Reverse degree distance of unicyclic graphs

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Abstract

The reverse degree distance is a connected graph invariant closely related to the
degree distance proposed in mathematical chemistry. We determine the unicyclic
graphs of given girth, number of pendant vertices and maximum degree, respec-
tively, with maximum reverse degree distances.

Keywords: Degree Distance, Reverse degree distance, Diameter, Unicyclic graph,
Pendant vertices, Maximum degree

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 the vertices $u$ and $v$ in $G$ and let $D_G(u) = \sum_{v \in V(G)} d_G(u, v)$. For
$u \in V(G)$, let $d_G(u)$ be the degree of $u$ in $G$. The degree distance of $G$ is defined as

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

It is a useful molecular descriptor [21]. Earlier as noted in [16, 20], this graph invariant
appeared to be part of the molecular topological index (or Schultz index) [19], which
may be expressed as $D'(G) + \sum_{u \in V(G)} d_G(u)^2$, see [12, 15, 17, 26], where the latter part

$$\sum_{u \in V(G)} d_G(u)^2$$

is known as the first Zagreb index [13, 14, 18]. Thus, the degree distance is
also called the true Schultz index in chemical literature [7].

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].

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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 [9] studied the ordering of unicyclic graphs with large degree distances, and bicyclic graphs were also considered in [10].

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 [12] 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., [4, 5].

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

$$rD'(G) = 2(n - 1)md - D'(G)$$

where $n$, $m$ and $d$ are the number of vertices, the number of edges and the diameter of $G$, respectively. Recall that, earlier, Balaban et al. [1] introduced the concept of reverse Wiener index, which is defined to be $\frac{n(n-1)d}{2} - W(G)$. If $G$ is a tree, then from the result of Gutman [12] mentioned above,

$$rD'(G) = 4 \left[ \frac{(n-1)^2d}{2} - W(G) \right] + n(n - 1).$$

Some properties of the reverse degree distance, especially for trees, have been given in [27]. There are two reasons for the study of this graph invariant. One is that the reverse degree distance itself is a topological index satisfying the basic requirement to be a branching index and with potential for application in chemistry [27]. The other is the study the reverse degree distance is actually the study the degree distance, which is important in both mathematical chemistry and in discrete mathematics.

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

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 $u$. 
Lemma 1 Let $G$ and $G^*$ be the two graphs in Fig. 1.

(i) If $V(N) = \{v\}$ and $G \not\cong G^*$, then $D'(G) > D'(G^*)$.

(ii) If $|V(M)|$, $|V(N)| \geq 3$, then $D'(G) > D'(G^*)$.

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 $H_1$ 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

$$
(d_s + d_t - 1)D_{H_1}(s) + 1 \cdot D_{H_1}(w) - d_sD_H(s) - d_tD_H(t)
$$

$$
= d_s[D_{H_1}(s) - D_H(s)] + d_t[D_{H_1}(s) - D_H(t)] + [D_{H_1}(w) - D_{H_1}(s)]
$$

$$
= -(d_s(|V(Q_2)| - 1) - d_t(|V(Q_1)| - 1) + (|V(Q_1)| + |V(Q_2)| - 2)
$$

$$
= -(d_s - 1)(|V(Q_2)| - 1) - (d_t - 1)(|V(Q_1)| - 1).
$$

Then

$$
D'(H_1) - D'(H)
$$

$$
= -(|V(Q_2)| - 1) \sum_{x \in V(Q_1) \setminus \{s\}} d_x - (|V(Q_1)| - 1) \sum_{x \in V(Q_2) \setminus \{t\}} d_x
$$

$$
+ (d_s + d_t - 1)D_{H_1}(s) + 1 \cdot D_{H_1}(w) - d_sD_H(s) - d_tD_H(t)
$$

$$
= -(|V(Q_2)| - 1) \sum_{x \in V(Q_1) \setminus \{s\}} d_x - (|V(Q_1)| - 1) \sum_{x \in V(Q_2) \setminus \{t\}} d_x
$$

$$
-(d_s - 1)(|V(Q_2)| - 1) - (d_t - 1)(|V(Q_1)| - 1) < 0,
$$

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

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

Lemma 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 $D'(G_{s,t}) > \min\{D'(G_{s+t,0}), D'(G_{0,s+t})\}$. 

3
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

\[
(d_u + s + t)D_{G_{s+t,0}}(u) - (d_u + s)D_{G_s,t}(u) + [d_vD_{G_{s+t,0}}(v) - (d_v + t)D_{G_s,t}(v)]
\]

\[
= (d_u + s)[D_{G_{s+t}}(u) - D_{G_s,t}(u)] + t[D_{G_{s+t,0}}(u) - D_{G_s,t}(v)]
\]

\[
+ d_v[D_{G_{s+t,0}}(v) - D_{G_s,t}(v)]
\]

\[
= -t \cdot d(u, v) \cdot (d_u + s) + t \left[ -sd(u, v) + \sum_{x \in V(G_0) \setminus \{u,v\}} (d(x, u) - d(x, v)) \right]
\]

\[
+ t \cdot d(u, v) \cdot d_v
\]

\[
= t \left[ (d_v - d_u - 2s)d(u, v) + \sum_{x \in V(G_0) \setminus \{u,v\}} (d(x, u) - d(x, v)) \right]
\]

and thus

\[
D'(G_{s+t,0}) - D'(G_{s,t})
\]

\[
= t \sum_{x \in V(G_0) \setminus \{u,v\}} d_x (d(x, u) - d(x, v))
\]

\[
- std(u, v) + t \left[ -sd(u, v) + \sum_{x \in V(G_0) \setminus \{u,v\}} (d(x, u) - d(x, v)) \right]
\]

\[
+ (d_u + s + t)D_{G_{s+t,0}}(u) - (d_u + s)D_{G_s,t}(u)
\]

\[
+ d_v[D_{G_{s+t,0}}(v) - (d_v + t)D_{G_s,t}(v)]
\]

\[
= t \sum_{x \in V(G_0) \setminus \{u,v\}} (d_x + 1)(d(x, u) - d(x, v)) - 2std(u, v)
\]

\[
+ t \left[ (d_v - d_u - 2s)d(u, v) + \sum_{x \in V(G_0) \setminus \{u,v\}} (d(x, u) - d(x, v)) \right]
\]

\[
= t \left[ (d_v - d_u - 4s)d(u, v) + \sum_{x \in V(G_0) \setminus \{u,v\}} (d_x + 2)(d(x, u) - d(x, v)) \right].
\]

Similarly, we have

\[
D'(G_{0,s+t}) - D'(G_{s,t})
\]

\[
= s \left[ (d_u - d_v - 4t)d(u, v) + \sum_{x \in V(G_0) \setminus \{u,v\}} (d_x + 2)(d(x, v) - d(x, u)) \right].
\]

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,
\[
D'(G_{0,s+t}) - D'(G_{s,t}) \leq s \left( (d_u - d_v - 4t)d(u, v) + (d_v - d_u - 4s)d(u, v) \right) = -4s(s + t)d(u, v) < 0.
\]
The result follows. \( \square \)

Let \( G \) and \( H \) be 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
\[
D'(H) - D'(G) = 2 \sum_{x \in V_1(H)} D_H(x) + \sum_{x \in V_2(H)} d^*_x D_H(x) - 2 \sum_{x \in V_1(G)} D_G(x) - \sum_{x \in V_2(G)} d_x D_G(x)
= 4[W(H) - W(G)] + \sum_{x \in V_2(H)} (d^*_x - 2) D_H(x) - \sum_{x \in V_2(G)} (d_x - 2) D_G(x).
\]

Let \( G^* \) be the unicyclic graph obtained from the 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 \( i \neq j \), \( a \geq 1 \) and \( b \geq 2 \). Label the vertices of the path \( P_b \) attached to \( v_j \) as \( u_1, \ldots, u_b \) 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 \( G^{(2)}_{v_j,h} \) the graph obtained from \( G^* \) by attaching \( h \) pendant vertices to \( v_t \), where \( 0 \leq t \leq m - 1 \).

**Lemma 3** Let \( n_1 = a + m - 1 \) and \( n_2 = b - t \) in \( G_{u_t,h}^{(1)} \). Then \( D' \left( G_{v_j,h}^{(2)} \right) - D' \left( G_{u_t,h}^{(1)} \right) = 2ht[2(n_2 - n_1) - 1] \).

**Proof** Let \( v \) be a pendant vertex attached to \( v_j \) in \( G_{v_j,h}^{(2)} \) (resp. \( u_t \) in \( G_{u_t,h}^{(1)} \)). Let \( G_1 = G_{v_j,h}^{(2)} \) and \( G_2 = G_{u_t,h}^{(1)} \). Then
\[
D' \left( G_{v_j,h}^{(2)} \right) - D' \left( G_{u_t,h}^{(1)} \right) = 4[W(G_1) - W(G_2)] - [D_{G_1}(u_b) - D_{G_2}(u_b)] - h[D_{G_1}(v) - D_{G_2}(v)] + (h + 1)D_{G_1}(v_j) - hD_{G_2}(u_t) - D_{G_2}(v_j) = 4ht(n_2 - n_1) - ht - ht(n_2 - n_1) + ht(n_2 - n_1) - ht = 2ht[2(n_2 - n_1) - 1],
\]
as desired. \( \square \)

By similar arguments as in Lemma 3, we have

**Lemma 4** 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 \( G = G_{v_t,h}^{(2)} \). If \( t \neq i \), then \( D' \left( G_{v_i,h}^{(2)} \right) - D' \left( G_{v_t,h}^{(2)} \right) = 4h[b(c - t_2) - at_1] \).
As usual, $G - V_1$ means the graph formed from the graph $G$ by deleting the vertices of $V_1 \subset V(G)$ and edges incident with these vertices, while $G - E_1$ means the graph formed from $G$ by deleting edges of $E_1 \subseteq E(G)$.

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 $3 \leq m \leq n - 1$ and $2 \leq d \leq n - \frac{m+1}{2}$. Let $P_s$ be a path on $s$ vertices. For $a \geq b \geq 0$ and $a \geq 1$, let $U^k_{n,m,d}(a,b)$ be the unicyclic graph obtained from the cycle $C_m = v_0v_1...v_{m-1}v_0$ by attaching a path $P_a$ to $v_0$ and a path $P_b$ to $v_1$ respectively (if $b = 0$, then by attaching only a path $P_a$ to $v_0$), where $a + b = d - \frac{m}{2}$, and attaching $n - d - \frac{m+1}{2}$ pendant vertices to $v_k$, where $0 \leq k \leq \frac{m}{2}$. 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 $v_1$ if $b \geq 1$, and $u_1 = v_{\frac{m}{2}}$ if $b = 0$, let $u$ be any of the pendant vertices attached to $v_0$.

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

Lemma 5 Let $n$, $m$ and $d$ be fixed integers with $3 \leq m \leq n - 2$ and $3 \leq d \leq n - \frac{m+1}{2}$. Then $D'(U_{n,m,d}(a,b))$ with $a \geq b$ and $a + b = d - \frac{m}{2}$ is minimum if and only if $(a,b) = (\gamma, \theta)$, $(\gamma-1, \theta+1)$ if $\alpha \geq 1$ is an integer with different parity as $d - \left\lceil \frac{m}{2} \right\rceil$, and $(a,b) = (\gamma, \theta)$ otherwise.

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

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

and if $a = d - \left\lceil \frac{m}{2} \right\rceil$ and $b = 0$, then

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

If
Lemma 6

Setting $u$ called the branches of $P$, a diametrical path of $D$ are pendant vertices attached to vertices that are nearest to them in $G$. Let $C$ be a unicyclic graph with $n$ vertices, girth $m$ and diameter $d$, where $2 \leq d \leq n - \left\lceil \frac{m+1}{2} \right\rceil$ and $3 \leq m \leq n - 2$. If $G \in \mathbb{U}(n,m,d)$, then $m = 3$ and $G = 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 of $T_i - v_i$ are called the branches of $G$ at $v_i$, each containing a neighbor of $v_i$ in $T_i$.

**Lemma 6** Let $n, m$ and $d$ be integers with $n \geq 6$, $3 \leq m \leq n - 2$ and $3 \leq d \leq n - \left\lceil \frac{m+1}{2} \right\rceil$, and let $\beta = \frac{1}{2}(d - \left\lceil \frac{m}{2} \right\rceil)$. If $G$ is a graph with minimum degree distance in $\mathbb{U}(n,m,d)$, then $G = U_{n,m,d}(a,b) = U^{0}_{n,m,d}(a,b)$ with $a \geq b$ or $G = U^{k}_{n,m,d}(\beta, \beta)$ for $k = 1, \ldots, \left\lceil \frac{m}{2} \right\rceil$.

**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 1 (ii) by setting $u = u_s$, $v = v_t$, $M$ to be the subgraph of $G$ consisting of the path $P(G)$ and 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 $v_i$, we 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 vertices in common as many as possible and $u_0$ is a pendant vertex.

Let $v_i = u_a$ (resp. $v_j = u_t$) be the first (resp. last) common vertex of $P(G)$ and $C_m$, where $0 < a \leq l \leq d$. By Lemma 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, 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 $s = v_q$. Let $N_q = \{v_{q_1}, \ldots, v_{q_r}\}$ be the set of pendant vertices attached to $v_q$. For $H = G - \{v_qv_{q_1}, \ldots, v_{q_r}v_q\} + \{v_qv_{q_1}, \ldots, v_{q_r}v_q\} \in \mathbb{U}(n,m,d)$, we have

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

$$D'(H^*) - D'(G) = 4[W(H^*) - W(G)] - [D_H(u_0) - D_G(u_0)] - [D_H(u_a) - D_G(u_a)]$$

$$-t[D_H(v_{qi}) - D_G(v_{qi})] + (t + 2)D_H(v_i) - tD_G(v_i) - 2D_G(v_i)$$

$$= -4dt \cdot d(v_i, v_i) + t \cdot d(v_i, v_i) + t \cdot d(v_i, v_i)$$

$$+ dt \cdot d(v_i, v_i) - dt \cdot d(v_i, v_i) - 2t \cdot d(v_i, v_i)$$

$$= -4dt \cdot d(v_i, v_i),$$

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

By Lemma 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 $x \in \{u_{i+1}, \ldots, u_{d-1}\}$, say $x = u_q$, where $l < q \leq d - 1$. Let $u_{qi}, u_{q2}, \ldots, u_{q6}$ be the pendant neighbors of $u_q$ outside $P(G)$. For $G_1 = G - \{u_qu_{q1}, u_qu_{q2}, \ldots, u_qu_{q6}\} + \{u_iu_{qi}, u_{qi}u_{q2}, \ldots, u_{qi}u_{q6}\} \in \mathbb{U}(n, m, d)$, using Lemma 3 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, $x \not\in \{u_{i+1}, u_{i+2}, \ldots, u_{d-1}\}$ if $l < d$. Moreover, if $a = b$ then by similar arguments, $x \not\in \{u_1, u_2, \ldots, u_{a-1}\}$, 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 that this is not true. Then $x = v_s$ for some $s$ with $0 \leq s \leq m - 1$ and $s \neq i$. Let $N_s = \{v_{s1}, \ldots, v_{sh}\}$ be the set of pendant vertices attached to $v_s$. Suppose that $d(v_i, v_j) = c, d(v_i, v_s) = t_1$ and $d(v_j, v_s) = t_2$, then $c \leq t_1 + t_2$. Consider $G_2 = G - \{v_sv_{s1}, \ldots, v_{sh}\} + \{v_{i}v_{s1}, \ldots, v_{i}v_{sh}\} \in \mathbb{U}(n, m, d)$. Note that if $l = d$, then $b = 0$. By Lemma 3, we have

$$D'(G_2) - D'(G) = 4h[b(c - t_2) - at_1] \leq 4h(bt_1 - at_1) = 4ht_1(b - a) < 0,$$

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

Next we prove that $d(v_i, v_j) = \lfloor \frac{m}{p} \rfloor$. If $l = d$, then this is obvious. Suppose that $l < d$ and $c = d(v_i, v_j) < \lfloor \frac{m}{p} \rfloor$. Let $v$ be the neighbor of $v_j$ on $C_m$ with $d(v_i, v) = c + 1$
(If \( \{v_i, v_{i+1}, \ldots, v_{j-1}, v_j\} \) is the shortest path from \( v_i \) to \( v_j \), then \( v = v_{j+1} \)). By our choice of \( P(G) \), we have \( b + c > \lceil \frac{m}{2} \rceil \), and then \( b > 1 \). Note that \( c > 0 \). Consider \( G_3 = G - \{v_ju_{i+1}\} + \{vu_{i+1}\} - \{u_{d-1}u_d\} + \{v_iu_d\} \in \mathbb{U}(n, m, d) \). If \( 1 \leq p \leq a - 1 \), then

\[
D'(G_3) - D'(G) = 4\{W(G_3) - W(G)\} - [D_{G_3}(u_0) - D_G(u_0)] - [D_{G_3}(u_d) - D_G(u_d)]
\]

By similar calculation, \( D'(G_3) - D'(G) = -2(2m-3)(b-1) - 4c(n-m-2b+1) < 0 \) holds also if \( p = a \). It follows that in either case \( D'(G_3) < D'(G) \), a contradiction. Thus, \( d(v_i, v_j) = \lceil \frac{m}{2} \rceil \) and \( h = n - d - \lceil \frac{m+1}{2} \rceil \).

Now we prove \( p = a \). Suppose that \( p \leq a - 1 \). Let \( u_{p_1}, u_{p_2}, \ldots, u_{p_h} \) be the pendant neighbors of \( u_p \) outside \( P(G) \). If \( b + m > a \), then \( p < b + m - 1 \), and for \( G_4 = G - \{u_{p_1}u_{p_1}, \ldots, u_{p}u_{p_p}\} + \{u_{p_1}u_{p_1}, \ldots, u_{p}u_{p_p}\} \in \mathbb{U}(n, m, d) \), using Lemma 3 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. Suppose that \( b + m \leq a \). Then \( b - (h-1) < a \).

Consider \( G_4 = G - \{u_{p_1}u_{p_1}, \ldots, u_{p}u_{p_p}\} + \{u_{p+1}u_{p_1}, \ldots, u_{p+1}u_{p_p}\} - \{u_0u_1\} + \{u_0u_d\} \in \mathbb{U}(n, m, d) \). If \( l < d \) and \( 1 \leq p \leq a - 2 \), then

\[
D'(G_4) - D'(G) = 4\{W(G_4) - W(G)\} + [D_{G_4}(u_0) - D_G(u_0)] + [D_{G_4}(u_d) - D_G(u_d)]
\]

By similar calculation, the inequality \( D'(G_4) - D'(G) < 0 \) holds also if \( l = d \) or \( p = a - 1 \).

Then, in any case, \( D'(G_4) < D'(G) \), a contradiction. Thus, \( p = a \).

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

**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 \( v_j \). 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 \( s \notin \{i, i+1, \ldots, j-1, j\} \).

Let \( N_s = \{v_{s_1}, \ldots, v_{s_h}\} \) be the set of pendant vertices attached to \( v_s \). Let \( d(v_i, v_s) = t_1 \) and \( d(v_j, v_s) = t_2 \). Then \( c < t_1 + t_2 \). For \( G_5 = G - \{v_sv_s, \ldots, v_sv_{sh}\} + \{v_iv_{s_1}, \ldots, v_iv_{s_h}\} \in \mathbb{U}(n, m, d) \), by Lemma 4 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 $c = d(v_i, v_j) \leq \lfloor \frac{m}{2} \rfloor$. Note that $d(v_i, v_{j+1}) = c + 1$. By our choice of $P(G)$, we have $b + c > \lfloor \frac{m}{2} \rfloor$, and then $b > 1$. Consider $G_6 = G - \{v_j u_{i+1}\} + \{v_{j+1} u_{i+1}\} - \{u_{d-1} u_d\} + \{v_s u_d\} \in \mathbb{U}(n, m, d)$. If $i + 1 \leq s \leq j - 1$, then

$$D'(G_6) - D'(G) = 4[W(G_6) - W(G)] - [D_{G_6}(u_0) - D_G(u_0)] - [D_{G_6}(u_d) - D_G(u_d)]$$

$$- h[D_{G_6}(v_{s_1}) - D_G(v_{s_1})] + [D_{G_6}(v_i) - D_G(v_i)]$$

$$+ (h + 1)D_{G_6}(v_s) - D_{G_6}(u_{d-1}) + D_{G_6}(v_{j+1}) - hD_G(v_s) - D_G(v_j)$$

$$= -2(2m - 3)(b - 1) - 4(j - s)(h + 1) < 0.$$  

By similar calculation, the inequality $D'(G_6) - D'(G), 0$ holds also if $s = i$ or $j$. In either 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 \ref{lem4}, we have $U^n_{n,m,d}(\beta, \beta)$ for $k = 0, 1, \ldots, \lfloor \frac{m}{2} \rfloor$ have equal degree distance, and thus $G = U^n_{n,m,d}(\beta, \beta)$ for $k = 0, 1, \ldots, \lfloor \frac{m}{2} \rfloor$.

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

**Theorem 1** Let $n, m$ and $d$ be integers with $n \geq 6$, $3 \leq m \leq n - 2$ and $3 \leq d \leq n - \lfloor \frac{m+1}{2} \rfloor$, and let $\alpha = \frac{(n - d - \lfloor \frac{m+1}{2} \rfloor)\lfloor \frac{m}{2} \rfloor}{n - d - \frac{m+1}{2}}$, $\beta = \frac{1}{2}(d - \lfloor \frac{m}{2} \rfloor)$.

(i) If $0 < \alpha < 1$ and $d - \lfloor \frac{m}{2} \rfloor$ is even, then $U^n_{n,m,d}(\beta, \beta)$ for $k = 0, 1, \ldots, \lfloor \frac{m}{2} \rfloor$ 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 $U^n_{n,m,d} = U^n_{n,m,d}(\beta + 1, \beta - 1)$ and $U^n_{n,m,d}(\beta, \beta)$ for $k = 0, 1, \ldots, \lfloor \frac{m}{2} \rfloor$ 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 $U^n_{n,m,d}$ and $U^n_{n,m,d}(\gamma - 1, \theta + 1)$ 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 either not an integer or an integer with the same parity as $d - \lfloor \frac{m}{2} \rfloor$, then $U^n_{n,m,d}$ is the unique graph in $\mathbb{U}(n, m, d)$ with minimum degree distance.

**Proof** Suppose that $G$ is a graph with minimum degree distance in $\mathbb{U}(n, m, d)$. By Lemma \ref{lem4} we have $G = U^n_{n,m,d}(a, b) = U^n_{n,m,d}(a, b)$ with $a \geq b$ or $G = U^n_{n,m,d}(\beta, \beta)$ for $k = 1, \ldots, \lfloor \frac{m}{2} \rfloor$. If $G = U^n_{n,m,d}(a, b)$, then we have by Lemma \ref{lem5} that $G = U^n_{n,m,d}$ or $U^n_{n,m,d}(\gamma - 1, \theta + 1)$ if $\alpha \geq 1$ is an integer with different parity as $d - \lfloor \frac{m}{2} \rfloor$, and $G = U^n_{n,m,d}$ otherwise.

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

Suppose that $d - \lfloor \frac{m}{2} \rfloor$ is even. Then either $G = U^n_{n,m,d}(\beta, \beta)$ for $k = 1, 2, \ldots, \lfloor \frac{m}{2} \rfloor$, or $G = U^n_{n,m,d}$, $U^n_{n,m,d}(\gamma - 1, \theta + 1)$ if $\alpha \geq 1$ is an odd integer, and $G = U^n_{n,m,d}$ otherwise.
If $\alpha = 0$, then $G = U_{n,m,d}$.

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

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

Suppose that $\alpha > 1$ is an odd integer. Then $G = U_{n,m,d}$, or $G = U_{n,m,d}^k(\beta, \beta)$ for $k = 1, 2, \ldots, \lfloor \frac{m}{4} \rfloor$. Let $h = n - d - \lfloor \frac{m+1}{2} \rfloor$. Then $\alpha = \frac{h \lfloor \frac{m}{2} \rfloor}{h + \lfloor \frac{m}{2} \rfloor}$ and $h > 0$. By the proof of Lemma 5, we have

$$D'(U_{n,m,d}^0(\beta, \beta)) - D'(U_{n,m,d}(\gamma, \theta))$$

$$= 2(\gamma - \theta) \left[ \frac{1}{2} (\theta - \gamma) \left( h + \left\lfloor \frac{m-1}{2} \right\rfloor + \frac{1}{2} \right) + h \left\lfloor \frac{m}{2} \right\rfloor \right]$$

$$> 2 \left[ -\frac{1}{2} (\alpha + 1) \left( h + \left\lfloor \frac{m-1}{2} \right\rfloor + \frac{1}{2} \right) + h \left\lfloor \frac{m}{2} \right\rfloor \right]$$

$$= \frac{h(\alpha - 1)}{\alpha} \left\lfloor \frac{m}{2} \right\rfloor > 0,$$

and then $D'(U_{n,m,d}^0(\beta, \beta)) > D'(U_{n,m,d}(\gamma, \theta)) = D'(U_{n,m,d}(\gamma - 1, \theta + 1))$. Thus $G = U_{n,m,d}$, $U_{n,m,d}(\gamma - 1, \theta + 1)$.

Suppose that $\alpha > 1$ is not an odd integer. Then $G = U_{n,m,d}$, or $G = U_{n,m,d}^k(\beta, \beta)$ for $k = 1, 2, \ldots, \lfloor \frac{m}{4} \rfloor$. By similar arguments as above, we have $D'(U_{n,m,d}^0(\beta, \beta)) > D'(U_{n,m,d})$. Thus $G = U_{n,m,d}$.

**Corollary 1** Let $G \in \mathbb{U}(n, m, d)$ with $n \geq 6$, $3 \leq m \leq n - 2$ and $3 \leq d \leq n - \lfloor \frac{m+1}{2} \rfloor$. Then $D'(G) \geq D'(U_{n,m,d})$.

### 4 Reverse degree distances 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 7** For $n \geq 6$, $3 \leq m \leq n - 2$ and $2 \leq d < n - \lfloor \frac{m+1}{2} \rfloor$, $D'(U_{n,m,d}) < D'(U_{n,m,d+1})$.

**Proof** Let $h = n - d - \lfloor \frac{m+1}{2} \rfloor$. Let $u_2$ be a pendant vertex attached to $v_0$ different from $u$ in $U_{n,m,d}$ if $h \geq 2$. 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 $U_{n,m,d}(\gamma, \theta) - \{u_0\} + \{uu_0\}$. Let $G_1 = U_{n,m,d+1}(\gamma + 1, \theta)$ and $G_2 = U_{n,m,d}(\gamma, \theta)$. If $\theta \geq 1$ and $h \geq 2$, then $D_{G_1}(v_{\lfloor \frac{m}{2} \rfloor}) - D_{G_2}(v_{\lfloor \frac{m}{2} \rfloor}) = D_{G_1}(u_1) - D_{G_2}(u_1)$, and thus

$$D'(U_{n,m,d+1}(\gamma + 1, \theta)) - D'(U_{n,m,d}(\gamma, \theta))$$

$$= 4[W(G_1) - W(G_2)] - (h - 1)[D_{G_1}(u_1) - D_{G_2}(u_2)]$$

$$= 4[W(G_1) - W(G_2)] - (h - 1)[D_{G_1}(u) - D_{G_2}(u_2)]$$

$$> 0$$

by Lemma 5. Therefore, $D'(G) < D'(U_{n,m,d+1})$. This completes the proof.

$\square$
Lemma 7, we have
\[-[D_{G_1}(u) - D_{G_2}(u)] + hD_{G_1}(v_0) - (h + 1)D_{G_2}(v_0) + D_{G_2}(u_0)\]
\[= 4\gamma(n - \gamma - 2) - \gamma(h - 1) - \gamma(n - \gamma - 2) + \gamma(n - \gamma + h - 1)\]
\[= -4\gamma^2 + 2(2n - 3)\gamma.\]

By similar calculation, the equality above holds also if \(\theta = 0\) or \(h = 1\). Thus
\[\tau D'(U_{n,m,d+1}(\gamma + 1, \theta)) - \tau D'(U_{n,m,d}(\gamma, \theta))\]
\[= 2n(n - 1) - [D'(U_{n,m,d+1}(\gamma + 1, \theta)) - D'(U_{n,m,d}(\gamma, \theta))]
\[= 4\gamma^2 - 2(2n - 3)\gamma + 2n^2 - 2n\]
\[\geq 4 \left(\frac{2n - 3}{4}\right)^2 - 2(2n - 3) \cdot \frac{2n - 3}{4} + 2n^2 - 2n\]
\[= n^2 + n - \frac{9}{4} > 0.\]

By Corollary \(\#\) we have \(\tau D'(U_{n,m,d+1}(\gamma + 1, \theta)) < \tau D'(U_{n,m,d+1})\), then the result follows. \(\square\)

**Theorem 2** Let \(G\) be a unicyclic graph with \(n\) vertices and girth \(m\), where \(n \geq 6\), \(3 \leq m \leq n - 2\). Then \(\tau D'(G) \leq \tau D'(U_{n,m,n-\lceil \frac{m+1}{2}\rceil})\) with equality if and only if \(G = U_{n,m,n-\lceil \frac{m+1}{2}\rceil}\).

**Proof** Let \(d\) be the diameter of \(G\). Then \(2 \leq d \leq n - \lceil \frac{m+1}{2}\rceil\). If \(d = n - \lceil \frac{m+1}{2}\rceil\), then \(\alpha = 0\), and by Theorem \(\#\) (iv), the result follows. If \(d = 2\), then \(G = U_{n,3,2}(1,0)\), and by Lemma \(\#\) we have \(\tau D'(U_{n,3,2}(1,0)) < \tau D'(U_{n,3,3})\). If \(3 \leq d < n - \lceil \frac{m+1}{2}\rceil\), then by Corollary \(\#\) and Lemma \(\#\) \(\tau D'(G) \leq \tau D'(U_{n,m,d}) < \tau D'(U_{n,m,n-\lceil \frac{m+1}{2}\rceil})\). \(\square\)

**Lemma 8** \([8]\) For \(n \geq 5, 3 \leq m \leq n - 1\) and \(3 \leq d \leq n - \lceil \frac{m+1}{2}\rceil\), let \(h = n - d - \lceil \frac{m+1}{2}\rceil\). Then
\[
W(U_{n,m,d}(a,b)) = \left(a + b + \frac{m}{2}\right) \left[\frac{m^2}{4}\right] + \left(a + 1\right) + \left(b + 1\right) + \frac{1}{2}ab \left(2 \left\lfloor \frac{m}{2}\right\rfloor + a + b + 2\right)
\]
\[+ m \left[\left(a + 1\right) + \left(b + 1\right)\right] + h \left(h - 1\right),\]
where \(a, b\) are integers with \(a + b = d - \lfloor \frac{m}{2}\rfloor\), \(a \geq b \geq 0\) and \(a \geq 1\).

By simple calculation, we have
Lemma 9 For $G = U_{n,m,d}(a,b)$ with $n \geq 5$, $3 \leq m \leq n - 1$ and $3 \leq d \leq n - \lfloor \frac{m+1}{2} \rfloor$, let $h = n - d - \lfloor \frac{m+1}{2} \rfloor$. Then

\[
D_G(v_0) = \left\lfloor \frac{m^2}{4} \right\rfloor + \frac{1}{2} a(a+1) + \frac{1}{2} b \left( b + 1 + 2 \left\lfloor \frac{m}{2} \right\rfloor \right) + h,
\]

\[
D_G(v_{\frac{n}{4}}) = \left\lfloor \frac{m^2}{4} \right\rfloor + \frac{1}{2} 2(2 \left\lfloor \frac{m}{2} \right\rfloor + b + 3) + 2(h - 1),
\]

\[
D_G(u_0) = \left\lfloor \frac{m^2}{4} \right\rfloor + a \left( \frac{1}{2} (a - 1) + m \right) + \frac{1}{2} b \left( 2a + 2 \left\lfloor \frac{m}{2} \right\rfloor + b + 1 \right) + h(a + 1),
\]

\[
D_G(u_1) = \left\lfloor \frac{m^2}{4} \right\rfloor + b \left( \frac{1}{2} (b - 1) + m \right) + \frac{1}{2} a \left( 2b + 2 \left\lfloor \frac{m}{2} \right\rfloor + a + 1 \right) + h \left( b + \left\lfloor \frac{m}{2} \right\rfloor + 1 \right).
\]

Lemma 10 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

\[
\delta'(U_{n,m,d}(a,0)) < \delta'(U_{n,m-2,d+1}(a + 2,0)).
\]

Proof Let $G_1 = U_{n,m-2,d+1}(a+2,0)$ and $G_2 = U_{n,m,d}(a,0)$. Note that $h = n - d - \lfloor \frac{m+1}{2} \rfloor = 0$. By Lemmas 8 and 9 we have

\[
\delta'(U_{n,m-2,d+1}(a + 2,0)) - \delta'(U_{n,m,d}(a,0)) = 4[W(G_1) - W(G_2)] - [D_{G_1}(u_0) - D_{G_2}(u_0)] + [D_{G_1}(v_0) - D_{G_2}(v_0)]
\]

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

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

Thus,

\[
\delta'(U_{n,m-2,d+1}(a + 2,0)) - \delta'(U_{n,m,d}(a,0)) = 2(n - 1)n - [\delta'(U_{n,m-2,d+1}(a + 2,0)) - \delta'(U_{n,m,d}(a,0))]
\]

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

\[= \begin{cases} 
5m^2 - 2(2n + 7)m + 2n^2 + 4n + 10 & \text{if } m \text{ is even} \\
5m^2 - 2(2n + 7)m + 2n^2 + 4n + 11 & \text{if } m \text{ is odd}
\end{cases}
\]

\[\geq 5m^2 - 2(2n + 7)m + 2n^2 + 4n + 10
\]

\[\geq 5 \cdot \left( \frac{2n + 7}{5} \right)^2 - 2(2n + 7) \cdot \frac{2n + 7}{5} + 2n^2 + 4n + 10
\]
Lemma 11 Let \( n, m \) and \( d \) be integers with \( 5 \leq m \leq n - 2, 3 \leq d \leq n - \left\lceil \frac{m+1}{2} \right\rceil \), and let \( a \) and \( b \) be integers with \( a + b = d - \left\lceil \frac{m}{2} \right\rceil \), \( a \geq b \geq 0 \) and \( a \geq 1 \). Then

\[
\rho' D' \left( U_{n,m,d}(a,b) \right) < \rho' D' \left( U_{n,m-2,d+1}(a+1,b+1) \right).
\]

Proof Let \( h = n - d - \left\lceil \frac{m+1}{2} \right\rceil \). 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 8 and 9 we have

\[
D'(U_{n,m-2,d+1}(a+1,b+1)) - D'(U_{n,m,d}(a,b)) = 4[W(G_1) - W(G_2)]
\]

\[
= (h+1)[D_{G_1}(v_0) - D_{G_2}(v_0)] + \left[ D_{G_1} \left( v_{\left\lceil \frac{m}{2} \right\rceil - 1} \right) - D_{G_2} \left( v_{\left\lceil \frac{m}{2} \right\rceil} \right) \right]
\]

\[
- h[D_{G_1}(u) - D_{G_2}(u)] - [D_{G_1}(u_0) - D_{G_2}(u_0)] - [D_{G_1}(u_1) - D_{G_2}(u_1)]
\]

\[
= 4 \left[ h \left( 2 + a - \left\lceil \frac{m+1}{2} \right\rceil \right) - 2 + ab + \left\lfloor \frac{m^2}{4} \right\rfloor \right]
\]

\[
+ \left( h + 1 \right) \left( 2 + a - \left\lceil \frac{m+1}{2} \right\rceil \right) + \left( 2 + b - \left\lceil \frac{m+1}{2} \right\rceil - h \right)
\]

\[
- h \left( 2 + a - \left\lceil \frac{m+1}{2} \right\rceil \right) - \left( b + \left\lceil \frac{m}{2} \right\rceil + h \right) - \left( a + \left\lceil \frac{m}{2} \right\rceil \right)
\]

\[
= -4b^2 + 4(n - m - 2h)b + 4n \left( \left\lceil \frac{m}{2} \right\rceil + h \right) - 2m^2 - 8mh
\]

\[
- 4(m - 1) \left( \left\lceil \frac{m}{2} \right\rceil - 1 \right) + 4 \left\lfloor \frac{m^2}{4} \right\rfloor - 4h^2 + 6h.
\]

If \( b = 0 \), then \( a = n - h - m \), and by similar calculation, the equality above holds also.

Thus,

\[
\rho' D'(U_{n,m-2,d+1}(a+1,b+1)) - \rho' D'(U_{n,m,d}(a,b)) = 2(n - 1)n - \left[D'(U_{n,m-2,d+1}(a+1,b+1)) - D'(U_{n,m,d}(a,b))\right]
\]

\[
= 4b^2 - 4(n - m - 2h)b
\]

\[
+ 2n^2 - 4n \left( \left\lceil \frac{m}{2} \right\rceil + h + \frac{1}{2} \right) + 2m^2 + 8mh + 4(m - 1) \left( \left\lceil \frac{m}{2} \right\rceil - 1 \right)
\]

\[
- 4 \left\lfloor \frac{m^2}{4} \right\rfloor + 4h^2 - 6h
\]

\[
\geq 4 \left( \frac{n - m - 2h}{2} \right)^2 - 4(n - m - 2h) \cdot \frac{n - m - 2h}{2}
\]
Among graphs in $\mathcal{U}$, $G$.

**Theorem 3** Among graphs in $\mathcal{U}$, the unique graph with maximum reverse degree distance for \(p\) is the unique graph with maximum reverse degree distance; the case $p = 0$ is trivial.

Any graph in $\mathcal{U}$ 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 $\mathcal{U}$.

**Theorem 3** Among graphs in $\mathcal{U}(n,p)$, where $n \geq 6$ and $1 \leq p \leq n - 4$,

(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 $U_{n,4,n-3}^k$ 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 $\left\lfloor \frac{n-p-1}{2} \right\rfloor = \frac{n+4}{6}$, $U_{n,3,n-p}$ 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, $\mathcal{U}(n,1) = \{U_{n,m,n-\left\lceil \frac{m+1}{2} \right\rceil}(n-m,0) : 3 \leq m \leq n - 1\}$. By Lemma 10, $D'(U_{n,m,n-\left\lceil \frac{m+1}{2} \right\rceil}(n-m,0)) < D'(U_{n,3,n-2}(n-3,0))$ for odd $m > 3$, and $D'(U_{n,m,n-\left\lceil \frac{m+1}{2} \right\rceil}(n-m,0)) < D'(U_{n,4,n-2}(n-4,0))$ 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

$$D'(U_{n,4,n-2}(n-4,0)) - D'(U_{n,3,n-2}(n-3,0))$$

$$= D'(U_{n,3,n-2}(n-3,0)) - D'(U_{n,4,n-2}(n-4,0))$$

Now the result follows. \(\square\)
\[= 4[W(G_2) - W(G_1)] + [D_{G_2}(v_0) - D_{G_1}(v_0)] - [D_{G_2}(u_0) - D_{G_1}(u_0)]\]
\[= 4(n - 4) + (n - 5) - 1 = 5n - 22 > 0.\]

Then (i) follows.

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

By Corollary 1 and Lemma 7, \(\mathcal{D}'(G) \leq \mathcal{D}'(U_{n,3,d}) \leq \mathcal{D}'(U_{n,3,n-p})\) for \(m = 3\), and \(\mathcal{D}'(G) \leq \mathcal{D}'(U_{n,4,d}) \leq \mathcal{D}'(U_{n,4,n-p})\) for \(m = 4\).

By Corollary 1 and Lemmas 7 and 11, if \(m \geq 5\), then for \(i = \lfloor \frac{m-3}{2} \rfloor\), we have

\[\mathcal{D}'(G) \leq \mathcal{D}'(U_{n,m,d}) \leq \mathcal{D}'(U_{n,m,n-p+2-\lfloor \frac{m+1}{2} \rfloor}(\gamma, \theta))\]
\[< \mathcal{D}'(U_{n,n-2i,n-p+2-\lfloor \frac{m+1}{2} \rfloor+i}(\gamma + i, \theta + i))\]
\[< \mathcal{D}'(U_{n,n-2i,n-p+2-\lfloor \frac{m+1}{2} \rfloor+i})\]
\[= \mathcal{D}'(U_{n,m-2i,n-p}).\]

Thus, \(\mathcal{D}'(G) \leq \mathcal{D}'(U_{n,3,n-p})\) for odd \(m > 3\), and \(\mathcal{D}'(G) < \mathcal{D}'(U_{n,4,n-p})\) for even \(m > 4\).

Note that \(U_{n,4,n-p} = U_{n,4,n-p}(\frac{n-p-2}{2}, \frac{n-p-2}{2})\) if \(p = 2, 3\) and \(n - p\) is even, \(U_{n,4,n-p} = U_{n,4,n-p}(\lfloor \frac{n-p}{2} \rfloor, \lfloor \frac{n-p-3}{2} \rfloor)\) if \(p = 2, 3\) and \(n - p\) is odd or \(4 \leq p \leq n - 4\), and \(U_{n,3,n-p} = U_{n,3,n-p}(\lfloor \frac{n-p}{2} \rfloor, \lfloor \frac{n-p-1}{2} \rfloor)\). 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. Note that \(\mathcal{D}'(U_{n,4,n-p}^0) = \mathcal{D}'(U_{n,4,n-p}^1)\) from Lemma 4.

It is easily seen that

\[\mathcal{D}'(U_{n,4,n-p}) - \mathcal{D}'(U_{n,3,n-p})\]
\[= \mathcal{D}'(U_{n,3,n-p}) - \mathcal{D}'(U_{n,4,n-p})\]
\[= 4[W(G_4) - W(G_3)] + (p - 1)[D_{G_4}(v_0) - D_{G_3}(v_0)]\]
\[+ [D_{G_4}(v_1) - D_{G_3}(v_2)] - (p - 2)[D_{G_4}(u) - D_{G_3}(u)]\]
\[+ [D_{G_4}(u_0) - D_{G_3}(u_0)] - [D_{G_4}(u_1) - D_{G_3}(u_1)]\]
\[= 4 \left(\frac{n - p - 2}{2} - p + 2\right) + (1 - p) + (2 - p) + (p - 2) + (1 - p) + (p - 2)\]
\[= 2n - 7p + 4 = \begin{cases} 2n - 10 > 0 & \text{if } p = 2 \text{ and } n \geq 6 \text{ is even} \\
2n - 17 > 0 & \text{if } p = 3 \text{ and } n > 7 \text{ is odd} \\
-3 & \text{if } p = 3 \text{ and } n = 7, \end{cases}\]

and thus (ii), (iii) and (iv) follow.

If \(p = n - 4\), then \(U_{n,4,n-p} = U_{n,4,4}(2, 0), U_{n,3,n-p} = U_{n,3,4}(2, 1)\), and it is easily checked that \(\mathcal{D}'(U_{n,4,4}) - \mathcal{D}'(U_{n,3,4}) = \mathcal{D}'(U_{n,3,4}) - \mathcal{D}'(U_{n,4,4}) = 2 - n < 0\). If \(p = 2, 3\) and \(n - p\) is odd, or \(4 \leq p \leq n - 5\), then by similar calculation as above, we have

\[\mathcal{D}'(U_{n,4,n-p}) - \mathcal{D}'(U_{n,3,n-p}) = 6 \left(\frac{n - p - 1}{2}\right) - n - 4,\]
and thus (v) follows easily. □
Let \( \Omega(n, \Delta) \) be the set of unicyclic graphs with \( n \) vertices and maximum degree \( \Delta \), where \( 2 \leq \Delta \leq n - 1 \). The cases \( \Delta = 2, n - 1 \) are trivial.

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

**Theorem 4** Among graphs in \( \Omega(n, \Delta) \), where \( n \geq 6 \) and \( 3 \leq \Delta \leq n - 3 \),

(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 \( U_{n,4,n-3}^k \) 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 \( U_{n,4,n-\Delta+1}^\gamma \) and \( U_{n,4,n-\Delta+1}^\gamma \) are the unique graphs with maximum reverse degree distance for \( \frac{n-\Delta}{6} > \frac{n+4}{6} \) and \( \frac{n-\Delta}{6} \leq \frac{n+4}{6} \), respectively.

**Proof** Let \( d \) be the diameter and let \( u \) be a vertex of degree \( \Delta \) in \( G \). A diametrical path \( P(G) \) contains at most \( \left\lfloor \frac{m}{2} \right\rfloor + 1 \) vertices of the cycle \( C_m \) and two neighbors of \( u \), but \( P(G) \) can not contain these vertices at the same time. Note that the cycle \( C_m \) contains at most two neighbors of \( u \). Thus \( d + 1 < n - (m + \Delta - 2) + \left\lfloor \frac{m}{2} \right\rfloor + 1 + 2 \) and then \( d \leq n - \Delta + 3 - \left\lfloor \frac{m+1}{2} \right\rfloor \).

By Corollary 1 and Lemmas 7 and 11, we have: \( 'D'(G) \leq 'D'(U_{n,3,d}) \leq 'D'(U_{n,3,n-\Delta+1}) \) for \( m = 3 \), \( 'D'(G) \leq 'D'(U_{n,4,d}) \leq 'D'(U_{n,4,n-\Delta+1}) \) for \( m = 4 \), and

\[
'D'(G) \leq 'D'(U_{n,m,d}) \leq 'D' \left( U_{n,m,n-\Delta+3-\left\lfloor \frac{m+1}{2} \right\rfloor}^\gamma \theta \right) \\
< 'D' \left( U_{n,m-2i,n-\Delta+3-\left\lfloor \frac{m+1}{2} \right\rfloor+i}^\gamma+i \theta+i \right) \\
\leq 'D' \left( U_{n,m-2i,n-\Delta+3-\left\lfloor \frac{m+1}{2} \right\rfloor+i}^\gamma+i \right) \\
= 'D' \left( U_{n,m-2i,n-\Delta+1}^\gamma+i \right)
\]

for \( m \geq 5 \), where \( i = \left\lfloor \frac{m-3}{2} \right\rfloor \).

Thus, \( 'D'(G) < 'D'(U_{n,3,n-\Delta+1}) \) for odd \( m > 3 \) and \( 'D'(G) < 'D'(U_{n,4,n-\Delta+1}) \) for even \( m > 4 \). Now the theorem follows by similar arguments as in the proof of Theorem 3. \( \square \)

Finally, we give the values of the maximum reverse degree distances in Theorem 3 and 4.
(i) For $U_{n,4,n-2}(n-4,0)$,
\[
D'(U_{n,4,n-2}(n-4,0)) = 4W(U_{n,4,n-2}(n-4,0)) + (3-2)D_{U_{n,4,n-2}(n-4,0)}(v_0) + (1-2)D_{U_{n,4,n-2}(n-4,0)}(u_0)
\]
\[
= 4W(U_{n,4,n-2}(n-4,0)) - 3(n-4)
\]
and thus,
\[
^rD'(U_{n,4,n-2}(n-4,0)) = 2(n-1)n(n-2) - D'(U_{n,4,n-2}(n-4,0))
\]
\[
= \frac{4}{3}n^3 - 6n^2 + \frac{47}{3}n - 36.
\]

(ii) For $U_{n,4,n-2}$,
\[
D'(U_{n,4,n-2}) = 4W(U_{n,4,n-2}) + (3-2)D_{U_{n,4,n-2}}(v_0) + (1-2)D_{U_{n,4,n-2}}(u_0)
\]
\[
+ (3-2)D_{U_{n,4,n-2}}(\{v_{\lfloor \frac{m}{2} \rfloor}\}) + (1-2)D_{U_{n,4,n-2}}(u_1)
\]
\[
= 4W(U_{n,4,n-2}(n-4,0)) - 3(n-4)
\]
and thus
\[
^rD'(U_{n,4,n-2}) = 2(n-1)n(n-2) - D'(U_{n,4,n-2})
\]
\[
= \begin{cases} 
\frac{4}{3}n^3 - \frac{2}{3}n^2 + \frac{11}{3}n - 12 & \text{if } n \text{ is even} \\
\frac{2}{3}n^3 - \frac{3}{3}n^2 + \frac{1}{3}n + \frac{27}{2} & \text{if } n \text{ is odd} 
\end{cases}
\]

(iii) For $U_{n,4,n-3}$ with odd $n$,
\[
D'(U_{n,4,n-3}) = 4W(U_{n,4,n-3}) + (4-2)D_{U_{n,4,n-3}}(v_0) + (1-2)D_{U_{n,4,n-3}}(u_0)
\]
\[
+ (1-2)D_{U_{n,4,n-3}}(u) + (3-2)D_{U_{n,4,n-3}}(\{v_{\lfloor \frac{m}{2} \rfloor}\})
\]
\[
+ (1-2)D_{U_{n,4,n-3}}(u_1)
\]
\[
= 4W(U_{n,4,n-3}) - \frac{1}{2}n^2 + \frac{19}{2}
\]
\[
= \frac{2}{3}n^3 - \frac{5}{2}n^2 + \frac{10}{3}n + \frac{47}{2}
\]
and thus
\[
^rD'(U_{n,4,n-3}) = 2(n-1)n(n-3) - D'(U_{n,4,n-3})
\]
\[
= \frac{4}{3}n^3 - \frac{11}{2}n^2 + \frac{8}{3}n - \frac{47}{2}.
\]

(iv) For $U_{n,4,n-p}$,
\[
D'(U_{n,4,n-p})
\[
\begin{aligned}
&= 4W(U_{n,4,n-p}) + [(p + 1) - 2]D_{U_{n,4,n-p}}(v_0)
+ (1 - 2)D_{U_{n,4,n-p}}(u_0) + (p - 2)(1 - 2)D_{U_{n,4,n-p}}(u)
+ (3 - 2)D_{U_{n,4,n-p}}(v_{\lfloor \frac{m}{2} \rfloor}) + (1 - 2)D_{U_{n,4,n-p}}(u_1)
\]
\[
= \begin{cases}
\frac{2}{3}n^3 - (p - \frac{1}{2})n^2 + (3p - \frac{17}{3})n + \frac{p^3}{3} - \frac{p^2}{2} + \frac{11p}{3} + 10 & \text{if } n - p \text{ is even}
\frac{2}{3}n^3 - (p - \frac{1}{2})n^2 + (3p - \frac{17}{3})n + \frac{p^3}{3} - \frac{p^2}{2} + \frac{11p}{3} + \frac{7}{2} & \text{if } n - p \text{ is odd}
\end{cases}
\]

and thus

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

(v) For \(U_{n,3,n-p},\)

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

and thus

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

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