\sum_{x\in V(G_0)\setminus\{u,v\}}(d_x+2)(d(x,v)-d(x,u))\Bigg].
\end{aligned}$$

If $D'(G_{s+t,0})\geq D'(G_{s,t})$, then

$$\sum_{x\in V(G_0)\setminus\{u,v\}}(d_x+2)(d(x,v)-d(x,u)) \;\leq\; (d_v-d_u-4s)d(u,v)$$

and thus

$$D'(G_{0,s+t})-D'(G_{s,t})$$

$$\begin{aligned} &\leq s\Big[(d_u - d_v - 4t)d(u,v) + (d_v - d_u - 4s)d(u,v)\Big] \\ &= -4s(s+t)d(u,v) < 0. \end{aligned}$$

The result follows. □

Now we give a technique to compare the degree distances of two connected graphs.

Let G and H be two connected graphs. Let $V_1(G) = \{x \in V(G) : d_G(x) = 2\}$ and $V_2(G) = V(G) \setminus V_1(G)$. Let $d_x = d_G(x)$ for $x \in V(G)$, and $d_x^* = d_H(x)$ for $x \in V(H)$. Then

$$\begin{aligned} &D'(H) - D'(G) \\ = \;& 2\sum_{x \in V_1(H)} D_H(x) + \sum_{x \in V_2(H)} d_x^* D_H(x) - 2\sum_{x \in V_1(G)} D_G(x) \\ &- \sum_{x \in V_2(G)} d_x D_G(x) \\ = \;& 4[W(H) - W(G)] + \sum_{x \in V_2(H)} (d_x^* - 2) D_H(x) \\ &- \sum_{x \in V_2(G)} (d_x - 2) D_G(x). \end{aligned}$$

Let P_n and C_n be the path and the cycle on n vertices, respectively.

Let G be the unicyclic graph obtained from a cycle $C_m = v_0 v_1 \ldots v_{m-1} v_0$ by attaching a path P_a and a path P_b to v_i and v_j, respectively, where $a \geq 1$ and $b \geq 2$. Label the vertices of the path P_b attached to v_j as $u_1, u_2, \ldots, u_b$ consecutively, where u_1 is adjacent to v_j in G. For integer $h \geq 1$, let $G^{(1)}_{u_t,h}$ be the graph obtained from G by attaching h pendant vertices to u_t, where $1 \leq t \leq b-1$, and $G^{(2)}_{v_t,h}$ be the graph obtained from G by attaching h pendant vertices to v_t, where $0 \leq t \leq m-1$.

Lemma 2.3. *Let $c = d_G(v_i, v_j)$, $t_1 = d_G(v_i, v_t)$ and $t_2 = d_G(v_j, v_t)$, where $G = G^{(2)}_{v_t,h}$. If $t \neq i$, then*

$$D'\left(G^{(2)}_{v_i,h}\right) - D'\left(G^{(2)}_{v_t,h}\right) = 4h[b(c - t_2) - at_1].$$

Proof. Denote by u^* the pendant vertex of the path attached to v_i in $G^{(2)}_{v_t,h}$, and v a pendant vertex attached to v_i in $G^{(2)}_{v_i,h}$ and v_t in $G^{(2)}_{v_t,h}$, respectively. Let $G_1 = G^{(2)}_{v_i,h}$ and $G_2 = G^{(2)}_{v_t,h}$. Note that $D_{G_1}(v_i) -$

$D_{G_2}(v_i) = D_{G_1}(u^*) - D_{G_2}(u^*)$, $D_{G_1}(v_j) - D_{G_2}(v_j) = D_{G_1}(u_b) - D_{G_2}(u_b)$, and $D_{G_1}(v_i) - D_{G_1}(v) = D_{G_2}(v_t) - D_{G_2}(v)$. If $i \neq j$ and $t \neq j$, then

$$\begin{aligned}
& D'\left(G^{(2)}_{v_i,h}\right) - D'\left(^{(2)}_{v_t,h}\right) \\
= \; & 4[W(G_1) - W(G_2)] - [D_{G_1}(u^*) - D_{G_2}(u^*)] \\
& +[D_{G_1}(v_j) - D_{G_2}(v_j)] - [D_{G_1}(u_b) - D_{G_2}(u_b)] \\
& -h[D_{G_1}(v) - D_{G_2}(v)] + (h+1)D_{G_1}(v_i) - hD_{G_2}(v_t) - D_{G_2}(v_i) \\
= \; & 4[W(G_1) - W(G_2)] - h[D_{G_1}(v) - D_{G_2}(v)] + h[D_{G_1}(v_i) - D_{G_2}(v_t)] \\
= \; & 4[W(G_1) - W(G_2)] \\
= \; & 4h[b(c - t_2) - at_1],
\end{aligned}$$

and if $i = j$ or $t = j$, then by similar argument, the result holds also. □

Lemma 2.4. *Let* $n_1 = a + m - 1$ *and* $n_2 = b - t$ *in* $G^{(1)}_{u_t,h}$. *Then*

$$D'\left(G^{(2)}_{v_j,h}\right) - D'\left(G^{(1)}_{u_t,h}\right) = 2ht[2(n_2 - n_1) - 1].$$

Proof. Denote by u^* the pendant vertex of the path attached to v_i in $G^{(1)}_{u_t,h}$, and v a pendant vertex attached to v_j in $G^{(2)}_{v_j,h}$ and u_t in $G^{(1)}_{u_t,h}$, respectively. Let $G_1 = G^{(2)}_{v_j,h}$ and $G_2 = G^{(1)}_{u_t,h}$. Note that $D_{G_1}(v_i) - D_{G_2}(v_i) = D_{G_1}(u^*) - D_{G_2}(u^*)$ and $D_{G_1}(v_j) - D_{G_1}(v) = D_{G_2}(u_t) - D_{G_2}(v)$. If $i \neq j$, then

$$\begin{aligned}
& D'\left(G^{(2)}_{v_j,h}\right) - D'\left(G^{(1)}_{u_t,h}\right) \\
= \; & 4[W(G_1) - W(G_2)] + [D_{G_1}(v_i) - D_{G_2}(v_i)] \\
& -[D_{G_1}(u^*) - D_{G_2}(u^*)] - [D_{G_1}(u_b) - D_{G_2}(u_b)] \\
& -h[D_{G_1}(v) - D_{G_2}(v)] + (h+1)D_{G_1}(v_j) - hD_{G_2}(u_t) - D_{G_2}(v_j) \\
= \; & 4[W(G_1) - W(G_2)] - [D_{G_1}(u_b) - D_{G_2}(u_b)] + [D_{G_1}(v_j) - D_{G_2}(v_j)] \\
= \; & 4ht(n_2 - n_1) - ht - ht \\
= \; & 2ht[2(n_2 - n_1) - 1],
\end{aligned}$$

and if $i = j$, then by similar argument, the result holds also. □

As usual, $G - E_1$ means the graph obtained from G by deleting the edges of $E_1 \subseteq E(G)$, and $G + E_2$ means the graph obtained from G by adding the edges of $E_2 \subseteq E(\overline{G})$, where $\overline{G}$ is the complement of G.

3. Minimum Degree Distance of Unicyclic Graphs with Given Girth and Diameter

In this section we determine the unicyclic graphs with minimum degree distance when the number of vertices, girth and diameter are given.

Let n, m and d be integers with $3 \le m \le n-1$ and $2 \le d \le n-\lfloor \frac{m+1}{2} \rfloor$. For $a \ge b \ge 0$ and $a \ge 1$, let $U^k_{n,m,d}(a,b)$ be the unicyclic graph obtained from the cycle $C_m = v_0v_1 \dots v_{m-1}v_0$ by attaching a path P_a to v_0 and a path P_b to $v_{\lfloor \frac{m}{2} \rfloor}$ respectively (if $b = 0$, then by attaching only a path P_a to v_0), where $a+b = d - \lfloor \frac{m}{2} \rfloor$, and attaching $n-d-\lfloor \frac{m+1}{2} \rfloor$ pendant vertices to v_k, where $0 \le k \le \lfloor \frac{m}{4} \rfloor$. Let $U_{n,m,d}(a,b) = U^0_{n,m,d}(a,b)$.

For $U_{n,m,d}(a,b)$, let u_0 be the pendant vertex on the path attached to v_0, let u_1 be the pendant vertex on the path attached to $v_{\lfloor \frac{m}{2} \rfloor}$ if $b \ge 1$, and $u_1 = v_{\lfloor \frac{m}{2} \rfloor}$ if $b = 0$, and let u be any of the pendant vertices attached to v_0.

Let $\alpha = \alpha(n,m,d) = \frac{\left(n-d-\lfloor \frac{m+1}{2} \rfloor\right)\lfloor \frac{m}{2} \rfloor}{n-d-\frac{1}{2}}$. Let γ and θ be integers such that $\gamma + \theta = d - \left\lfloor \frac{m}{2} \right\rfloor$ and $\gamma - \theta$ is an integer as large as possible but no more than $\alpha + 1$. Let $U_{n,m,d} = U_{n,m,d}(\gamma,\theta) = U^0_{n,m,d}(\gamma,\theta)$.

Lemma 3.1. *Let n, m and d be fixed integers with $3 \le m \le n-2$ and $3 \le d \le n-\lfloor \frac{m+1}{2} \rfloor$. Then $D'\left(U_{n,m,d}(a,b)\right)$ with $a \ge b$ and $a+b = d-\left\lfloor \frac{m}{2} \right\rfloor$ is minimum if and only if $(a,b) = (\gamma,\theta)$, $(\gamma-1,\theta+1)$ if $\alpha \ge 1$ is an integer with different parity as $d - \left\lfloor \frac{m}{2} \right\rfloor$, and $(a,b) = (\gamma,\theta)$ otherwise.*

Proof. Let $h = n-d-\lfloor \frac{m+1}{2} \rfloor$. Let w be the neighbor of u_0 in $U_{n,m,d}(a,b)$. Note that for $a-b \ge 2$, $U_{n,m,d}(a-1,b+1) \cong U_{n,m,d}(a,b)-\{u_0w\}+\{u_0u_1\}$. Let $G_1 = U_{n,m,d}(a-1,b+1)$ and $G_2 = U_{n,m,d}(a,b)$. If $a \ge b \ge 1$, then

$$\begin{aligned} & D'(U_{n,m,d}(a-1,b+1)) - D'(U_{n,m,d}(a,b)) \\ = \; & 4[W(G_1) - W(G_2)] - h[D_{G_1}(u) - D_{G_2}(u)] \\ & -[D_{G_1}(u_0) - D_{G_2}(u_0)] + [D_{G_1}(v_{\lfloor \frac{m}{2} \rfloor}) - D_{G_2}(v_{\lfloor \frac{m}{2} \rfloor})] \\ & +(h+1)[D_{G_1}(v_0) - D_{G_2}(v_0)] - D_{G_1}(w) + D_{G_2}(u_1) \\ = \; & 4\left[(1-a+b)\left(h + \left\lfloor \frac{m-1}{2} \right\rfloor + \frac{1}{2}\right) + h\left\lfloor \frac{m}{2} \right\rfloor\right], \end{aligned}$$

and if $a = d - \lfloor \frac{m}{2} \rfloor$ and $b = 0$, then

$$\begin{aligned} & D'(U_{n,m,d}(a-1,b+1)) - D'(U_{n,m,d}(a,b)) \\ = \; & 4[W(G_1) - W(G_2)] - h[D_{G_1}(u) - D_{G_2}(u)] \\ & -[D_{G_1}(u_0) - D_{G_2}(u_0)] + (h+1)[D_{G_1}(v_0) - D_{G_2}(v_0)] \end{aligned}$$

$$+D_{G_1}(v_{\lfloor \frac{m}{2} \rfloor}) - D_{G_1}(w)$$
$$= 4\left[(1-a)\left(h + \left\lfloor \frac{m-1}{2} \right\rfloor + \frac{1}{2}\right) + h\left\lfloor \frac{m}{2} \right\rfloor\right].$$

Thus $D'(U_{n,m,d}(a-1,b+1)) \geq D'(U_{n,m,d}(a,b))$ if and only if $a-b \leq \alpha+1$, and $D'(U_{n,m,d}(a-1,b+1)) = D'(U_{n,m,d}(a,b))$ if and only if $a-b = \alpha+1$. Thus $D'(U_{n,m,d}(a,b))$ is minimum if and only if $a-b$ is as large as possible with $a-b \leq \alpha+1$. Note that $a-b = \alpha+1$ if and only if $\alpha \geq 1$ is an integer with different parity as $d - \left\lfloor \frac{m}{2} \right\rfloor$. The result follows. □

Let $\mathbb{U}(n,m,d)$ be the set of unicyclic graphs with n vertices, girth m and diameter d, where $2 \leq d \leq n - \lfloor \frac{m+1}{2} \rfloor$ and $3 \leq m \leq n-2$. If $G \in \mathbb{U}(n,m,2)$, then $m = 3$ and $G \cong U_{n,3,2}(1,0)$.

Let G be a unicyclic graph with n vertices and let $C_m = v_0v_1 \ldots v_{m-1}v_0$ be its unique cycle. Then $G - E(C_m)$ consists of m trees $T_0, T_1, \ldots, T_{m-1}$, where $v_i \in V(T_i)$ for $i = 0, 1, \ldots, m-1$. If the degree of v_i is at least three, then the components obtained from T_i by deleting the vertex v_i (and its incident edges) are called the branches of G at v_i, each containing a neighbor of v_i in T_i.

Lemma 3.2. *Let n, m and d be integers with $3 \leq m \leq n-2$ and $3 \leq d \leq n - \lfloor \frac{m+1}{2} \rfloor$, and let $\beta = \frac{1}{2}(d - \lfloor \frac{m}{2} \rfloor)$. If G is a graph with minimum degree distance in $\mathbb{U}(n,m,d)$, then $G \cong U_{n,m,d}(a,b) = U^0_{n,m,d}(a,b)$ with $a \geq b$ or $G \cong U^k_{n,m,d}(\beta,\beta)$ for $k = 1, 2, \ldots, \lfloor \frac{m}{4} \rfloor$.*

Proof. Let $C_m = v_0v_1 \ldots v_{m-1}v_0$ be the unique cycle of G, and let $P(G) = u_0u_1 \ldots u_d$ be a diametrical path of G. Let $d(x,y) = d_G(x,y)$ for $x, y \in V(G)$.

Suppose that $P(G)$ has no common vertices with C_m. Let u_s and v_t be the vertices such that $d(u_s, v_t) = \min\{d(u,v) : u \in V(P(G)), v \in V(C_m)\}$. Using Lemma 2.1 (ii) by setting $u = u_s$, $v = v_t$, M to be the subgraph of G consisting of the path $P(G)$ and the trees attached to u_i for all $1 \leq i \leq d-1$ and $i \neq s$, N to be the subgraph of G by deleting all branches at v_t, we can obtain a graph G^* for which $P(G^*)$ $(= P(G))$ and the cycle C_m have exactly one common vertex and $D'(G^*) < D'(G)$, a contradiction. Thus $P(G)$ and C_m have at least one common vertex. We may choose $P(G)$ such that $P(G)$ and the cycle C_m have common vertices as many as possible and u_0 is a pendant vertex.

Let u_a and u_l be the common vertices of $P(G)$ and C_m such that they have the smallest and largest subscript, respectively, among vertices in $P(G)$, where $0 < a \leq l \leq d$. Let $u_a = v_i$ and $u_l = v_j$. By Lemma 2.1 (i), all vertices outside C_m except those in T_i and T_j are pendant vertices attached to vertices that are nearest to them in C_m, all vertices in T_i and T_j except those in $P(G)$ are pendant vertices attached to vertices that are nearest to them in $P(G)$.

Suppose that $P(G)$ and C_m have only one common vertex, i.e., $i = j$, $a = l$ and $l < d$. By the choice of $P(G)$, we have $a \geq 2$. By Lemma 2.2, all pendant vertices in G except u_0 and u_d are actually attached to some vertex, say s, of G.

Suppose that $s \in \{v_0, v_1, \ldots, v_{m-1}\} \setminus \{v_i\}$, say $s = v_q$. Denote by $v_{q_1}, v_{q_2}, \ldots, v_{q_t}$ the pendant neighbors of v_q. Let $H = G - \{v_q v_{q_1}, v_q v_{q_2}, \ldots, v_q v_{q_t}\} + \{v_i v_{q_1}, v_i v_{q_2}, \ldots, v_i v_{q_t}\}$. Then $H \in \mathbb{U}(n, m, d)$. By Lemma 2.3, we have

$$D'(H) - D'(G) = -4dt \cdot d(v_q, v_i) < 0,$$

a contradiction. Thus $s \in \{u_1, u_2, \ldots, u_{d-1}\}$. Suppose without loss of generality that $s \in \{u_a, u_{a+1}, \ldots, u_{d-1}\}$. Let $H^* = G - \{u_{a-2}u_{a-1}\} + \{u_{a-2}v_{i-1}\}$. Then $H^* \in \mathbb{U}(n, m, d)$. Note that the (diametrical) path $P(H^*) = u_0 u_1 \ldots u_{a-2} v_{i-1} v_i u_{a+1} u_{a+2} \ldots u_d$ has more than one common vertex with the cycle C_m and the same length as $P(G)$. Then

$$\begin{aligned} D'(H^*) - D'(G) &= 4[W(H^*) - W(G)] - [D_{H^*}(u_0) - D_G(u_0)] \\ &\quad + D_{H^*}(v_{i-1}) - D_{H^*}(u_{a-1}) \\ &= -4(m-2)(a-1) + (m-2) - 2a - m + 4 \\ &= -2(a-1)(2m-3) < 0, \end{aligned}$$

and thus $D'(H^*) < D'(G)$, a contradiction. It follows that $P(G)$ and C_m have at least two common vertices, i.e., $a < l$.

By Lemma 2.2, all pendant vertices in G except u_0 and u_d are actually attached to some vertex, say x, in G. Thus x has exactly $h = n - m - a - (d - l)$ pendant neighbors outside $P(G)$. Let $b = d - l$. Assume that $a \geq b$.

Suppose that $l < d$ and $x \in \{u_{l+1}, u_{l+2}, \ldots, u_{d-1}\}$, say $x = u_q$, where $l < q \leq d-1$. Let $u_{q_1}, u_{q_2}, \ldots, u_{q_h}$ be the pendant neighbors of u_q outside $P(G)$. Let $G_1 = G - \{u_q u_{q_1}, u_q u_{q_2}, \ldots, u_q u_{q_h}\} + \{u_l u_{q_1}, u_l u_{q_2}, \ldots, u_l u_{q_h}\}$. Then $G_1 \in \mathbb{U}(n, m, d)$. Using Lemma 2.4 by setting $t = q - l$, $n_1 = a + m - 1$ and $n_2 = b - t$, and noting that $n_1 > n_2$ since $a \geq b$, we have

$$D'(G_1) - D'(G) = 2h(q-l)[2(n_2 - n_1) - 1] < 0,$$

and then $D'(G_1) < D'(G)$, a contradiction. Thus $x \notin \{u_{l+1}, u_{l+2}, \ldots, u_{d-1}\}$ if $l < d$. Moreover, if $a = b$, then by similar argument, $x \notin \{u_1, u_2, \ldots, u_{a-1}\}$, and thus $x \in \{v_0, v_1, \ldots, v_{m-1}\}$.

Case 1. $a > b$.

First we prove that $x \in \{u_1, u_2, \ldots, u_a\}$. Suppose to the contrary that $x = v_s$ with $0 \le s \le m-1$ and $s \ne i$. Denote by $v_{s_1}, v_{s_2}, \ldots, v_{s_h}$ the pendant neighbors of v_s. Suppose that $d(v_i, v_j) = c$, $d(v_i, v_s) = t_1$ and $d(v_j, v_s) = t_2$, then $c \le t_1 + t_2$. Let $G_2 = G - \{v_s v_{s_1}, v_s v_{s_2}, \ldots, v_s v_{s_h}\} + \{v_i v_{s_1}, v_i v_{s_2}, \ldots, v_i v_{s_h}\}$. Then $G_2 \in \mathbb{U}(n, m, d)$. Note that $b = 0$ if $l = d$. By Lemma 2.3, we have

$$\begin{aligned} D'(G_2) - D'(G) &= 4h[b(c - t_2) - at_1] \le 4h(bt_1 - at_1) \\ &= 4ht_1(b - a) < 0, \end{aligned}$$

and then $D'(G_2) < D'(G)$, a contradiction. Thus $x \in \{u_1, u_2, \ldots, u_a\}$, say $x = u_p$ with $1 \le p \le a$.

Next we prove that $d(v_i, v_j) = \lfloor \frac{m}{2} \rfloor$. If $l = d$, then it is obvious. Suppose that $l < d$ and $c = d(v_i, v_j) < \lfloor \frac{m}{2} \rfloor$. Let v be the neighbor of v_j on C_m with $d(v_i, v) = c + 1$ ($v = v_{j+1}$ if $\{v_i, v_{i+1}, \ldots, v_{j-1}, v_j\}$ is a shortest path from v_i to v_j). By the choice of $P(G)$, we have $b + c > \lfloor \frac{m}{2} \rfloor$, and then $b > 1$. Let $G_3 = G - \{v_j u_{l+1}\} + \{v u_{l+1}\} - \{u_{d-1} u_d\} + \{v_i u_d\}$. Then $G_3 \in \mathbb{U}(n, m, d)$. If $1 \le p \le a - 1$, then

$$\begin{aligned} & D'(G_3) - D'(G) \\ = \; & 4[W(G_3) - W(G)] - [D_{G_3}(u_0) - D_G(u_0)] - [D_{G_3}(u_d) - D_G(u_d)] \\ & + 2D_{G_3}(v_i) + D_{G_3}(v) - D_{G_3}(u_{d-1}) - D_G(v_i) - D_G(v_j) \\ = \; & -2(2m - 3)(b - 1) - 4c(n - m - 2b + 1) < 0, \end{aligned}$$

if $p = a$, then by similar calculation,

$$D'(G_3) - D'(G) = -2(2m - 3)(b - 1) - 4c(n - m - 2b + 1) < 0.$$

It follows that $D'(G_3) < D'(G)$ for $1 \le p \le a$, a contradiction. Thus $d(v_i, v_j) = \lfloor \frac{m}{2} \rfloor$ and $h = n - d - \lfloor \frac{m+1}{2} \rfloor$.

Now we prove that $p = a$. Suppose to the contrary that $p \le a - 1$. Let $u_{p_1}, u_{p_2}, \ldots, u_{p_h}$ be the pendant neighbors of u_p outside $P(G)$. Suppose first that $b + m > a$. Then $p < b + m - 1$. Let $G_4 = G - \{u_p u_{p_1}, u_p u_{p_2}, \ldots, u_p u_{p_h}\} + \{u_a u_{p_1}, u_a u_{p_2}, \ldots, u_a u_{p_h}\}$. Then $G_4 \in \mathbb{U}(n, m, d)$. Using Lemma 2.4 by setting $t = a - p$, $n_1 = b + m - 1$ and $n_2 = p$, we have

$$D'(G_4) - D'(G) \;=\; 2h(a - p)[2p - 2(b + m - 1) - 1] < 0,$$

and thus $D'(G_4) < D'(G)$, a contradiction. Now suppose that $b + m \le a$. Then $b - (h - 1) < a$. Let $G_4 = G - \{u_p u_{p_1}, u_p u_{p_2}, \ldots, u_p u_{p_h}\} +$

$\{u_{p+1}u_{p_1}, u_{p+1}u_{p_2}, \ldots, u_{p+1}u_{p_h}\} - \{u_0u_1\} + \{u_0u_d\}$. Then $G_4 \in \mathbb{U}(n, m, d)$. If $l < d$ and $1 \leq p \leq a-2$, then

$$\begin{aligned} & D'(G_4) - D'(G) \\ = \; & 4[W(G_4) - W(G)] + [D_{G_4}(u_a) - D_G(u_a)] + [D_{G_4}(u_l) - D_G(u_l)] \\ & -[D_{G_4}(u_0) - D_G(u_0)] - h[D_{G_4}(u_{p_1}) - D_G(u_{p_1})] \\ & +hD_{G_4}(u_{p+1}) - D_{G_4}(u_1) - hD_G(u_p) + D_G(u_d) \\ = \; & 2\left(2\left\lfloor \frac{m-1}{2} \right\rfloor + 1\right)(b - a + 1 - h) < 0. \end{aligned}$$

By similar calculation, $D'(G_4) - D'(G) < 0$ holds also if $l = d$ or $p = a-1$. Then in any case we have $D'(G_4) < D'(G)$, a contradiction. Thus $p = a$.

Now we have proved that $G \cong U_{n,m,d}(a, b)$, where $a > b$ and $a + b = d - \lfloor \frac{m}{2} \rfloor$.

Case 2. $a = b$.

Note that $x \in \{v_0, v_1, \ldots, v_{m-1}\}$, say $x = v_s$. Assume that $v_iv_{i+1}\ldots v_{j-1}v_j$ is a shortest path from v_i to v_j in G. Obviously, $m \geq 2(j-i)$. If $m = 2(j-i)$, then by symmetry, we may assume that $i \leq s \leq j$. Suppose that $m > 2(j-i)$ and $s \notin \{i, i+1, \ldots, j-1, j\}$. Denote by $v_{s_1}, v_{s_2}, \ldots, v_{s_h}$ the pendant neighbors of v_s. Let $d(v_i, v_j) = j - i = c$, $d(v_i, v_s) = t_1$ and $d(v_j, v_s) = t_2$. Then $c < t_1 + t_2$. Let $G_5 = G - \{v_sv_{s_1}, v_sv_{s_2}, \ldots, v_sv_{s_h}\} + \{v_iv_{s_1}, v_iv_{s_2}, \ldots, v_iv_{s_h}\}$. Then $G_5 \in \mathbb{U}(n, m, d)$. By Lemma 2.3, we have

$$D'(G_5) - D'(G) = 4h[b(c - t_2) - at_1] = 4ha(c - t_1 - t_2) < 0,$$

and then $D'(G_5) < D'(G)$, a contradiction. Thus $i \leq s \leq j$.

Suppose that $c = d(v_i, v_j) < \lfloor \frac{m}{2} \rfloor$. Note that $d(v_i, v_{j+1}) = c + 1$. By the choice of $P(G)$, we have $b + c > \lfloor \frac{m}{2} \rfloor$, and then $b > 1$. Let $G_6 = G - \{v_ju_{l+1}\} + \{v_{j+1}u_{l+1}\} - \{u_{d-1}u_d\} + \{v_su_d\}$. Then $G_6 \in \mathbb{U}(n, m, d)$. If $i + 1 \leq s \leq j - 1$, then

$$\begin{aligned} & D'(G_6) - D'(G) \\ = \; & 4[W(G_6) - W(G)] - [D_{G_6}(u_0) - D_G(u_0)] - [D_{G_6}(u_d) - D_G(u_d)] \\ & -h[D_{G_6}(v_{s_1}) - D_G(v_{s_1})] + [D_{G_6}(v_i) - D_G(v_i)] \\ & +(h+1)D_{G_6}(v_s) - D_{G_6}(u_{d-1}) + D_{G_6}(v_{j+1}) - hD_G(v_s) - D_G(v_j) \\ = \; & -2(2m-3)(b-1) - 4(j-s)(h+1) < 0. \end{aligned}$$

By similar calculation, $D'(G_6) - D'(G) < 0$ holds also if $s = i$ or j. In any case, we have $D'(G_6) < D'(G)$, a contradiction. Thus $d(v_i, v_j) = \lfloor \frac{m}{2} \rfloor$ and $h = n - d - \lfloor \frac{m+1}{2} \rfloor$. By Lemma 2.3, we have $U^k_{n,m,d}(\beta, \beta)$ for

$k = 0, 1, \ldots, \lfloor \frac{m}{4} \rfloor$ have equal degree distance, and thus $G \cong U^k_{n,m,d}(\beta, \beta)$ for $k = 0, 1, \ldots, \lfloor \frac{m}{4} \rfloor$.

By combining Cases 1 and 2, we have $G \cong U_{n,m,d}(a, b) = U^0_{n,m,d}(a, b)$ with $a \geq b$ or $G \cong U^k_{n,m,d}(\beta, \beta)$ for $k = 1, 2, \ldots, \lfloor \frac{m}{4} \rfloor$. □

Theorem 3.3. *Let n, m and d be integers with $3 \leq m \leq n-2$ and $3 \leq d \leq n - \lfloor \frac{m+1}{2} \rfloor$, and let $\alpha = \frac{(n-d-\lfloor \frac{m+1}{2} \rfloor)\lfloor \frac{m}{2} \rfloor}{n-d-\frac{1}{2}}$, $\beta = \frac{1}{2}(d - \lfloor \frac{m}{2} \rfloor)$.*

- (i) *If $0 < \alpha < 1$ and $d - \lfloor \frac{m}{2} \rfloor$ is even, then $U^k_{n,m,d}(\beta, \beta)$ for $k = 0, 1, \ldots, \lfloor \frac{m}{4} \rfloor$ are the unique graphs in $\mathbb{U}(n, m, d)$ with minimum degree distance.*
- (ii) *If $\alpha = 1$ and $d - \lfloor \frac{m}{2} \rfloor$ is even, then $U_{n,m,d} = U_{n,m,d}(\beta+1, \beta-1)$ and $U^k_{n,m,d}(\beta, \beta)$ for $k = 0, 1, \ldots, \lfloor \frac{m}{4} \rfloor$ are the unique graphs in $\mathbb{U}(n, m, d)$ with minimum degree distance.*
- (iii) *If $\alpha > 1$ is an integer with different parity as $d - \lfloor \frac{m}{2} \rfloor$, then $U_{n,m,d}$ and $U_{n,m,d}(\gamma-1, \theta+1)$ are the unique graphs in $\mathbb{U}(n, m, d)$ with minimum degree distance.*
- (iv) *If $\alpha = 0$, or $0 < \alpha \leq 1$ and $d - \lfloor \frac{m}{2} \rfloor$ is odd, or $\alpha > 1$ is not an integer or is an integer with the same parity as $d - \lfloor \frac{m}{2} \rfloor$, then $U_{n,m,d}$ is the unique graph in $\mathbb{U}(n, m, d)$ with minimum degree distance.*

Proof. Suppose that G is a graph in $\mathbb{U}(n, m, d)$ with minimum degree distance. By Lemma 3.2, we have $G \cong U_{n,m,d}(a, b) = U^0_{n,m,d}(a, b)$ with $a \geq b$ or $G \cong U^k_{n,m,d}(\beta, \beta)$ for $k = 1, 2, \ldots, \lfloor \frac{m}{4} \rfloor$. If $G \cong U_{n,m,d}(a, b)$, then we have by Lemma 3.1 that $G \cong U_{n,m,d}$ or $U_{n,m,d}(\gamma-1, \theta+1)$ if $\alpha \geq 1$ is an integer with different parity as $d - \lfloor \frac{m}{2} \rfloor$, and $G \cong U_{n,m,d}$ otherwise.

If $d - \lfloor \frac{m}{2} \rfloor$ is odd, then $G \cong U_{n,m,d}$ or $U_{n,m,d}(\gamma-1, \theta+1)$ if $\alpha \geq 1$ is an even integer, and $G \cong U_{n,m,d}$ otherwise.

Suppose in the following that $d - \lfloor \frac{m}{2} \rfloor$ is even. Then $G \cong U^k_{n,m,d}(\beta, \beta)$ for $k = 1, 2, \ldots, \lfloor \frac{m}{4} \rfloor$, or $G \cong U_{n,m,d}$, $U_{n,m,d}(\gamma-1, \theta+1)$ if $\alpha \geq 1$ is an odd integer, and $G \cong U_{n,m,d}$ otherwise.

If $\alpha = 0$, then $G \cong U_{n,m,d}$.

If $0 < \alpha < 1$, then $G \cong U^k_{n,m,d}(\beta, \beta)$ for $k = 0, 1, \ldots, \lfloor \frac{m}{4} \rfloor$.

Suppose that $\alpha = 1$. Then $G \cong U_{n,m,d}$, $U_{n,m,d}(\gamma-1, \theta+1)$, or $G \cong U^k_{n,m,d}(\beta, \beta)$ for $k = 1, 2, \ldots, \lfloor \frac{m}{4} \rfloor$. Since $(\gamma-1, \theta+1) = (\beta, \beta)$, we have $G \cong U_{n,m,d}$, or $U^k_{n,m,d}(\beta, \beta)$ for $k = 0, 1, \ldots, \lfloor \frac{m}{4} \rfloor$.

Suppose that $\alpha > 1$ is an odd integer. Then $G \cong U_{n,m,d}$, $U_{n,m,d}(\gamma - 1, \theta + 1)$, or $G \cong U^k_{n,m,d}(\beta, \beta)$ for $k = 1, 2, \ldots, \lfloor \frac{m}{4} \rfloor$. By Lemmas 2.3 and 3.1, we have

$$\begin{aligned} & D'(U^k_{n,m,d}(\beta,\beta)) = D'(U^0_{n,m,d}(\beta,\beta)) \\ > \quad & D'(U_{n,m,d}(\gamma,\theta)) = D'\left(U_{n,m,d}(\gamma-1,\theta+1)\right) \end{aligned}$$

for $k = 1, 2, \ldots, \lfloor \frac{m}{4} \rfloor$. Thus $G \cong U_{n,m,d}$ or $U_{n,m,d}(\gamma - 1, \theta + 1)$.

Suppose that $\alpha > 1$ is not an odd integer. Then $G \cong U_{n,m,d}$, or $G \cong U^k_{n,m,d}(\beta, \beta)$ for $k = 1, 2, \ldots, \lfloor \frac{m}{4} \rfloor$. By Lemmas 2.3 and 3.1, we have

$$D'(U^k_{n,m,d}(\beta,\beta)) = D'(U^0_{n,m,d}(\beta,\beta)) > D'(U_{n,m,d}(\gamma,\theta))$$

for $k = 1, 2, \ldots, \lfloor \frac{m}{4} \rfloor$. Thus $G \cong U_{n,m,d}$. □

Corollary 3.4. *Let $G \in \mathbb{U}(n, m, d)$ with $3 \le m \le n - 2$ and $3 \le d \le n - \lfloor \frac{m+1}{2} \rfloor$. Then*

$$D'(G) \ge D'\left(U_{n,m,d}\right).$$

4. Maximum Reverse Degree Distance of Unicyclic Graphs

In this section we determine the unicyclic graphs on n vertices with maximum reverse degree distances when girth, number of pendant vertices and maximum degree are given, respectively.

Lemma 4.1. *For $3 \le m \le n - 2$ and $2 \le d < n - \left\lfloor \frac{m+1}{2} \right\rfloor$,*

$${}^{r}D'(U_{n,m,d}) < {}^{r}D'(U_{n,m,d+1}).$$

Proof. Let $h = n - d - \lfloor \frac{m+1}{2} \rfloor$. Let u_2 be a pendant neighbor of v_0 different from u in $U_{n,m,d}$ if $h \ge 2$. Recall that $U_{n,m,d} = U_{n,m,d}(\gamma, \theta)$. Note that we may obtain $U_{n,m,d+1}(\gamma+1, \theta)$ from $U_{n,m,d}(\gamma, \theta)$ by deleting the edge uv_0 and adding the edge uu_0. Let $G_1 = U_{n,m,d+1}(\gamma + 1, \theta)$ and $G_2 = U_{n,m,d}(\gamma, \theta)$. If $\theta \ge 1$ and $h \ge 2$, then $D_{G_1}\left(v_{\lfloor \frac{m}{2} \rfloor}\right) - D_{G_2}\left(v_{\lfloor \frac{m}{2} \rfloor}\right) = D_{G_1}(u_1) - D_{G_2}(u_1)$, and thus

$$\begin{aligned} & D'(U_{n,m,d+1}(\gamma+1,\theta)) - D'(U_{n,m,d}(\gamma,\theta)) \\ = \quad & 4[W(G_1) - W(G_2)] - (h-1)[D_{G_1}(u_2) - D_{G_2}(u_2)] \\ & -[D_{G_1}(u) - D_{G_2}(u)] + hD_{G_1}(v_0) - (h+1)D_{G_2}(v_0) + D_{G_2}(u_0) \\ = \quad & 4\gamma(n-\gamma-2) - (h-1)\gamma - \gamma(n-\gamma-2) + \gamma(n-\gamma+h-1) \\ = \quad & -4\gamma^2 + 2(2n-3)\gamma. \end{aligned}$$

If $\theta = 0$ or $h = 1$, then by similar calculation, we also have $D'(U_{n,m,d+1}(\gamma + 1, \theta)) - D'(U_{n,m,d}(\gamma, \theta)) = -4\gamma^2 + 2(2n-3)\gamma$. Thus

$$\begin{aligned} & {}^{r}D'(U_{n,m,d+1}(\gamma+1,\theta)) - {}^{r}D'(U_{n,m,d}(\gamma,\theta)) \\ = \;& 2(n-1)n - [D'(U_{n,m,d+1}(\gamma+1,\theta)) - D'(U_{n,m,d}(\gamma,\theta))] \\ = \;& 4\gamma^2 - 2(2n-3)\gamma + 2n^2 - 2n \\ \geq \;& 4\left(\frac{2n-3}{4}\right)^2 - 2(2n-3)\cdot\frac{2n-3}{4} + 2n^2 - 2n \\ = \;& n^2 + n - \frac{9}{4} > 0. \end{aligned}$$

By Corollary 3.4, we have ${}^{r}D'(U_{n,m,d+1}(\gamma+1,\theta)) \leq {}^{r}D'(U_{n,m,d+1})$. Then the result follows clearly. □

Theorem 4.2. *Let G be a unicyclic graph with n vertices and girth m, where $3 \leq m \leq n-2$. Then*

$${}^{r}D'(G) \leq {}^{r}D'\left(U_{n,m,n-\lfloor\frac{m+1}{2}\rfloor}\right)$$

with equality if and only if $G \cong U_{n,m,n-\lfloor\frac{m+1}{2}\rfloor}$.

Proof. Let d be the diameter of G. Then $2 \leq d \leq n - \lfloor\frac{m+1}{2}\rfloor$. If $d = n - \lfloor\frac{m+1}{2}\rfloor$, then $\alpha = 0$, and by Theorem 3.3 (iv),

$${}^{r}D'(G) \leq {}^{r}D'\left(U_{n,m,n-\lfloor\frac{m+1}{2}\rfloor}\right)$$

with equality if and only if $G \cong U_{n,m,n-\lfloor\frac{m+1}{2}\rfloor}$. If $d = 2$, then $G \cong U_{n,3,2}(1,0)$, similar to the proof of Lemma 4.1, we have ${}^{r}D'(U_{n,3,2}(1,0)) < {}^{r}D'(U_{n,3,3})$. If $3 \leq d < n - \lfloor\frac{m+1}{2}\rfloor$, then by Corollary 3.4 and Lemma 4.1,

$${}^{r}D'(G) \leq {}^{r}D'(U_{n,m,d}) < {}^{r}D'\left(U_{n,m,n-\lfloor\frac{m+1}{2}\rfloor}\right).$$

Then the result follows easily. □

Lemma 4.3. [7] *For $3 \leq m \leq n-1$ and $3 \leq d \leq n - \lfloor\frac{m+1}{2}\rfloor$, let $h = n - d - \lfloor\frac{m+1}{2}\rfloor$. Then*

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

$$+h\left[\left\lfloor\frac{m^2}{4}\right\rfloor+m+\frac{1}{2}a(a+3)+\frac{1}{2}b\left(2\left\lfloor\frac{m}{2}\right\rfloor+b+3\right)\right]+h(h-1),$$

where a, b *are integers with* $a+b=d-\left\lfloor\frac{m}{2}\right\rfloor$, $a \geq b \geq 0$ *and* $a \geq 1$.

By simple calculation, we have

Lemma 4.4. *For* $G=U_{n,m,d}(a,b)$ *with* $3 \leq m \leq n-1$ *and* $3 \leq d \leq n-\lfloor\frac{m+1}{2}\rfloor$, *let* $h=n-d-\left\lfloor\frac{m+1}{2}\right\rfloor$. *Then*

$$\begin{aligned}
D_G(v_0) &= \left\lfloor\frac{m^2}{4}\right\rfloor+\frac{1}{2}a(a+1)+\frac{1}{2}b\left(b+1+2\left\lfloor\frac{m}{2}\right\rfloor\right)+h,\\
D_G\left(v_{\lfloor\frac{m}{2}\rfloor}\right) &= \left\lfloor\frac{m^2}{4}\right\rfloor+\frac{1}{2}a\left(a+1+2\left\lfloor\frac{m}{2}\right\rfloor\right)+\frac{1}{2}b(b+1)\\
&\quad +h\left(1+\left\lfloor\frac{m}{2}\right\rfloor\right),\\
D_G(u) &= \left\lfloor\frac{m^2}{4}\right\rfloor+m+\frac{1}{2}a(a+3)+\frac{1}{2}b\left(2\left\lfloor\frac{m}{2}\right\rfloor+b+3\right)\\
&\quad +2(h-1),\\
D_G(u_0) &= \left\lfloor\frac{m^2}{4}\right\rfloor+a\left[\frac{1}{2}(a-1)+m\right]+\frac{1}{2}b\left(2a+2\left\lfloor\frac{m}{2}\right\rfloor+b+1\right)\\
&\quad +h(a+1),\\
D_G(u_1) &= \left\lfloor\frac{m^2}{4}\right\rfloor+b\left[\frac{1}{2}(b-1)+m\right]+\frac{1}{2}a\left(2b+2\left\lfloor\frac{m}{2}\right\rfloor+a+1\right)\\
&\quad +h\left(b+\left\lfloor\frac{m}{2}\right\rfloor+1\right).
\end{aligned}$$

Lemma 4.5. *Let* n *and* m *be integers with* $5 \leq m \leq n-1$. *Let* $d=n-\lfloor\frac{m+1}{2}\rfloor$ *and* $a=n-m$. *Then*

$$^rD'(U_{n,m,d}(a,0)) < {}^rD'(U_{n,m-2,d+1}(a+2,0)).$$

Proof. Let $G_1=U_{n,m-2,d+1}(a+2,0)$ and $G_2=U_{n,m,d}(a,0)$. Note that $h=n-d-\left\lfloor\frac{m+1}{2}\right\rfloor=0$. By Lemmas 4.3 and 4.4, we have

$$\begin{aligned}
&D'(U_{n,m-2,d+1}(a+2,0))-D'(U_{n,m,d}(a,0))\\
=\ & 4[W(G_1)-W(G_2)]-[D_{G_1}(u_0)-D_{G_2}(u_0)]\\
&+[D_{G_1}(v_0)-D_{G_2}(v_0)]\\
=\ & 4\left[-\frac{3}{2}m^2+\left(n+\frac{9}{2}\right)m+\left\lfloor\frac{m^2}{4}\right\rfloor-2n-4\right]-(m-2)\\
&+(2n-3m+4)
\end{aligned}$$

$$= \quad -6m^2 + 2(2n+7)m + 4\left\lfloor \frac{m^2}{4} \right\rfloor - 6n - 10.$$

Thus

$$\begin{aligned}
& {}^{r}\!D'(U_{n,m-2,d+1}(a+2,0)) - {}^{r}\!D'(U_{n,m,d}(a,0)) \\
= \;& 2(n-1)n - [D'(U_{n,m-2,d+1}(a+2,0)) - D'(U_{n,m,d}(a,0))] \\
= \;& 6m^2 - 2(2n+7)m - 4\left\lfloor \frac{m^2}{4} \right\rfloor + 2n^2 + 4n + 10 \\
= \;& \begin{cases} 5m^2 - 2(2n+7)m + 2n^2 + 4n + 10 & \text{if } m \text{ is even} \\ 5m^2 - 2(2n+7)m + 2n^2 + 4n + 11 & \text{if } m \text{ is odd} \end{cases} \\
\geq \;& 5m^2 - 2(2n+7)m + 2n^2 + 4n + 10 \\
\geq \;& 5 \cdot \left(\frac{2n+7}{5}\right)^2 - 2(2n+7) \cdot \frac{2n+7}{5} + 2n^2 + 4n + 10 \\
= \;& \frac{1}{5}(6n^2 - 8n + 1) > 0.
\end{aligned}$$

The result follows. □

Lemma 4.6. *Let n, m and d be integers with $5 \leq m \leq n-2$, $3 \leq d \leq n - \lfloor \frac{m+1}{2} \rfloor$, and let a and b be integers with $a + b = d - \lfloor \frac{m}{2} \rfloor$, $a \geq b \geq 0$ and $a \geq 1$. Then*

$$ {}^{r}\!D'\left(U_{n,m,d}(a,b)\right) < {}^{r}\!D'\left(U_{n,m-2,d+1}(a+1,b+1)\right).$$

Proof. Let $h = n - d - \lfloor \frac{m+1}{2} \rfloor$. Let $G_1 = U_{n,m-2,d+1}(a+1,b+1)$ and $G_2 = U_{n,m,d}(a,b)$. If $b \geq 1$, then by Lemmas 4.3 and 4.4, we have

$$\begin{aligned}
& D'(U_{n,m-2,d+1}(a+1,b+1)) - D'(U_{n,m,d}(a,b)) \\
= \;& 4[W(G_1) - W(G_2)] \\
& +(h+1)[D_{G_1}(v_0) - D_{G_2}(v_0)] + \left[D_{G_1}\left(v_{\lfloor \frac{m}{2} \rfloor - 1}\right) - D_{G_2}\left(v_{\lfloor \frac{m}{2} \rfloor}\right)\right] \\
& -h[D_{G_1}(u) - D_{G_2}(u)] - [D_{G_1}(u_0) - D_{G_2}(u_0)] \\
& -[D_{G_1}(u_1) - D_{G_2}(u_1)] \\
= \;& 4\left[h\left(2 + a - \left\lfloor \frac{m+1}{2} \right\rfloor\right) - 2 + ab + \left\lfloor \frac{m^2}{4} \right\rfloor \right. \\
& \left. + \left\lfloor \frac{m}{2} \right\rfloor (a+b+1) + \frac{3}{2}m - \frac{m^2}{2}\right] \\
& +(h+1)\left(2 + a - \left\lfloor \frac{m+1}{2} \right\rfloor\right) + \left(2 + b - \left\lfloor \frac{m+1}{2} \right\rfloor - h\right)
\end{aligned}$$

$$
\begin{aligned}
& -h\left(2+a-\left\lfloor\frac{m+1}{2}\right\rfloor\right)-\left(b+\left\lfloor\frac{m}{2}\right\rfloor+h\right)-\left(a+\left\lfloor\frac{m}{2}\right\rfloor\right)\\
= & -4b^2+4(n-m-2h)b+4n\left(\left\lfloor\frac{m}{2}\right\rfloor+h\right)-2m^2-8mh\\
& -4(m-1)\left(\left\lfloor\frac{m}{2}\right\rfloor-1\right)+4\left\lfloor\frac{m^2}{4}\right\rfloor-4h^2+6h.
\end{aligned}
$$

If $b=0$, then by similar calculation, we also have the right most expression for $D'(U_{n,m-2,d+1}(a+1,b+1))-D'(U_{n,m,d}(a,b))$ as above. Thus

$$
\begin{aligned}
& {}^{r}D'(U_{n,m-2,d+1}(a+1,b+1))-{}^{r}D'(U_{n,m,d}(a,b))\\
= & \ 2(n-1)n-[D'(U_{n,m-2,d+1}(a+1,b+1))-D'(U_{n,m,d}(a,b))]\\
= & \ 4b^2-4(n-m-2h)b\\
& +2n^2-4n\left(\left\lfloor\frac{m}{2}\right\rfloor+h+\frac{1}{2}\right)+2m^2+8mh\\
& +4(m-1)\left(\left\lfloor\frac{m}{2}\right\rfloor-1\right)-4\left\lfloor\frac{m^2}{4}\right\rfloor+4h^2-6h\\
\geq & \ 4\left(\frac{n-m-2h}{2}\right)^2-4(n-m-2h)\cdot\frac{n-m-2h}{2}\\
& +2n^2-4n\left(\left\lfloor\frac{m}{2}\right\rfloor+h+\frac{1}{2}\right)+2m^2+8mh\\
& +4(m-1)\left(\left\lfloor\frac{m}{2}\right\rfloor-1\right)-4\left\lfloor\frac{m^2}{4}\right\rfloor+4h^2-6h\\
= & \begin{cases} 2m^2+2(2h-3)m+n^2-2n+4-6h & \text{if } m \text{ is even}\\ 2m^2+2(2h-3)m+n^2-2n+4-6h & \\ +2n-2m+3 & \text{if } m \text{ is odd}\end{cases}\\
\geq & \ 2m^2+2(2h-3)m+n^2-2n+4-6h\\
\geq & \ 2\cdot 5^2+2(2h-3)\cdot 5+n^2-2n+4-6h\\
= & \ n^2-2n+24+14h>0.
\end{aligned}
$$

Now the result follows. □

Let $\mathcal{U}(n,p)$ be the set of unicyclic graphs with n vertices and p pendant vertices, where $0\leq p\leq n-3$. The case $p=0$ is trivial.

Any graph in $\mathcal{U}(n, n-3)$ may be obtained by attaching $n-3$ pendant vertices to vertices of a triangle, and then it is easily seen that $U_{n,3,3}$ attains maximum reverse degree distance in $\mathcal{U}(n, n-3)$.

Theorem 4.7. *Among graphs in $\mathcal{U}(n,p)$ with $1 \leq p \leq n-4$,*

(i) *if $p = 1$, then $U_{n,4,n-2}(n-4, 0)$ is the unique graph with maximum reverse degree distance*;

(ii) *if $p = 2$, then $U_{n,4,n-2}$ is the unique graph with maximum reverse degree distance*;

(iii) *if $p = 3$ and $n = 7$, then $U_{7,3,4}$ is the unique graph with maximum reverse degree distance*;

(iv) *if $p = 3$ and $n > 7$ is odd, then $U^k_{n,4,n-3}(\frac{n-5}{2}, \frac{n-5}{2})$ for $k = 0, 1$ are the unique graphs with maximum reverse degree distance*;

(v) *if $p = 3$ and $n \geq 6$ is even, or $4 \leq p \leq n-4$, then $U_{n,4,n-p}$ is the unique graph with maximum reverse degree distance for $\left\lfloor \frac{n-p-1}{2} \right\rfloor > \frac{n+4}{6}$, $U_{n,3,n-p}$ and $U_{n,4,n-p}$ are the unique graphs with maximum reverse degree distance for $\left\lfloor \frac{n-p-1}{2} \right\rfloor = \frac{n+4}{6}$, and $U_{n,3,n-p}$ is the unique graph with maximum reverse degree distance for $\left\lfloor \frac{n-p-1}{2} \right\rfloor < \frac{n+4}{6}$.*

Proof. Obviously, $\mathcal{U}(n,1) = \left\{U_{n,m,n-\lfloor \frac{m+1}{2} \rfloor}(n-m, 0) : 3 \leq m \leq n-1\right\}$. By Lemma 4.5, ${}^r\!D'(U_{n,m,n-\lfloor \frac{m+1}{2} \rfloor}(n-m, 0)) < {}^r\!D'(U_{n,3,n-2}(n-3,0))$ for odd $m > 3$, and ${}^r\!D'(U_{n,m,n-\lfloor \frac{m+1}{2} \rfloor}(n-m, 0)) < {}^r\!D'(U_{n,4,n-2}(n-4,0))$ for even $m > 4$. Let $G_1 = U_{n,4,n-2}(n-4,0)$ and $G_2 = U_{n,3,n-2}(n-3,0)$. It is easily seen that

$$\begin{aligned} & {}^r\!D'(U_{n,4,n-2}(n-4,0)) - {}^r\!D'(U_{n,3,n-2}(n-3,0)) \\ = \; & D'(U_{n,3,n-2}(n-3,0)) - D'(U_{n,4,n-2}(n-4,0)) \\ = \; & 4[W(G_2) - W(G_1)] + [D_{G_2}(v_0) - D_{G_1}(v_0)] \\ & -[D_{G_2}(u_0) - D_{G_1}(u_0)] \\ = \; & 4(n-4) + (n-5) - 1 = 5n - 22 > 0. \end{aligned}$$

Then (i) follows.

Suppose that $2 \leq p \leq n-4$. Let $G \in \mathcal{U}(n,p)$, and let d and m be, respectively, the diameter and girth of G. A diametrical path of G contains at most $\lfloor \frac{m}{2} \rfloor + 1$ vertices on C_m and two pendant vertices, and then at most $\left(\lfloor \frac{m}{2} \rfloor + 1\right) + 2 + (n-m-p) = n-p+3-\lfloor \frac{m+1}{2} \rfloor$ vertices in G, implying that $d \leq n-p+2-\lfloor \frac{m+1}{2} \rfloor$.

Note that $U_{n,4,n-p} = U_{n,4,n-p}\left(\frac{n-p-2}{2}, \frac{n-p-2}{2}\right)$ if $p = 2, 3$ and $n-p$ is even, $U_{n,4,n-p} = U_{n,4,n-p}\left(\left\lfloor\frac{n-p}{2}\right\rfloor, \left\lfloor\frac{n-p-3}{2}\right\rfloor\right)$ if $p = 2, 3$ and $n-p$ is odd or $4 \le p \le n-4$, and $U_{n,3,n-p} = U_{n,3,n-p}\left(\left\lfloor\frac{n-p}{2}\right\rfloor, \left\lfloor\frac{n-p-1}{2}\right\rfloor\right)$.

By Corollary 3.4 and Lemma 4.1,

$$ {}^{r}D'(G) \le {}^{r}D'(U_{n,3,d}) \le {}^{r}D'(U_{n,3,n-p}) $$

with equalities if and only if $G \cong U_{n,3,n-p}$ for $m = 3$, and

$$ {}^{r}D'(G) \le {}^{r}D'(U_{n,4,d}) \le {}^{r}D'(U_{n,4,n-p}) $$

with equalities if and only if $G \cong U^k_{n,4,n-p}\left(\frac{n-p-2}{2}, \frac{n-p-2}{2}\right)$ with $k = 0, 1$ if $p = 2, 3$ and $n-p$ is even, and $G \cong U_{n,4,n-p}$ if $p = 2, 3$ and $n-p$ is odd or $4 \le p \le n-4$ for $m = 4$. If $m \ge 5$, then by Corollary 3.4 and Lemmas 4.1 and 4.6, we have

$$
\begin{aligned}
{}^{r}D'(G) &\le {}^{r}D'(U_{n,m,d}) \le {}^{r}D'\left(U_{n,m,n-p+2-\lfloor\frac{m+1}{2}\rfloor}(\gamma,\theta)\right) \\
&< {}^{r}D'\left(U_{n,m-2i,n-p+2-\lfloor\frac{m+1}{2}\rfloor+i}(\gamma+i,\theta+i)\right) \\
&\le {}^{r}D'\left(U_{n,m-2i,n-p+2-\lfloor\frac{m+1}{2}\rfloor+i}\right) \\
&= {}^{r}D'\left(U_{n,m-2i,n-p}\right),
\end{aligned}
$$

where $i = \lfloor\frac{m-3}{2}\rfloor$. Thus ${}^{r}D'(G) < {}^{r}D'(U_{n,3,n-p})$ for odd $m > 3$, and ${}^{r}D'(G) < {}^{r}D'(U_{n,4,n-p})$ for even $m > 4$. We need only to compare ${}^{r}D'(U_{n,3,n-p})$ with ${}^{r}D'(U_{n,4,n-p})$. Let $G_3 = U_{n,4,n-p}$ and $G_4 = U_{n,3,n-p}$.

Suppose that $p = 2, 3$ and $n-p$ is even. By Lemma 2.3,

$$
\begin{aligned}
D'\left(U_{n,4,n-p}\right) &= D'\left(U^0_{n,4,n-p}\left(\frac{n-p-2}{2}, \frac{n-p-2}{2}\right)\right) \\
&= D'\left(U^1_{n,4,n-p}\left(\frac{n-p-2}{2}, \frac{n-p-2}{2}\right)\right).
\end{aligned}
$$

It is easily seen that

$$
\begin{aligned}
& {}^{r}D'(U_{n,4,n-p}) - {}^{r}D'(U_{n,3,n-p}) \\
=\ & D'(U_{n,3,n-p}) - D'(U_{n,4,n-p}) \\
=\ & 4[W(G_4) - W(G_3)] + (p-1)[D_{G_4}(v_0) - D_{G_3}(v_0)] \\
& + [D_{G_4}(v_1) - D_{G_3}(v_2)] - (p-2)[D_{G_4}(u) - D_{G_3}(u)] \\
& - [D_{G_4}(u_0) - D_{G_3}(u_0)] - [D_{G_4}(u_1) - D_{G_3}(u_1)]
\end{aligned}
$$

$$= 4\left(\frac{n-p-2}{2} - p + 2\right) + (1-p) + (2-p) + (p-2)$$
$$+(1-p) + (p-2)$$
$$= 2n - 7p + 4 = \begin{cases} 2n-10 > 0 & \text{if } p = 2 \text{ and } n \geq 6 \text{ is even} \\ -3 & \text{if } p = 3 \text{ and } n = 7 \\ 2n-17 > 0 & \text{if } p = 3 \text{ and } n > 7 \text{ is odd,} \end{cases}$$

and thus (iii) and (iv) follow.

If $p = 2, 3$ and $n - p$ is odd, or $4 \leq p \leq n - 4$, then by a similar calculation as above, we have

$${}^{r}D'(U_{n,4,n-p}) - {}^{r}D'(U_{n,3,n-p}) = 6\left\lfloor \frac{n-p-1}{2} \right\rfloor - n - 4,$$

and thus (ii) and (v) follow easily. □

Let $\mathfrak{U}(n, \Delta)$ be the set of unicyclic graphs with n vertices and maximum degree Δ, where $2 \leq \Delta \leq n-1$. The cases $\Delta = 2, n-1$ are trivial.

It is easily checked that $U_{n,3,3}$ attains maximum reverse degree distance in $\mathfrak{U}(n, n-2)$.

Theorem 4.8. *Among graphs in $\mathfrak{U}(n, \Delta)$ with $3 \leq \Delta \leq n-3$,*

(i) *if $\Delta = 3$, then $U_{n,4,n-2}$ is the unique graph with maximum reverse degree distance*;

(ii) *if $\Delta = 4$ and $n = 7$, then $U_{7,3,4}$ is the unique graph with maximum reverse degree distance*;

(iii) *if $\Delta = 4$ and $n > 7$ is odd, then $U^k_{n,4,n-3}(\frac{n-5}{2}, \frac{n-5}{2})$ for $k = 0, 1$ are the unique graphs with maximum reverse degree distance*;

(iv) *if $\Delta = 4$ and $n \geq 6$ is even, or $5 \leq \Delta \leq n-3$, then $U_{n,4,n-\Delta+1}$ is the unique graph with maximum reverse degree distance for $\lfloor \frac{n-\Delta}{2} \rfloor > \frac{n+4}{6}$, $U_{n,3,n-\Delta+1}$ and $U_{n,4,n-\Delta+1}$ are the unique graphs with maximum reverse degree distance for $\lfloor \frac{n-\Delta}{2} \rfloor = \frac{n+4}{6}$, and $U_{n,3,n-\Delta+1}$ is the unique graph with maximum reverse degree distance for $\lfloor \frac{n-\Delta}{2} \rfloor < \frac{n+4}{6}$.*

Proof. Let $G \in \mathfrak{U}(n, \Delta)$, and let d and m be the diameter and girth of G respectively.

First we show that $d \leq n - \Delta + 3 - \lfloor \frac{m+1}{2} \rfloor$. Let u be a vertex of degree Δ in G, and let N_u be the union of vertex u and its neighbors in G. Among the vertices in $V(C_m) \cup N_u$, any diametrical path of G, say

$P(G)$ with $|P(G) \cup V(C_m)| \leq 1$, $P(G)$ contains at most $3 \leq \lfloor \frac{m}{2} \rfloor + 2$ vertices. On the other hand, any diametrical path of G, say $P(G)$ with $|P(G) \cup V(C_m)| \geq 2$, contains at most $\lfloor \frac{m}{2} \rfloor + 1$ vertices of the cycle C_m, at most three vertices in $N_u \setminus V(C_m)$ if $u \notin V(C_m)$, and at most one vertex in $N_u \setminus V(C_m)$ if $u \in V(C_m)$. Thus among the vertices in $V(C_m) \cup N_u$, $P(G)$ contains at most $\lfloor \frac{m}{2} \rfloor + 4$ vertices if $u \notin V(C_m)$, and at most $\lfloor \frac{m}{2} \rfloor + 2$ vertices if $u \in V(C_m)$. Note that $|V(C_m) \cap N_u| \leq 1$ if $u \notin V(C_m)$, and $|V(C_m) \cap N_u| = 3$ if $u \in V(C_m)$. If $u \notin V(C_m)$, then $P(G)$ contains at most $\left\lfloor \frac{m}{2} \right\rfloor + 4 + (n - |V(C_m) \cup N_u|)$ vertices, and thus

$$\begin{aligned} d &\leq \left\lfloor \frac{m}{2} \right\rfloor + 4 + (n - |V(C_m) \cup N_u|) - 1 \\ &= \left\lfloor \frac{m}{2} \right\rfloor + 4 + n - |V(C_m)| - |N_u| + |V(C_m) \cap N_u| - 1 \\ &\leq \left\lfloor \frac{m}{2} \right\rfloor + 4 + n - m - (\Delta + 1) + 1 - 1 \\ &= n - \Delta + 3 - \left\lfloor \frac{m+1}{2} \right\rfloor . \end{aligned}$$

Similarly, if $u \in V(C_m)$, then

$$d \leq \left\lfloor \frac{m}{2} \right\rfloor + 2 + (n - |V(C_m) \cup N_u|) - 1 \leq n - \Delta + 3 - \left\lfloor \frac{m+1}{2} \right\rfloor .$$

By Corollary 3.4 and Lemmas 4.1 and 4.6, we have

$${}^{r}D'(G) \leq {}^{r}D'(U_{n,3,d}) \leq {}^{r}D'\left(U_{n,3,n-\Delta+1}\right)$$

for $m = 3$,

$${}^{r}D'(G) \leq {}^{r}D'\left(U_{n,4,d}\right) \leq {}^{r}D'(U_{n,4,n-\Delta+1})$$

for $m = 4$, and

$$\begin{aligned} {}^{r}D'(G) &\leq {}^{r}D'(U_{n,m,d}) \leq {}^{r}D'\left(U_{n,m,n-\Delta+3-\lfloor \frac{m+1}{2} \rfloor}(\gamma, \theta)\right) \\ &< {}^{r}D'\left(U_{n,m-2i,n-\Delta+3-\lfloor \frac{m+1}{2} \rfloor + i}(\gamma + i, \theta + i)\right) \\ &\leq {}^{r}D'\left(U_{n,m-2i,n-\Delta+3-\lfloor \frac{m+1}{2} \rfloor + i}\right) \\ &= {}^{r}D'\left(U_{n,m-2i,n-\Delta+1}\right) \end{aligned}$$

for $m \geq 5$, where $i = \lfloor \frac{m-3}{2} \rfloor$. Thus ${}^{r}D'(G) \leq {}^{r}D'\left(U_{n,3,n-\Delta+1}\right)$ for odd $m \geq 3$, and ${}^{r}D'(G) \leq {}^{r}D'\left(U_{n,4,n-\Delta+1}\right)$ for even $m \geq 4$. Now the theorem follows by similar arguments appeared in the proof of Theorem 4.7. $\square$

Finally, we give the values of the maximum reverse degree distances in Theorems 4.7 and 4.8.

(i) For $U_{n,4,n-2}(n-4,0)$ with $n \geq 6$,

$$\begin{aligned}
& D'(U_{n,4,n-2}(n-4,0)) \\
= \;& 4W(U_{n,4,n-2}(n-4,0)) + (3-2)D_{U_{n,4,n-2}(n-4,0)}(v_0) \\
& +(1-2)D_{U_{n,4,n-2}(n-4,0)}(u_0) \\
= \;& 4W(U_{n,4,n-2}(n-4,0)) - 3(n-4) \\
= \;& \frac{2}{3}n^3 - \frac{35}{3}n + 36,
\end{aligned}$$

and thus

$$\begin{aligned}
{}^{r}D'(U_{n,4,n-2}(n-4,0)) &= 2(n-1)n(n-2) - D'(U_{n,4,n-2}(n-4,0)) \\
&= \frac{4}{3}n^3 - 6n^2 + \frac{47}{3}n - 36.
\end{aligned}$$

(ii) For $U_{n,4,n-2}$ with $n \geq 6$,

$$\begin{aligned}
& D'(U_{n,4,n-2}) \\
= \;& 4W(U_{n,4,n-2}) + (3-2)D_{U_{n,4,n-2}}(v_0) + (1-2)D_{U_{n,4,n-2}}(u_0) \\
& +(3-2)D_{U_{n,4,n-2}}(v_2) + (1-2)D_{U_{n,4,n-2}}(u_1) \\
= \;& \begin{cases} \frac{2}{3}n^3 - \frac{3}{2}n^2 + \frac{1}{3}n + 12 & \text{if } n \text{ is even} \\ \frac{2}{3}n^3 - \frac{3}{2}n^2 + \frac{1}{3}n + \frac{27}{2} & \text{if } n \text{ is odd,} \end{cases}
\end{aligned}$$

and thus

$$\begin{aligned}
{}^{r}D'(U_{n,4,n-2}) &= 2(n-1)n(n-2) - D'(U_{n,4,n-2}) \\
&= \begin{cases} \frac{4}{3}n^3 - \frac{9}{2}n^2 + \frac{11}{3}n - 12 & \text{if } n \text{ is even} \\ \frac{4}{3}n^3 - \frac{9}{2}n^2 + \frac{11}{3}n - \frac{27}{2} & \text{if } n \text{ is odd.} \end{cases}
\end{aligned}$$

(iii) For $U_{n,4,n-3}$ with odd $n \geq 7$,

$$\begin{aligned}
& D'(U_{n,4,n-3}) \\
= \;& 4W(U_{n,4,n-3}) + (4-2)D_{U_{n,4,n-3}}(v_0) + (1-2)D_{U_{n,4,n-3}}(u_0) \\
& +(1-2)D_{U_{n,4,n-3}}(u) + (3-2)D_{U_{n,4,n-3}}(v_2) \\
& +(1-2)D_{U_{n,4,n-3}}(u_1) \\
= \;& 4W(U_{n,4,n-3}) - \frac{1}{2}n^2 + \frac{19}{2} \\
= \;& \frac{2}{3}n^3 - \frac{5}{2}n^2 + \frac{10}{3}n + \frac{47}{2},
\end{aligned}$$

and thus

$$\begin{aligned} {}^{r}D'(U_{n,4,n-3}) &= 2(n-1)n(n-3) - D'(U_{n,4,n-3}) \\ &= \frac{4}{3}n^3 - \frac{11}{2}n^2 + \frac{8}{3}n - \frac{47}{2}. \end{aligned}$$

(iv) For $U_{n,4,n-p}$ with $3 \le p \le n-4$,

$$\begin{aligned} & D'(U_{n,4,n-p}) \\ = \; & 4W(U_{n,4,n-p}) + [(p+1)-2]D_{U_{n,4,n-p}}(v_0) \\ & +(1-2)D_{U_{n,4,n-p}}(u_0) + (p-2)(1-2)D_{U_{n,4,n-p}}(u) \\ & +(3-2)D_{U_{n,4,n-p}}(v_2) + (1-2)D_{U_{n,4,n-p}}(u_1) \\ = \; & \begin{cases} \frac{2}{3}n^3 - \left(p-\frac{1}{2}\right)n^2 + \left(3p-\frac{17}{3}\right)n + \frac{p^3}{3} - \frac{p^2}{2} + \frac{11p}{3} + 10 & \text{if } n-p \text{ is even} \\ \frac{2}{3}n^3 - \left(p-\frac{1}{2}\right)n^2 + \left(3p-\frac{17}{3}\right)n + \frac{p^3}{3} - \frac{p^2}{2} + \frac{14p}{3} + \frac{7}{2} & \text{if } n-p \text{ is odd,} \end{cases} \end{aligned}$$

and thus

$$\begin{aligned} & {}^{r}D'(U_{n,4,n-p}) \\ = \; & 2(n-1)n(n-p) - D'(U_{n,4,n-p}) \\ = \; & \begin{cases} \frac{4}{3}n^3 - \left(p+\frac{5}{2}\right)n^2 - \left(p-\frac{17}{3}\right)n - \frac{p^3}{3} + \frac{p^2}{2} - \frac{11p}{3} - 10 & \text{if } n-p \text{ is even} \\ \frac{4}{3}n^3 - \left(p+\frac{5}{2}\right)n^2 - \left(p-\frac{17}{3}\right)n - \frac{p^3}{3} + \frac{p^2}{2} - \frac{14p}{3} - \frac{7}{2} & \text{if } n-p \text{ is odd.} \end{cases} \end{aligned}$$

(v) For $U_{n,3,n-p}$ with $3 \le p \le n-4$,

$$\begin{aligned} & D'(U_{n,3,n-p}) \\ = \; & 4W(U_{n,3,n-p}) + [(p+1)-2]D_{U_{n,3,n-p}}(v_0) \\ & +(1-2)D_{U_{n,3,n-p}}(u_0) + (p-2)(1-2)D_{U_{n,3,n-p}}(u) \\ & +(3-2)D_{U_{n,3,n-p}}(v_1) + (1-2)D_{U_{n,3,n-p}}(u_1) \\ = \; & \begin{cases} \frac{2}{3}n^3 - \left(p-\frac{1}{2}\right)n^2 + \left(3p-\frac{11}{3}\right)n + \frac{p^3}{3} - \frac{p^2}{2} + \frac{2p}{3} & \text{if } n-p \text{ is even} \\ \frac{2}{3}n^3 - \left(p-\frac{1}{2}\right)n^2 + \left(3p-\frac{11}{3}\right)n + \frac{p^3}{3} - \frac{p^2}{2} + \frac{5p}{3} - \frac{7}{2} & \text{if } n-p \text{ is odd,} \end{cases} \end{aligned}$$

and thus

$${}^{r}D'(U_{n,3,n-p})$$

$$
\begin{aligned}
&= 2(n-1)n(n-p) - D'(U_{n,3,n-p}) \\
&= \begin{cases} \frac{4}{3}n^3 - \left(p+\frac{5}{2}\right)n^2 - \left(p-\frac{11}{3}\right)n - \frac{p^3}{3} + \frac{p^2}{2} - \frac{2p}{3} \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{if } n-p \text{ is even} \\ \frac{4}{3}n^3 - \left(p+\frac{5}{2}\right)n^2 - \left(p-\frac{11}{3}\right)n - \frac{p^3}{3} + \frac{p^2}{2} - \frac{5p}{3} + \frac{7}{2} \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{if } n-p \text{ is odd.} \end{cases}
\end{aligned}
$$

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