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DETOUR INDEX OF A CLASS OF UNICYCLIC GRAPHS

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Abstract

The detour index of a connected graph is defined as the sum of detour distances between all unordered pairs of vertices. We determine the n-vertex unicyclic graphs whose vertices on its unique cycle all have degree at least three with the first, the second and the third smallest and largest detour indices respectively for $n \geq 7$.

1 Introduction

Let G be a simple connected graph with vertex set $V(G)$. For $u, v \in V(G)$, the distance $d(u, v)$ or $d_G(u, v)$ between u and v in G is the length of a shortest path connecting them [1], and the detour distance $l(u, v)$ or $l_G(u, v)$ between u and v in G is the length of a longest path connecting them [2, 3]. Note that $d(u, u) = l(u, u) = 0$ for any $u \in V(G)$.

The Wiener index of the graph G is defined as [4, 5]

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u, v).$$

As one of the oldest topological indices, the Wiener index has found various applications in chemical research [6] and has also been studied extensively in mathematics [7–10].

The detour index of the graph G is defined as [11–13]

$$\omega(G) = \sum_{\{u,v\} \subseteq V(G)} l(u, v).$$

This graph invariant has found applications in QSPR and QSAR studies, see the work of Lukovits [13], Trinajstić *et al.* [14], Rücker and Rücker [15], and Nikolić *et al.* [16]. For the computation aspect of the detour index, see the work of Lukovits

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and Razinger [17], Trinajstić *et al.* [16], and Rücker and Rücker [15]. Related work may be found in [19, 20].

In [21], Zhou and Cai established some basic properties of the detour index, especially, they gave bounds for the detour index, determined the n-vertex unicyclic graphs with the first, the second and the third smallest and largest detour indices respectively for $n \geq 5$, and determined the n-vertex unicyclic graphs of cycle length r with minimum and maximum detour indices respectively where $3 \leq r \leq n-2$.

A unicyclic graph is fully loaded if vertices on its unique cycle all have degree at least three. In the present paper, in continuation of the study on the detour index, we determine the n-vertex fully loaded unicyclic graphs with the first, the second and the third smallest and largest detour indices respectively for $n \geq 7$.

2 Preliminaries

For a connected graph G with $u \in V(G)$, let $W_u(G) = \sum_{v \in V(G)} d(u,v)$ and $\omega_u(G) = \sum_{v \in V(G)} l(u,v)$. Let S_n and P_n be the n-vertex star and path, respectively.

Lemma 1. [7] *Let T be an n-vertex tree different from S_n and P_n. Then*

$$(n-1)^2 = W(S_n) < W(T) < W(P_n) = \frac{n^3-n}{6}.$$

We will also use the following lemmas.

Lemma 2. [21] *Let T be an n-vertex tree with $u \in V(T)$, where u is not the center if $T = S_n$ and u is not a terminal vertex if $T = P_n$. Let x and y be the center of the star S_n and a terminal vertex of the path P_n, respectively. Then*

$$n-1 = W_x(S_n) < W_u(T) < W_y(P_n) = \frac{n(n-1)}{2}.$$

An n-vertex tree of diameter 3 is of the form $T_{n;a,b}$ formed by attaching a and b pendent vertices to the two vertices of P_2, respectively, where $a+b = n-2$ and $a, b \geq 1$. Let $S'_n = T_{n;n-3,1}$ for $n \geq 4$ and let $S''_n = T_{n;n-4,2}$ for $n \geq 6$.

Lemma 3. [21] *Among the n-vertex trees with $n \geq 6$, S'_n and S''_n are respectively the unique graphs with the second and the third smallest Wiener indices, which are equal to n^2-n-2 and n^2-7, respectively.*

Lemma 4. [21] *Let T be an n-vertex tree with $n \geq 6$, $u \in V(T)$, $T \neq S_n$, where u is not a vertex of maximal degree if $T = S'_n$ or $T = S''_n$. Let x and y be the vertices of maximal degrees in S'_n and S''_n, respectively. Then $n = W_x(S'_n) < W_y(S''_n) = n+1 \leq W_u(T)$.*

Let C_n be the n-vertex cycle with $n \geq 3$.

Lemma 5. [21] *Let u be a vertex on the cycle C_r with $r \geq 3$. Then $\omega_u(C_r) = \frac{1}{4}(3r^2 - 4r + \varepsilon_r)$ and $\omega(C_r) = \frac{1}{8}r(3r^2 - 4r + \varepsilon_r)$ where $\varepsilon_r = 1$ if r is odd and $\varepsilon_r = 0$ if r is even.*

Let $C_r(T_1, T_2, \ldots, T_r)$ be the graph constructed as follows. Let the vertices of the cycle C_r be labeled consecutively by $v_1, v_2, \ldots, v_r$. Let $T_1, T_2, \ldots, T_r$ be vertex–disjoint trees such that T_i and the cycle C_r share exactly one common vertex v_i for $i = 1, 2, \ldots, r$. Then any n-vertex unicyclic graph G with a cycle on r vertices is of the form $C_r(T_1, T_2, \ldots, T_r)$, where $\sum\limits_{i=1}^{r} |T_i| = n$, and $|H| = |V(H)|$ for a graph H.

Lemma 6. [21] *Let $G = C_r(T_1, T_2, \ldots, T_r)$. Suppose that trees T_i and T_j are nontrivial stars. Let $x \in V(T_i)$, $y \in V(T_j)$ with $x \neq v_i$ and $y \neq v_j$. If $\omega_x(G) \leq \omega_y(G)$, then $\omega(G - v_j y + v_i y) < \omega(G)$.*

Lemma 7. [21] *Let $G = C_r(T_1, T_2, \ldots, T_r)$. Then*

$$\omega(G) = \sum_{i=1}^{r} W(T_i) + \sum_{1 \leq i < j \leq r} \left[|T_i| \cdot W_{v_j}(T_j) + |T_j| \cdot W_{v_i}(T_i) + |T_i| \cdot |T_j| \cdot l_{C_r}(v_i, v_j) \right].$$

For $n \geq 6$, let $\mathbb{U}_n$ be the set of n-vertex fully loaded unicyclic graphs. For $3 \leq r \leq \lfloor \frac{n}{2} \rfloor$, let $\mathbb{U}_{n,r}$ be the set of graphs in $\mathbb{U}_n$ with cycle length r.

3 Fully loaded unicyclic graphs with small detour indices

For $3 \leq r \leq \lfloor \frac{n}{2} \rfloor$, let $S_{n,r} = C_r(T_1, T_2, \ldots, T_r)$ with $T_1 = \cdots = T_{r-1} = P_2$ and $T_r = S_{n-2(r-1)}$ with center v_r.

Lemma 8. *For $3 \leq r \leq \lfloor \frac{n}{2} \rfloor$,*

$$\omega(S_{n,r}) = \begin{cases} n^2 + \frac{3r^2-6r-1}{2} n + \frac{-3r^3+4r^2+r}{2} & \text{if } r \text{ is odd,} \\ n^2 + \frac{3r^2-6r-2}{2} n + \frac{-3r^3+4r^2+2r}{2} & \text{if } r \text{ is even.} \end{cases}$$

Proof. Let $u_i \neq v_i$ be the pendent vertex of $T_i = P_2$ for $i = 1, 2, \ldots, r-1$, and let $u_j \neq v_r$, $j = r, r+1, \ldots, n-r$, be the pendent vertices of $T_r = S_{n-2(r-1)}$. To compute $\omega(S_{n,r})$, consider the contributions of the pairs of vertices in the cycle, the pairs of pendent vertices, and the pairs with one vertex in the cycle and the other a pendent vertex. It is easily seen that

$$
\begin{aligned}
\omega(S_{n,r}) &= \sum_{1\le i<j\le r} l(v_i,v_j) + \sum_{1\le i<j\le n-r} l(u_i,u_j) + \sum_{i=1}^{r}\sum_{j=1}^{n-r} l(v_i,u_j) \\
&= \omega(C_r) + \sum_{1\le i<j\le r} l(u_i,u_j) + 2\binom{n-2r}{2} + (n-2r)\left[2+\sum_{i=1}^{r-1} l(u_r,u_i)\right] \\
&\quad + \sum_{i=1}^{r}\sum_{j=1}^{r} l(v_i,u_j) + \sum_{i=1}^{r}\sum_{j=r+1}^{n-r} l(v_i,u_j) \\
&= \omega(C_r) + \sum_{1\le i<j\le r} [l(v_i,v_j)+2] + 2\binom{n-2r}{2} \\
&\quad +(n-2r)\left[2+\sum_{i=1}^{r-1}(l(v_r,v_i)+2)\right] \\
&\quad + \sum_{i=1}^{r}\sum_{j=1}^{r}[l(v_i,v_j)+1] + \sum_{i=1}^{r}\sum_{j=r+1}^{n-r}[l(v_i,v_r)+1] \\
&= \omega(C_r)+\omega(C_r)+2\binom{r}{2}+2\binom{n-2r}{2} \\
&\quad +(n-2r)\left[2+\omega_{v_r}(C_r)+2(r-1)\right] \\
&\quad +2\omega(C_r)+r^2+(n-2r)(\omega_{v_r}(C_r)+r) \\
&= 4\omega(C_r)+2(n-2r)\omega_{v_r}(C_r)+(n-1)(n-r).
\end{aligned}
$$

Now the result follows from Lemma 5. □

Proposition 1. *Let $G \in \mathbb{U}_{n,r}$ with $3 \le r \le \lfloor \frac{n}{2} \rfloor$. Then $\omega(G) \ge \omega(S_{n,r})$ with equality if and only if $G = S_{n,r}$.*

Proof. Let $G = C_r(T_1, T_2, \ldots, T_r)$ be a graph with the smallest detour index among graphs in $\mathbb{U}_{n,r}$. We need only to show that $G = S_{n,r}$.

By Lemmas 1, 2 and 7, T_i is a star with center v_i for $i = 1, 2, \ldots, r$. Suppose that $|T_i|$, $|T_j| \ge 3$ with $i \ne j$. Let $x \in V(T_i)$, $y \in V(T_j)$ with $x \ne v_i$, $y \ne v_j$. Suppose without loss of generality that $\omega_x(G) \le \omega_y(G)$. By Lemma 6, $\omega(G - v_jy + v_iy) < \omega(G)$, a contradiction. Thus there can not be two trees of $T_1, T_2, \ldots, T_r$ with at least three vertices in G, i.e., $G = S_{n,r}$. □

Let Γ_n be the set of graphs $C_3(T_1, T_2, T_3)$ in $\mathbb{U}_n$ with $|T_1| = |T_2| = 2$. Let Ψ_n be the set of graphs $C_3(T_1, T_2, T_3)$ in $\mathbb{U}_n$ with $|T_3| \ge |T_2| \ge \max\{|T_1|, 3\}$. Let Φ_n be the set of graphs in $\mathbb{U}_n$ with cycle length at least four. Then $\mathbb{U}_n = \Gamma_n \cup \Psi_n \cup \Phi_n$.

For $n \ge 7$, let B'_n be the graph in Γ_n formed by attaching a path P_2 and $n-7$ pendent vertices to the vertex of degree two in $C_3(P_2, P_2, P_1)$, and for $n \ge 8$, let B''_n be the graph in Γ_n formed by attaching a star S_3 at its center and $n-8$ pendent vertices to the vertex of degree two in $C_3(P_2, P_2, P_1)$.

Lemma 9. *Among the graphs in Γ_n, B'_n for $n \geq 7$ and B''_n for $n \geq 8$ are the unique graphs respectively with the second and the third smallest detour indices, which are equal to $n^2 + 5n - 24$ and $n^2 + 6n - 29$, respectively.*

Proof. The case $n = 7$ is trivial. Let $G = C_3(T_1, T_2, T_3) \in \Gamma_n$ with $n \geq 8$. Note that $|T_1| = |T_2| = 2$. By Lemma 7, we have

$$\begin{aligned} \omega(G) &= 1 + 1 + W(T_3) + 2 + 2 + 8 + 2\,[2W_{v_3}(T_3) + n - 4 + 4(n-4)] \\ &= 10n - 26 + W(T_3) + 4W_{v_3}(T_3), \end{aligned}$$

which, together with Lemmas 3 and 4, implies that B'_n and B''_n are the unique graphs in Γ_n with the second and the third smallest detour indices, which are equal to $n^2 + 5n - 24$ and $n^2 + 6n - 29$, respectively. □

Let $S_n(a, b, c) = C_3(T_1, T_2, T_3)$ with $|T_1| = a$, $|T_2| = b$, $|T_3| = c$, $a + b + c = n$, and $a, b, c \geq 2$, where T_1 (T_2, T_3, respectively) is a star with center v_1 (v_2, v_3, respectively).

Lemma 10. *Among the graphs in Ψ_n, $S_n(2, 3, n-5)$ for $n \geq 8$ is the unique graph with the smallest detour index, which is equal to $n^2 + 6n - 35$, and $C_3(P_2, P_3, S_3)$ with v_2 being a terminal vertex of P_3 and v_3 being the center of S_3 for $n = 8$, $S_9(3, 3, 3)$ for $n = 9$, and $S_n(2, 4, n-6)$ for $n = 10, 11$ are the unique graphs with the second smallest detour index, which is equal to* 82 *for $n = 8$,* 102 *for $n = 9$, and $n^2 + 8n - 53$ for $n = 10, 11$.*

Proof. For $n \geq 8$, let $G = C_3(T_1, T_2, T_3) \in \Psi_n$ with $c \geq b \geq \max\{a, 3\}$, where $|T_1| = a$, $|T_2| = b$, $|T_3| = c$, and $a + b + c = n$.

Suppose first that $G = S_n(a, b, c)$ and $G \neq S_n(2, 3, n-5)$. It is easily seen that $\omega_x(G) \leq \omega_y(G)$ for pendent vertices $x \in V(T_3)$ and $y \in V(T_1) \cup V(T_2)$. By Lemma 6, we have

$$\omega(S_n(a, b, c)) \geq \omega(S_n(2, b, a + c - 2)) \geq \omega(S_n(2, 3, n-5)),$$

and at least one of the two inequalities is strict. If $G \neq S_n(a, b, c)$, then by Lemmas 1, 2 and 7, we have $\omega(G) > \omega(S_n(a, b, c)) \geq \omega(S_n(2, 3, n-5)) = n^2 + 6n - 35$. Thus $S_n(2, 3, n-5)$ for $n \geq 8$ is the unique graph in Ψ_n with the smallest detour index, which is equal to $n^2 + 6n - 35$.

Now we determine the graphs with the second smallest detour index in Ψ_n for $8 \leq n \leq 11$. It is trivial if $n = 8$. Suppose that $n = 9, 10, 11$. Let $G \in \Psi_n$ with $G \neq S_n(2, 3, n-5)$. Let G_1 be the graph obtained from $S_n(2, 3, n-5)$ by moving a pendent vertex at v_2 to the other pendent vertex, and G_2 the graph obtained from $S_n(2, 3, n-5)$ by moving a pendent vertex at v_3 to one other pendent vertex. If in G, $T_1 = P_2$ and $T_2 = S_3$ with v_2 its center, then by Lemma 7, $\omega(G) = 13n - 41 + W(T_3) + 5W_{v_3}(T_3)$, which, by Lemmas 1, 2, 3 and 4, is minimum when T_3 is not the star with center v_3 if and only if $T_3 = S'_{n-5}$ with v_3 its vertex of maximal degree, i.e., $G = G_2$. If $(a, b) = (2, 3)$, then by Lemmas 1, 2 and 7, $\omega(G) \geq \min\{\omega(G_1), \omega(G_2)\} = n^2 + 7n - 38$, and thus $\omega(G) \geq 106 > 102 = \omega(S_9(3, 3, 3))$

if $n = 9$, and $\omega(G) > n^2 + 8n - 53 = \omega(S_n(2, 4, n-6))$ if $n = 10, 11$. Suppose that $(a, b) \neq (2, 3)$. By Lemmas 1, 2 and 7, $\omega(G) \geq \omega(S_n(a, b, c))$ with equality if and only if $G = S_n(a, b, c)$. If $n = 9$, then $(a, b, c) = (3, 3, 3)$. If $n = 10$, then $(a, b, c) = (2, 4, 4), (3, 3, 4)$. If $n = 11$, then $(a, b, c) = (2, 4, 5), (3, 3, 5), (3, 4, 4)$.

Note that $\omega(S_{10}(3, 3, 4)) = 129 > 127 = \omega(S_{10}(2, 4, 4))$ and $\omega(S_{11}(3, 4, 4)) = 160 > \omega(S_{11}(3, 3, 5)) = 158 > \omega(S_{11}(2, 4, 5)) = 156$. The result follows easily. □

Proposition 2. *Among the graphs in* $\mathbb{U}_n$,

(*i*) $S_{n,3}$ *for* $n \geq 6$ *is the unique graph with the smallest detour index, which is equal to* $n^2 + 4n - 21$;

(*ii*) B'_7 *for* $n = 7$, $S_n(2, 3, n-5)$ *for* $8 \leq n \leq 10$, $S_{11}(2, 3, 6)$ *and* B'_{11} *for* $n = 11$, *and* B'_n *for* $n \geq 12$ *are the unique graphs with the second smallest detour index, which is equal to* 60 *for* $n = 7$, $n^2 + 6n - 35$ *for* $8 \leq n \leq 10$, 152 *for* $n = 11$, *and* $n^2 + 5n - 24$ *for* $n \geq 12$;

(*iii*) B'_8 *for* $n = 8$, B'_9 *and* $S_9(3, 3, 3)$ *for* $n = 9$, B'_{10} *for* $n = 10$, $S_{11}(2, 4, 5)$ *for* $n = 11$, *and* $S_n(2, 3, n-5)$ *for* $n \geq 12$ *are the unique graphs with the third smallest detour index, which is equal to* 80 *for* $n = 8$, 102 *for* $n = 9$, 126 *for* $n = 10$, 156 *for* $n = 11$, *and* $n^2 + 6n - 35$ *for* $n \geq 12$.

Proof. If r is odd with $3 \leq r \leq \lfloor \frac{n}{2} \rfloor - 1$, then by Lemma 8,

$$\omega(S_{n,r+1}) - \omega(S_{n,r}) = -\frac{1}{2}(9r^2 - 6nr + 4n - 3) = -\frac{9}{2}(r - r_1)(r - r_2),$$

where $r_1 = \frac{n - \sqrt{(n-3)(n-1)}}{3} < \frac{n-(n-3)}{3} = 1 < 3$, $r_2 = \frac{n + \sqrt{(n-3)(n-1)}}{3} > \frac{n+n-3}{3} = \frac{2}{3}n - 1 > \lfloor \frac{n}{2} \rfloor - 1$, and thus $r_1 < r < r_2$, implying that $\omega(S_{n,r+1}) > \omega(S_{n,r})$. If r is even with $4 \leq r \leq \lfloor \frac{n}{2} \rfloor - 1$, then by Lemma 8,

$$\omega(S_{n,r+1}) - \omega(S_{n,r}) = -\frac{1}{2}(9r^2 + 2r - 6nr + 2n - 2) = -\frac{9}{2}(r - r_3)(r - r_4),$$

where $r_3 = \frac{3n - 1 - \sqrt{(3n-4)^2 + 3}}{9} < \frac{3n-1-(3n-4)}{9} = \frac{1}{3} < 4$, $r_4 = \frac{3n - 1 + \sqrt{(3n-4)^2 + 3}}{9} > \frac{3n-1+3n-4}{9} = \frac{2}{3}n - \frac{5}{9} > \lfloor \frac{n}{2} \rfloor - 1$, and thus $r_3 < r < r_4$, implying that $\omega(S_{n,r+1}) > \omega(S_{n,r})$. It follows that $\omega(S_{n,r})$ is increasing with respect to $r \in \{3, 4, \ldots, \lfloor \frac{n}{2} \rfloor\}$. By Proposition 1 and Lemma 8, $S_{n,3}$ for $n \geq 6$ is the unique graph in $\mathbb{U}_n$ with the smallest detour index, which is equal to $n^2 + 4n - 21$, proving (*i*). Moreover, $S_{n,4}$ for $n \geq 8$ is the unique graph in Φ_n with the smallest detour index, which is equal to $n^2 + 11n - 60$.

Now we prove (*ii*). The case $n = 7$ is trivial. For $n \geq 8$, the graphs in $\mathbb{U}_n$ with the second smallest detour index are just the graphs in $\mathbb{U}_n \setminus \{S_{n,3}\} = (\Gamma_n \setminus \{S_{n,3}\}) \cup \Psi_n \cup \Phi_n$ with the smallest detour index, which, by Lemmas 9 and 10, is equal to $\min\{\omega(B'_n), \omega(S_n(2, 3, n-5)), \omega(S_{n,4})\} = \min\{n^2 + 5n - 24, n^2 + 6n - 35, n^2 + 11n - 60\}$, i.e., $n^2 + 6n - 35$ for $8 \leq n \leq 10$, $n^2 + 5n - 24 = n^2 + 6n - 35 = 152$ for $n = 11$, and $n^2 + 5n - 24$ for $n \geq 12$. Then (*ii*) follows.

From (*i*) and (*ii*) and by Lemmas 9 and 10, we find that the graphs in $\mathbb{U}_n$ for $n \geq 8$ with the third smallest detour index are just the graphs in $\mathbb{U}_n \setminus \{S_{n,3}, S_n(2, 3, n-$

$5)\} = (\Gamma_n \setminus \{S_{n,3}\}) \cup (\Psi_n \setminus \{S_n(2,3,n-5)\} \cup \Phi_n$ for $8 \le n \le 10$, $\mathbb{U}_{11} \setminus \{S_{11,3}, B'_{11}, S_{11}(2,3,6)\} = (\Gamma_{11} \setminus \{S_{11,3}, B'_{11}\}) \cup (\Psi_{11} \setminus \{S_{11}(2,3,6)\} \cup \Phi_{11}$ for $n = 11$ and $\mathbb{U}_n \setminus \{S_{n,3}, B'_n\} = (\Gamma_n \setminus \{S_{n,3}, B'_n\}) \cup \Psi_n \cup \Phi_n$ for $n \ge 12$ with the smallest detour index, which is equal to

$$\min\{\omega(B'_8), \omega(C_3(P_2,P_3,S_3)), \omega(S_{8,4})\} = \min\{80, 82, 92\} = 80 \text{ for } n = 8,$$

$$\min\{\omega(B'_9), \omega(S_9(3,3,3)), \omega(S_{9,4})\} = \min\{102, 102, 120\} = 102 \text{ for } n = 9,$$

$$\min\{\omega(B'_{10}), \omega(S_{10}(2,4,4)), \omega(S_{10,4})\} = \min\{126, 127, 150\} = 126 \text{ for } n = 10,$$

$$\min\{\omega(B''_{11}), \omega(S_{11}(2,4,5)), \omega(S_{11,4})\} = \min\{158, 156, 182\} = 156 \text{ for } n = 11,$$

and

$$\begin{aligned} & \min\{\omega(B''_n), \omega(S_n(2,3,n-5)), \omega(S_{n,4})\} \\ = \; & \min\{n^2+6n-29, n^2+6n-35, n^2+11n-60\} \\ = \; & n^2+6n-35 \end{aligned}$$

for $n \ge 12$. Now (iii) follows easily. $\square$

4 Fully loaded unicyclic graphs with large detour indices

For $3 \le r \le \lfloor \frac{n}{2} \rfloor$, let $P_{n,r} = C_r(T_1, T_2, \ldots, T_r)$ with $T_1 = \cdots = T_{r-1} = P_2$ and $T_r = P_{n-2(r-1)}$ with a terminal vertex v_r.

Lemma 11. *For* $3 \le r \le \lfloor \frac{n}{2} \rfloor$,

$$\omega(P_{n,r}) = \begin{cases} \frac{1}{6}[n^3 + (-3r^2+12r-10)n + 7r^3 - 24r^2 + 17r] & \text{if } r \text{ is odd,} \\ \frac{1}{6}[n^3 + (-3r^2+12r-13)n + 7r^3 - 24r^2 + 20r] & \text{if } r \text{ is even.} \end{cases}$$

Proof. To compute $\omega(P_{n,r})$, consider the contributions of the pairs of vertices in its subgraph $G_1 = C_r(P_2, P_2, \ldots, P_2)$, the pairs of vertices in the subgraph P_{n-2r} (obtained from $P_{n,r}$ by deleting vertices of G_1), and the pairs with one vertex in G_1 and the other vertex in P_{n-2r}. It is easily seen that

$$\begin{aligned} \omega(P_{n,r}) \; = \; & \omega(G_1) + W(P_{n-2r}) \\ & + \sum_{j=1}^{n-2r} \left[j + j + 1 + \sum_{i=1}^{r-1} (j + 1 + l(v_r, v_i) + j + 1 + l(v_r, v_i) + 1) \right] \\ = \; & 4\omega(C_r) + 2r^2 - r + W(P_{n-2r}) \\ & + 2(n-2r)\omega_{v_r}(C_r) + rn^2 + (-4r^2+4r-2)n + 4r^3 - 8r^2 + 4r \\ = \; & 4\omega(C_r) + W(P_{n-2r}) + 2(n-2r)\omega_{v_r}(C_r) \\ & + rn^2 + (-4r^2+4r-2)n + 4r^3 - 6r^2 + 3r. \end{aligned}$$

Now the result follows from Lemmas 1 and 5. $\square$

Proposition 3. *Let $G \in \mathbb{U}_{n,r}$ with $3 \le r \le \lfloor \frac{n}{2} \rfloor$. Then $\omega(G) \le \omega(P_{n,r})$ with equality if and only if $G = P_{n,r}$.*

Proof. Let $G = C_r(T_1, T_2, \ldots, T_r)$ be a graph with the largest detour index among graphs in $\mathbb{U}_{n,r}$. We need only to show that $G = P_{n,r}$.

By Lemmas 1, 2 and 7, T_i is a path with v_i as one of its terminal vertices for each $i = 1, 2, \ldots, r$. Suppose that $|T_i|, |T_j| \ge 3$ with $i \ne j$. Let $x \ne v_i$ and $y \ne v_j$ be terminal vertices of T_i and T_j, respectively. Suppose without loss of generality that $\omega_x(G) \ge \omega_y(G)$. Let z be the neighbor of y in G. Then for $G' = G - zy + xy \in \mathbb{U}_{n,r}$, we have

$$\begin{aligned}
\omega(G') - \omega(G) &= \omega_y(G') - \omega_y(G) \\
&= \omega_x(G') + n - 2 - \omega_y(G) \\
&= \omega_x(G) + 1 - l_G(x, y) + n - 2 - \omega_y(G) \\
&= \omega_x(G) - \omega_y(G) + n - 1 - l_G(x, y) > 0,
\end{aligned}$$

and thus $\omega(G') > \omega(G)$, a contradiction. Thus there can not be two trees of $T_1, T_2, \ldots, T_r$ with at least three vertices in G, i.e., $G = P_{n,r}$. $\square$

For even n, let $S'_{n,\frac{n-2}{2}} = C_{\frac{n-2}{2}}\left(T_1, T_2, \ldots, T_{\frac{n-2}{2}}\right)$, where $T_1 = P_4$ with a center v_1, and $T_i = P_2$ for $i \ne 1$, and let $S''_{n,\frac{n-2}{2}} = C_{\frac{n-2}{2}}\left(T_1, T_2, \ldots, T_{\frac{n-2}{2}}\right)$, where $T_1 = S_4$ with a pendent vertex v_1, and $T_i = P_2$ for $i \ne 1$. For even n and integer i with $i = 2, 3, \ldots, \lfloor \frac{n+2}{4} \rfloor$, let $Q_{n,\frac{n-2}{2}}(1, i) = C_{\frac{n-2}{2}}\left(T_1, T_2, \ldots, T_{\frac{n-2}{2}}\right)$, where $T_1 = P_3$ with a terminal vertex v_1, $T_i = P_3$ with a terminal vertex v_i, and $T_j = P_2$ for $j \ne 1, i$.

Lemma 12. *Among the graphs in $\mathbb{U}_{n,\frac{n-2}{2}}$ with even $n \ge 8$, $Q_{n,\frac{n-2}{2}}(1, 2)$ is the unique graph with the second largest detour index, which is equal to $\frac{1}{16}(3n^3 - 6n^2 + 40n - 80)$ for $n \equiv 0 \pmod 4$, and $\frac{1}{16}(3n^3 - 6n^2 + 36n - 88)$ for $n \equiv 2 \pmod 4$.*

Proof. For any graph $C_{\frac{n-2}{2}}\left(T_1, T_2, \ldots, T_{\frac{n-2}{2}}\right) \in \mathbb{U}_{n,\frac{n-2}{2}}$, there are at most two trees T_i and T_j with three vertices. By Proposition 3, the graphs in $\mathbb{U}_{n,\frac{n-2}{2}}$ with the second largest detour index are just the graphs in $\mathbb{U}_{n,\frac{n-2}{2}} \setminus \{P_{n,\frac{n-2}{2}}\}$ with the largest detour index. Except $P_{n,\frac{n-2}{2}}$, there are three graphs $S_{n,\frac{n-2}{2}}$, $S'_{n,\frac{n-2}{2}}$ and $S''_{n,\frac{n-2}{2}}$ in $\mathbb{U}_{n,\frac{n-2}{2}}$ with exactly one tree (T_1) with four vertices. Similarly to the proof of Lemma 9, we have $\omega\left(S''_{n,\frac{n-2}{2}}\right) > \omega\left(S'_{n,\frac{n-2}{2}}\right) > \omega\left(S_{n,\frac{n-2}{2}}\right)$, where $\omega\left(S''_{n,\frac{n-2}{2}}\right)$ is equal to $\frac{1}{16}(3n^3 - 6n^2 + 32n - 80)$ for $n \equiv 0 \pmod 4$ and $\frac{1}{16}(3n^3 - 6n^2 + 28n - 88)$ for $n \equiv 2 \pmod 4$. Let $G = C_{\frac{n-2}{2}}\left(T_1, T_2, \ldots, T_{\frac{n-2}{2}}\right)$ be a graph in $\mathbb{U}_{n,\frac{n-2}{2}}$ with exactly two trees of at least three vertices. Suppose without loss of generality that $|T_1| = |T_i| = 3$ for $2 \le i \le \lfloor \frac{n+2}{4} \rfloor$. Then T_1 and T_i are both paths on three vertices. For fixed i, by Lemmas 1, 2 and 7, $\omega(G)$ is maximum if and only if v_1 is a terminal vertex of T_1 and v_i is a terminal vertex of T_i, i.e., if and only if $G = Q_{n,\frac{n-2}{2}}(1, i)$.

It is easily seen that

$$\begin{aligned}
\omega\left(Q_{n,\frac{n-2}{2}}(1,i)\right) &= \omega\left(C_{\frac{n-2}{2}}(P_2,P_2,\ldots,P_2)\right)+4+\frac{n-2}{2}-(i-1)\\
&\quad +2\left[1+2+\sum_{j=2}^{r}(5+2l(v_1,v_j))\right]\\
&= \omega\left(C_{\frac{n-2}{2}}(P_2,P_2,\ldots,P_2)\right)+4\omega_{v_1}\left(C_{\frac{n-2}{2}}\right)+\frac{11n-20}{2}-i,
\end{aligned}$$

which is decreasing with respect to $i \in \left\{2,3,\ldots,\lfloor\frac{n+2}{4}\rfloor\right\}$. Thus $Q_{n,\frac{n-2}{2}}(1,2)$ is the unique graph with the largest detour index among the graphs in $\mathbb{U}_{n,\frac{n-2}{2}}$ with exactly two trees of at least three vertices, which is equal to $\frac{1}{16}(3n^3-6n^2+40n-80)$ for $n \equiv 0 \pmod 4$, and $\frac{1}{16}(3n^3-6n^2+36n-88)$ for $n \equiv 2 \pmod 4$. Since $\omega\left(Q_{n,\frac{n-2}{2}}(1,2)\right) > \omega\left(S''_{n,\frac{n-2}{2}}\right)$, the result follows easily. $\square$

Proposition 4. (1) *If n is odd with $n \geq 7$, then among the graphs in $\mathbb{U}_n$,*

(1.1) $P_{n,\frac{n-1}{2}}$ *is the unique graph with the largest detour index, which is equal to* $\frac{1}{16}(3n^3-3n^2+13n-45)$ *for $n \geq 7$ and $n \equiv 1 \pmod 4$, and* $\frac{1}{16}(3n^3-3n^2+17n-41)$ *for $n \geq 7$ and $n \equiv 3 \pmod 4$;*

(1.2) $P_{9,3}$ *for $n=9$, and $S_{n,\frac{n-1}{2}}$ for $n=7$ and $n \geq 11$ are the unique graphs with the second largest detour index, which is equal to 56 for $n=7$, 124 for $n=9$,* $\frac{1}{16}(3n^3-3n^2-3n+3)$ *for $n \geq 11$ and $n \equiv 1 \pmod 4$, and* $\frac{1}{16}(3n^3-3n^2+n+7)$ *for $n \geq 11$ and $n \equiv 3 \pmod 4$;*

(1.3) $C_3(P_2,P_3,P_4)$ *with v_2 a terminal vertex of P_3 and v_3 a terminal vertex of P_4 for $n=9$, and $P_{n,\frac{n-3}{2}}$ for $n \geq 11$ are the unique graphs with the third largest detour index, which is equal to 122 for $n=9$,* $\frac{1}{16}(3n^3-9n^2+89n-275)$ *for $n \geq 11$ and $n \equiv 1 \pmod 4$, and* $\frac{1}{16}(3n^3-9n^2+85n-287)$ *for $n \geq 11$ and $n \equiv 3 \pmod 4$.*

(2) *If n is even with $n \geq 6$, then among the graphs in $\mathbb{U}_n$,*

(2.1) $P_{n,\frac{n}{2}}$ *is the unique graph with the largest detour index, which is equal to* $\frac{1}{16}(3n^3-8n)$ *for $n \geq 6$ and $n \equiv 0 \pmod 4$, and* $\frac{1}{16}(3n^3-4n)$ *for $n \geq 6$ and $n \equiv 2 \pmod 4$;*

(2.2) $P_{n,\frac{n-2}{2}}$ *is the unique graph with the second largest detour index, which is equal to* $\frac{1}{16}(3n^3-6n^2+48n-128)$ *for $n \geq 8$ and $n \equiv 0 \pmod 4$, and* $\frac{1}{16}(3n^3-6n^2+44n-136)$ *for $n \geq 8$ and $n \equiv 2 \pmod 4$;*

(2.3) $Q_{8,3}(1,2)$ *for $n=8$, $P_{10,3}$ for $n=10$, and $Q_{n,\frac{n-2}{2}}(1,2)$ for $n \geq 12$ are the unique graphs with the third largest detour index, which is equal to 87 for $n=8$, 169 for $n=10$,* $\frac{1}{16}(3n^3-6n^2+40n-80)$ *for $n \geq 12$ and $n \equiv 0 \pmod 4$, and* $\frac{1}{16}(3n^3-6n^2+36n-88)$ *for $n \geq 12$ and $n \equiv 2 \pmod 4$.*

Proof. If r is odd with $3 \le r \le \lfloor \frac{n}{2} \rfloor - 1$, then by Lemma 11,

$$\begin{aligned} 2[\omega(P_{n,r+1}) - \omega(P_{n,r})] &= (2-2r)n + 7r^2 - 8r + 1 \\ &\ge (2-2r)\cdot 2(r+1) + 7r^2 - 8r + 1 \\ &= 3r^2 - 8r + 5 > 0, \end{aligned}$$

and thus $\omega(P_{n,r+1}) > \omega(P_{n,r})$. If r is even with $4 \le r \le \lfloor \frac{n}{2} \rfloor - 1$, then by Lemma 11,

$$\begin{aligned} 2[\omega(P_{n,r+1}) - \omega(P_{n,r})] &= (4-2r)n + 7r^2 - 10r \\ &\ge (4-2r)\cdot 2(r+1) + 7r^2 - 10r \\ &= 3r^2 - 6r + 8 > 0, \end{aligned}$$

and thus $\omega(P_{n,r+1}) > \omega(P_{n,r})$. It follows that $\omega(P_{n,r})$ is increasing with respect to $r \in \left\{3, 4, \ldots, \lfloor \frac{n}{2} \rfloor\right\}$.

Suppose that n is odd. By the above property of $\omega(P_{n,r})$, Proposition 3 and Lemma 11, $P_{n,\frac{n-1}{2}}$ is the unique graph in $\mathbb{U}_n$ with the largest detour index, which is equal to $\frac{1}{16}(3n^3 - 3n^2 + 13n - 45)$ for $n \ge 7$ and $n \equiv 1 \pmod 4$, and $\frac{1}{16}(3n^3 - 3n^2 + 17n - 41)$ for $n \ge 7$ and $n \equiv 3 \pmod 4$. Then (1.1) follows.

Since $\mathbb{U}_7 = \{P_{7,3}, S_{7,3}\}$, we have from (1.1) the result in (1.2) for $n = 7$. Suppose that $n \ge 9$. Note that $\mathbb{U}_{n,\frac{n-1}{2}} \setminus \left\{P_{n,\frac{n-1}{2}}\right\} = \left\{S_{n,\frac{n-1}{2}}\right\}$. By the above discussion, $P_{n,\frac{n-3}{2}}$ is the unique graph in $\mathbb{U}_n$ whose cycle length is at most $\frac{n-3}{2}$ with the largest detour index, and then the graphs in $\mathbb{U}_n$ with the second largest detour index are just the graphs $S_{n,\frac{n-1}{2}}$ and $P_{n,\frac{n-3}{2}}$ with larger detour index.

Since $\omega\left(S_{n,\frac{n-1}{2}}\right) - \omega\left(P_{n,\frac{n-3}{2}}\right)$ is negative for $n = 9$ and positive for $n \ge 11$, $P_{n,3}$ for $n = 9$ and $S_{n,\frac{n-1}{2}}$ for $n \ge 11$ are the unique graphs in $\mathbb{U}_n$ with the second largest detour index, which is equal to 124 for $n = 9$, $\frac{1}{16}(3n^3 - 3n^2 - 3n + 3)$ for $n \ge 11$ and $n \equiv 1 \pmod 4$, and $\frac{1}{16}(3n^3 - 3n^2 + n + 7)$ for $n \ge 11$ and $n \equiv 3 \pmod 4$. It also follows that $P_{n,\frac{n-3}{2}}$ for $n \ge 11$ is the unique graph in $\mathbb{U}_n$ with the third largest detour index, which is equal to $\frac{1}{16}(3n^3 - 9n^2 + 89n - 275)$ for $n \equiv 1 \pmod 4$, and $\frac{1}{16}(3n^3 - 9n^2 + 85n - 287)$ for $n \equiv 3 \pmod 4$. We are left with the case $n = 9$. Note that the third largest detour index of graphs in $\mathbb{U}_9$ is equal to the largest detour index of graphs in $(\Gamma_9 \setminus \{P_{9,3}\}) \cup \Psi_9 \cup (\Phi_9 \setminus \{P_{9,4}\})$. By direct checking, the largest detour index of graphs in $\Gamma_9 \setminus \{P_{9,3}\}$ is 118, in $\Phi_9 \setminus \{P_{9,4}\}$ is 120, and in Ψ_9 is 122, which is achieved uniquely by the graph $C_3(P_2, P_3, P_4)$ with v_2 a terminal vertex of P_3 and v_3 a terminal vertex of P_4, and thus this graph is the unique graph in $\mathbb{U}_9$ with the third largest detour index, which is equal to 122. Then (1.2) and (1.3) follow.

Now suppose that n is even. By the above property of $\omega(P_{n,r})$, Proposition 3 and Lemma 11, $P_{n,\frac{n}{2}}$ is the unique graph in $\mathbb{U}_n$ with the largest detour index, which is equal to $\frac{1}{16}(3n^3 - 8n)$ for $n \ge 6$ and $n \equiv 0 \pmod 4$, and $\frac{1}{16}(3n^3 - 4n)$ for $n \ge 6$ and $n \equiv 2 \pmod 4$, while $P_{n,\frac{n-2}{2}}$ is the unique graph with the second largest detour index, which is equal to $\frac{1}{16}(3n^3 - 6n^2 + 48n - 128)$ for $n \ge 8$ and $n \equiv 0 \pmod 4$, and $\frac{1}{16}(3n^3 - 6n^2 + 44n - 136)$ for $n \geq 8$ and $n \equiv 2 \pmod 4$. Then (2.1) and (2.2) follow.

Now we prove (2.3). From (2.1) and (2.2) and by Lemma 12 and the property of $\omega(P_{n,r})$, we find that the graphs in $\mathbb{U}_n$ with the third largest detour index are just the graphs in $\mathbb{U}_n \setminus \left\{P_{n,\frac{n}{2}}, P_{n,\frac{n-2}{2}}\right\}$ with the largest detour index, which is equal to $\omega(Q_{8,3}(1,2)) = 87$ for $n = 8$ and $\max\left\{\omega\left(Q_{n,\frac{n-2}{2}}(1,2)\right), \omega\left(P_{n,\frac{n-4}{2}}\right)\right\}$ for even $n \geq 10$. By Lemma 11, we have

$$\omega(P_{n,\frac{n-4}{2}}) = \begin{cases} \frac{1}{16}(3n^3 - 12n^2 + 136n - 512) & \text{if } n \equiv 0 \pmod 4, \\ \frac{1}{16}(3n^3 - 12n^2 + 140n - 496) & \text{if } n \equiv 2 \pmod 4. \end{cases}$$

Since $\omega(Q_{10,4}(1,2)) < \omega(P_{10,3})$ for $n = 10$ and $\omega\left(Q_{n,\frac{n-2}{2}}(1,2)\right) > \omega\left(P_{n,\frac{n-4}{2}}\right)$ for even $n \geq 12$, (2.3) follows easily. $\square$

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