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ON DETOUR INDEX

Bo Zhou* **and Xiaochun Cai**

Department of Mathematics, South China Normal University, Guangzhou 510631, P. R. China

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Abstract

The detour index of a connected graph is defined as the sum of the detour distances (lengths of longest paths) between unordered pairs of vertices of the graph. We give bounds for the detour index, determine the graphs with minimum and maximum detour indices respectively in the class of n-vertex unicyclic graphs with cycle length r, where $3 \le r \le n-2$, and the graphs with the first, the second and the third smallest and largest detour indices respectively in the class of n-vertex unicyclic graphs for $n \ge 5$.

1. INTRODUCTION

Let G be a connected graph with vertex set $V(G)$. The distance between vertices u and v in G is the length (number of edges) of a shortest path between them, denoted by $d(u, v|G)$. The Wiener index [1] of the graph G is defined as [2]

$$W(G) = \frac{1}{2} \sum_{u,v \in V(G)} d(u, v|G).$$

See [3–6] for more details on the Wiener index.

*E-mail: zhoubo@scnu.edu.cn

The detour distance [7–9] (also under the name elongation) between vertices u and v in the graph G is the length of a longest path between them, denoted by $l(u,v|G)$. Note that $l(u,u|G) = 0$ for any $u \in V(G)$, see [10] for a discussion. The detour index of the graph G is defined as [8–11]

$$\omega(G) = \frac{1}{2} \sum_{u,v \in V(G)} l(u,v|G).$$

If we use the notion of the detour matrix [8, 9], which is an $n \times n$ matrix whose (i,j)-element is $l(v_i, v_j|G)$ with $V(G) = \{v_1, v_2, \ldots, v_n\}$, then the detour index is equal to the half–sum of the (off–diagonal) elements of the detour matrix. Lukovits [11] investigated the use of the detour index in quantitative structure–activity relationship (QSAR) studies. Following the work in [11], Trinajstić *et al.* [12] analyzed the use of the detour index and compared its application and that of the Wiener index in structure–boiling point modeling, while Rücker and Rücker [10] also probed the detour index as a descriptor for boiling points of acyclic and cyclic alkanes. It was found that the detour index in combination with the Wiener index is very efficient in structure–boiling point modeling of acyclic and cyclic saturated hydrocarbons. Lukovits and Razinger [13] proposed an algorithm for the detection of the longest path between any two vertices of a graph, which was used to derive analytical formulas for the detour index of fused bicyclic structures. Trinajstić *et al.* [14] and Rücker and Rücker [10] proposed computer methods for computing the detour distances and hence for computing the detour index. Related work may be found in, e.g., [15]. For more details on the properties and chemical applications of the detour index, one may refer to [16].

We establish some properties of the detour index. We give bounds for the detour index, determine the graphs with minimum and maximum detour indices respectively in the class of n-vertex unicyclic graphs with cycle length r, where $3 \le r \le n-2$, and the graphs with the first, the second and the third smallest and largest detour indices respectively in the class of n-vertex unicyclic graphs for $n \ge 5$.

2. PRELIMINARIES

For the connected graph G with $u \in V(G)$, let $D(u|G) = \sum_{v \in V(G)} d(u,v|G)$ and $L(u|G) = \sum_{v \in V(G)} l(u,v|G)$. Then

$$W(G) = \frac{1}{2} \sum_{u \in V(G)} D(u|G),$$

$$\omega(G) = \frac{1}{2} \sum_{u \in V(G)} L(u|G).$$

Let S_n, P_n and C_n be the n-vertex star, path and cycle, respectively.

Lemma 1. [5] *Let T be a n-vertex tree different from S_n and P_n. Then $(n-1)^2 = W(S_n) < W(T) < W(P_n) = \frac{n^3-n}{6}$.*

The following lemma is obvious.

Lemma 2. *Let T be an n-vertex tree with $u \in V(T)$, where $n \geq 3$. Let x and y be the center of the star S_n and a terminal vertex of the path P_n, respectively. Then $n-1 = D(x|S_n) \leq D(u|T) \leq D(y|P_n) = \frac{n(n-1)}{2}$. Left equality holds exactly when $T = S_n$ and $u = x$, and right equality holds exactly when $T = P_n$ and u is a terminal vertex.*

Any 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 $n \geq 5$. Let T be a tree with edge set $E(T)$. For any $e \in E(T)$, $n_{T,1}(e)$ and $n_{T,2}(e)$ denote respectively the number of vertices of T lying on the two sides of e. It has been known [1, 3, 5] that $W(T) = \sum_{e \in E(T)} n_{T,1}(e) \cdot n_{T,2}(e)$. By this and the fact that the function $k(n-k)$ is increasing for $1 \leq k \leq \frac{n}{2}$, we may easily have the following lemma.

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

Proof. For any n-vertex tree T with diameter at least 4, there are at least two edges whose end vertices have degree at least 2, and then $W(T) \geq 2 \times 2 \times (n-2) + (n-3) \times 1 \times (n-1) = n^2 - 5$. For any n-vertex tree T of diameter 3, say $T = T_{n;a,b}$ with $a+b = n-2$ and $a, b \geq 1$, we have $W(T) = (a+1)(b+1)+(n-2)\times 1 \times (n-1)$ and thus if $T \neq S'_n$ then $W(T) \geq 3(n-3)+(n-2)(n-1) = W(S''_n) = n^2-7 > n^2-n-2 = W(S'_n)$ with equality if and only if $T = S''_n$. Now the result follows from Lemma 1. ■

Also, the following lemma is obvious.

Lemma 4. *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 vertex of maximal degree of S'_n and S''_n, respectively. Then $n = D(x|S'_n) < D(y|S''_n) \leq D(u|T)$.*

Recall that a unicyclic graph is a connected graph with a unique cycle. Let the vertices of the cycle C_r be labelled 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 have exactly one vertex v_i in common for $1 \leq i \leq r$. Such a unicyclic graph is denoted by $C_r(T_1, T_2, \ldots, T_r)$. Obviously, any n-vertex unicyclic graph G with cycle length r is of the form $C_r(T_1, T_2, \ldots, T_r)$, where $\sum_{i=1}^{r} |T_i| = n$ with $|T_i| = |V(T_i)|$.

Lemma 5. *Let $G = C_r(T_1, T_2, \ldots, T_r)$. Then*

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

Proof. It is easily seen that

$$\omega(G) = \sum_{i=1}^{r} W(T_i) + \sum_{1 \leq i < j \leq r} \sum_{x \in V(T_i)} \sum_{y \in V(T_j)} \left[d(x, v_i|G) + d(v_j, y|G) + l(v_i, v_j|G) \right].$$

Note that

$$\begin{aligned}
& \sum_{1 \leq i < j \leq r} \sum_{x \in V(T_i)} \sum_{y \in V(T_j)} \left[d(x, v_i|G) + d(v_j, y|G) + l(v_i, v_j|G) \right] \\
= & \sum_{1 \leq i < j \leq r} \left[\sum_{x \in V(T_i)} d(x, v_i|T_i) \sum_{y \in V(T_j)} 1 + \sum_{y \in V(T_j)} d(v_j, y|T_j) \sum_{x \in V(T_i)} 1 \right. \\
& \left. + l(v_i, v_j|C_r) \sum_{x \in V(T_i)} \sum_{y \in V(T_j)} 1 \right] \\
= & \sum_{1 \leq i < j \leq r} \left[|T_j| D(v_i|T_i) + |T_i| D(v_j|T_j) + |T_i||T_j| l(v_i, v_j|C_r) \right].
\end{aligned}$$

The result follows. ■

Lemma 6. [11] *Let $r \geq 3$ be an integer. Then $\omega(C_r) = \frac{1}{8} r(3r^2 - 4r + r_0)$ where $r_0 = 1$ if r is odd and $r_0 = 0$ if r is even.*

Let K_n be the complete graph with n vertices. Let $K_{a,b}$ be the complete bipartite graph with two partite sets having a and b vertices, respectively. For non-adjacent distinct vertices u and v of the graph G, $G + uv$ denotes the graph formed from G by adding the edge uv.

3. BOUNDS FOR THE DETOUR INDEX

We give basic lower and upper bounds for the detour index in terms of the number of vertices. A graph is said to be Hamilton–connected if each pair of distinct vertices are connected by a Hamilton path (a path containing all vertices of the graph).

Proposition 1. *Let G be a connected graph with $n \geq 3$ vertices. Then*

$$(n-1)^2 \leq \omega(G) \leq \frac{n(n-1)^2}{2}$$

with left equality if and only if $G = S_n$ and with right equality if and only if G is a Hamilton–connected graph.

Proof. For $u, v \in V(G)$, it is easily seen that $l(u, v|G) \leq n-1$ with equality if and only if there is a path of length $n-1$ between vertices u and v. Thus $\omega(G) \leq (n-1) \cdot \frac{n(n-1)}{2} = \frac{n(n-1)^2}{2}$ with equality if and only if there is a path of length $n-1$ between each pair of distinct vertices, i.e., G is a Hamilton–connected graph.

On the other hand, for any spanning tree T of G, we have $l(u, v|G) \geq d(u, v|T)$ and then $\omega(G) \geq W(T)$ with equality if and only if $G = T$. Recall that $W(T) \geq (n-1)^2$ with equality if and only if $T = S_n$ (see Lemma 1). Thus $\omega(G) \geq (n-1)^2$ with equality if and only if $G = T = S_n$. ■

If $G(n)$ is an n-vertex Hamilton–connected graph, then $G(3) = K_3$, $G(4) = K_4$, $G(5) = K_5 - 2K_2$ (K_5 with two independent edges deleted), $K_5 - K_2$ (K_5 with one edge deleted), or K_5. Moon [17] showed that for $n \geq 4$ there exist Hamilton–connected graphs with $\lfloor \frac{3n+1}{2} \rfloor$ edges. Since $\lfloor \frac{3n+1}{2} \rfloor < \frac{n(n-1)}{2}$ if and only if $n \geq 5$, there are n-vertex Hamilton–connected graphs with $\lfloor \frac{3n+1}{2} \rfloor + i$ edges with $i = 0, 1, \ldots, \frac{n(n-1)}{2} - \lfloor \frac{3n+1}{2} \rfloor$. Thus, the upper bound in Proposition 1 is attained for every $n \geq 3$, and for $n \geq 5$, we have a class of n-vertex Hamilton–connected graphs each of which has the same detour index (actually have the same detour matrix).

Recall that $l(u, v|G) \leq l(u, v|G + uv)$ for any pair of non-adjacent distinct vertices u and v in the connected n-vertex graph G and then $\omega(G) \leq \omega(G + uv)$. The equality may be attained even if the number of edges of G is less than $\lfloor \frac{3n+1}{2} \rfloor$. See, e.g., [18], the graphs G_1 and G_2 have equal detour index (actually have equal detour matrix), where $G_1 = K_{2,3}$ and G_2 is formed from G_1 by adding an edge between the two vertices of degree three.

Proposition 2. *Let G be a connected bipartite graph with $n \geq 2$ vertices. Then*

$$(n-1)^2 \leq \omega(G) \leq \begin{cases} \frac{1}{2}(n-1)^3 & \text{if } n \text{ is odd} \\ \frac{1}{4}n(2n^2 - 5n + 4) & \text{if } n \text{ is even} \end{cases}$$

with left equality if and only if $G = S_n$ *and with right equality if and only if* $G = K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$.

Proof. The left inequality has been shown in the previous proposition. Suppose that $V(G) = V_1 \cup V_2$ is the bipartition of G with $n_1 = |V_1| \le |V_2| = n_2$. Evidently, $n_1 + n_2 = n$. For distinct vertices u and v, $l(u,v|G) \le 2n_1 - 2$ if $u, v \in V_1$, $l(u,v|G) \le 2n_1$ if $u, v \in V_2$ and $n_1 < n_2$, and $l(u,v|G) \le 2n_1 - 1$ if $u \in V_1$ and $v \in V_2$. Thus, if $n_1 = n_2$ then $\omega(G) \le (2n_1 - 2) \cdot \frac{n_1(n_1-1)}{2} \cdot 2 + (2n_1 - 1) \cdot n_1 n_2 = \frac{1}{4} n(2n^2 - 5n + 4)$, and if $n_1 < n_2$ then $\omega(G) \le (2n_1 - 2) \cdot \frac{n_1(n_1-1)}{2} + 2n_1 \cdot \frac{n_2(n_2-1)}{2} + (2n_1 - 1) \cdot n_1 n_2 = n_1(n-1)^2 \le \lfloor \frac{n-1}{2} \rfloor (n-1)^2 < \frac{1}{4} n(2n^2 - 5n + 4)$.

If n is odd then $\omega(G) \le \frac{1}{2}(n-1)^3$ with equality if and only if $n_1 = \lfloor \frac{n-1}{2} \rfloor$, and for distinct vertices u and v, $l(u,v|G) = 2n_1 - 2$ if $u, v \in V_1$, $l(u,v|G) = 2n_1$ if $u, v \in V_2$, and $l(u,v|G) = 2n_1 - 1$ if $u \in V_1$ and $v \in V_2$, i.e., $G = K_{\frac{n-1}{2}, \frac{n+1}{2}}$. If n is even then $\omega(G) \le \frac{1}{4} n(2n^2 - 5n + 4)$ with equality if and only if $n_1 = n_2$, and for distinct vertices u and v, $l(u,v|G) = 2n_1 - 2$ if $u, v \in V_1$ or if $u, v \in V_2$, and $l(u,v|G) = 2n_1 - 1$ if $u \in V_1$ and $v \in V_2$, i.e., $G = K_{\frac{n}{2}, \frac{n}{2}}$. ■

From the proof above, we know that if G is a connected bipartite graph with n vertices and an (n_1, n_2)-bipartition where $n_1 < n_2$ then $\omega(G) \le n_1(n-1)^2$ with equality if and only if $G = K_{n_1, n_2}$.

4. THE DETOUR INDICES OF UNICYCLIC GRAPHS

For integers r and n with $3 \le r \le n$, let $\mathbb{U}_{n,r}$ be the set of n-vertex unicyclic graphs with cycle length r.

For integers n and r with $3 \le r \le n-1$, let $S_{n,r}$ be the graph formed by attaching $n - r$ pendent vertices to a vertex of the cycle C_r. Let $S_{n,n} = C_n$.

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

Proof. The result holds trivially for $r = n-1, n$. Suppose that $r \le n-2$. Assume that $G = C_r(T_1, T_2, \ldots, T_r)$ is a graph in $\mathbb{U}_{n,r}$ with minimum detour index. We need only to show that $G = S_{n,r}$.

By Lemmas 1, 2 and 5, T_i is a star with center v_i for $i = 1, 2, \ldots, r$.

Suppose that $|T_i|, |T_j| \ge 2$ with $i \ne j$. Let $x \in V(T_i), y \in V(T_j)$ with $x \ne v_i$, $y \ne v_j$, and suppose without loss of generality that $L(x|G) \le L(y|G)$. Consider $G' = G - v_j y + v_i y \in \mathbb{U}_{n,r}$. The detour matrices of G and G' differ only in their entries in the row (and column) corresponding to y, the sum of which is $L(y|G)$ and $L(y|G')$, respectively. Thus

$$\begin{aligned}\omega(G') - \omega(G) &= L(y|G') - L(y|G) \\ &= L(x|G') - L(y|G) \\ &= L(x|G) + 2 - l(x, y|G) - L(y|G) \\ &= L(x|G) - L(y|G) - l(v_i, v_j|C_r) < 0,\end{aligned}$$

and then $\omega(G') < \omega(G)$, a contradiction. Thus, there can not be in G two trees T_i and T_j with at least two vertices, i.e., $G = S_{n,r}$. ■

Lemma 7. *For* $3 \le r \le n$, $\omega(S_{n,r}) = (n-r)(n-1) + \frac{1}{8}(2n-r)(3r^2 - 4r + r_0)$.

Proof. Setting T_1 to be a star with center v_1, $n_1 = |T_1| = n - r + 1$, $n_i = |T_i| = 1$ for $i = 2, \ldots, r$ in $C_r(T_1, T_2, \ldots, T_r)$, we get $S_{n,r}$. Then $W(T_1) = (n_1 - 1)^2$, $D(v_1|T_1) = n_1 - 1$, $W(T_i) = 0$ and $D(v_i|T_i) = n_i - 1 = 0$ for $i = 2, \ldots, r$. By Lemma 5,

$$\begin{aligned}\omega(S_{n,r}) &= W(T_1) + \sum_{1 \le i < j \le r} D(v_i|T_i) + \sum_{1 \le i < j \le r} |T_i| l(v_i, v_j|C_r) \\ &= (n_1 - 1)^2 + \sum_{1 \le i < j \le r} (n_i - 1) + \sum_{1 \le i < j \le r} n_i l(v_i, v_j|C_r) \\ &= (n-r)^2 + (n-r)(r-1) + \sum_{1 \le i < j \le r} n_i l(v_i, v_j|C_r) \\ &= (n-r)(n-1) + (n-r)L(v_1|C_r) + \omega(C_r) \\ &= (n-r)(n-1) + \left(\frac{2n}{r} - 1\right)\omega(C_r).\end{aligned}$$

Now the result follows from Lemma 6. ■

Let Γ_n be the set of n-vertex unicyclic graphs with cycle length 3, such that for any $G = C_3(T_1, T_2, T_3) \in \Gamma_n$, $|T_1| = n - 2$ and $|T_2| = |T_3| = 1$.

For $n \ge 5$, let B'_n be the n-vertex unicyclic graph formed by attaching $n - 5$ pendent vertices and a path P_2 to one vertex of a triangle. For $n \ge 6$, let B''_n be the n-vertex unicyclic graph formed by attaching $n - 6$ pendent vertices and the star S_3 at its center vertex to one vertex of a triangle. Evidently, B'_n, $B''_n \in \Gamma_n$.

Lemma 8. *Among the graphs in* Γ_n *with* $n \ge 6$, B'_n *and* B''_n *are respectively the unique graphs with the second and the third smallest detour indices, which are equal to* $n^2 + n - 6$ *and* $n^2 + 2n - 11$, *respectively.*

Proof. The result holds trivially for $n = 6, 7$. Suppose that $n \geq 8$. Let $G = C_3(T_1, T_2, T_3) \in \Gamma_n$. Note that $|T_1| = n - 2 \geq 6$ and $W(T_2) = W(T_3) = 0$. By Lemma 5, we have

$$\begin{aligned} \omega(G) &= W(T_1) + \sum_{1 \leq i < j \leq 3} [D(v_i|T_i) + |T_i| l(v_i, v_j|C_3)] \\ &= W(T_1) + 2D(v_1|T_1) + 4n - 6, \end{aligned}$$

which, together with Lemmas 3 and 4, implies that B'_n and B''_n are respectively the unique graphs in Γ_n with the second and the third smallest detour indices, where

$$\begin{aligned} \omega(B'_n) &= W(S'_{n-2}) + 2(n - 3 + 1) + 4n - 6 = n^2 + n - 6, \\ \omega(B''_n) &= W(S''_{n-2}) + 2(n - 3 + 2) + 4n - 6 = n^2 + 2n - 11. \end{aligned}$$

This proves the result. $\blacksquare$

Let $\mathcal{U}_n$ be the set of n-vertex unicyclic graphs with $n \geq 3$.

Let $S_n(a, b, c)$ be the n-vertex unicyclic graph formed by attaching $a - 1$, $b - 1$ and $c - 1$ pendent vertices to the three vertices of a triangle, respectively, where $a \geq b \geq c \geq 1$ and $a + b + c = n$.

Proposition 4. *Among graphs in $\mathcal{U}_n$,*

- *$S_{n,3} = S_n(n - 2, 1, 1)$ for $n \geq 3$ is the unique graph with the smallest detour index, which is equal to $n^2 - 3$;*
- *B'_5 and $S_5(2, 2, 1)$ for $n = 5$, and B'_n for $n \geq 6$ are the unique graphs with the second smallest detour index, which is $n^2 + n - 6$;*
- *B''_n and $S_n(n - 3, 2, 1)$ for $n \geq 6$ are the unique graphs with the third smallest detour index, which is equal to $n^2 + 2n - 11$.*

Proof. If $n = 3$, the result is evident. Suppose that $n \geq 4$ and $3 \leq r \leq n$. Note that $\omega(S_{n,r}) = (n - r)(n - 1) + \frac{1}{8}(2n - r)(3r^2 - 4r + r_0)$. If r is odd with $r \leq n - 1$, then by Lemma 7,

$$\omega(S_{n,r+1}) - \omega(S_{n,r}) = -\frac{1}{8}\left(9r^2 - 12nr + 12n - 9\right) = -\frac{3}{8}\left[3r - (4n - 3)\right](r - 1) > 0,$$

and if r is even with $r \leq n - 1$, then

$$r_1 = \frac{1}{9}\left[6n - 1 + \sqrt{(6n - 7)^2 + 24}\right] > n,$$

$$r_2 = \frac{1}{9}\left[6n - 1 - \sqrt{(6n-7)^2 + 24}\right] < 3$$

and thus by by Lemma 7,

$$\omega(S_{n,r+1}) - \omega(S_{n,r}) = -\frac{1}{8}\left[9r^2 - (12n-2)r + 8n - 8\right] = -\frac{9}{8}(r - r_1)(r - r_2) > 0.$$

It follows that $\omega(S_{n,r})$ is increasing for $r \in \{3, 4, \ldots, n\}$. Then, for $3 \leq r \leq n$, $\omega(S_{n,r}) \geq \omega(S_{n,3})$ with equality if and only if $r = 3$. By Proposition 3, $S_{n,3} = S_n(n-2, 1, 1)$ is the unique n-vertex unicyclic graph with the smallest detour index, which is equal to $n^2 - 3$ by Lemma 7.

Let Φ_n be the set of n-vertex unicyclic graphs of cycle length at least 4. Let $\Psi_n = \mathcal{U}_n \setminus (\Gamma_n \cup \Phi_n)$.

Suppose that $n \geq 5$. From the discussion above, we know that $S_{n,4}$ is the unique graph in Φ_n with the smallest detour index, which is equal to $n^2+3n-12$ by Lemma 7.

Obviously, $\Gamma_5 \cup \Psi_5 = \{S_5(3,1,1), S_5(2,2,1), B_5'\}$. Note that $\omega(S_5(2,2,1)) = \omega(B_5') = 24 < \omega(S_{5,4})$. The result holds for $n = 5$. Suppose that $n \geq 6$.

By Lemma 8, B_n' and B_n'' are respectively the unique graphs in Γ_n with the second and the third smallest detour index, which is equal to $n^2 + n - 6$ and $n^2 + 2n - 11$, respectively.

For any graph $G = C_3(T_1, T_2, T_3) \in \Psi_n$, if it is not of the form $S_n(a, b, c)$, then by Lemmas 1 and 5, there are a, b and c such that $\omega(G) > \omega\left(S_n(a, b, c)\right) = (n-1)(n-3) + 2(ab + bc + ca)$ with $a \geq b \geq 2$, $c \geq 1$ and $a + b + c = n$. Thus it is easily checked that $S_n(n-3, 2, 1)$ is the unique graph in Ψ_n with the smallest detour index, which is equal to $n^2 + 2n - 11$.

It follows that the detour indices of the graphs in $\mathcal{U}_n$ may be ordered as:

$$\begin{aligned}
\omega\left(S_n(n-2,1,1)\right) = n^2 - 3 \;&<\; \omega(B_n') = n^2 + n - 6 \\
&<\; \omega(B_n'') = \omega(S_n(n-3,2,1)) = n^2 + 2n - 11 \\
&<\; \cdots
\end{aligned}$$

which implies the result for $n \geq 6$. ■

Let n and r be integers with $3 \leq r \leq n-1$. For integers a and b with $a \geq b \geq 0$ and $a + b = n - r$, let $Q_{n,r}(a, b)$ be the unicyclic graph obtained by attaching respectively a path P_a and a path P_b at one terminal vertex to two adjacent vertices of the cycle C_r (if $b = 0$ then only a path P_a is attached to a vertex of C_r). Let $\mathcal{Q}_{n,r} = \{Q_{n,r}(a, b) : a + b = n - r, a \geq b \geq 0\}$. In particular, $Q_{n,n-1}(1, 0) = S_{n,n-1}$. Let $Q_{n,n}(0, 0) = C_n$.

Proposition 5. *Let $G \in \mathbb{U}_{n,r}$ and $H \in \mathcal{Q}_{n,r}$ where $3 \le r \le n$. Then $\omega(G) \le \omega(H)$ with equality if and only if $G \in \mathcal{Q}_{n,r}$.*

Proof. The result holds trivially for $r = n-1, n$. Suppose that $r \le n-2$. Assume that $G = C_r(T_1, T_2, \dots, T_r)$ is a graph in $\mathbb{U}_{n,r}$ with maximum detour index. We need only to show that $G \in \mathcal{Q}_{n,r}$ and any two graphs in $\mathcal{Q}_{n,r}$ have equal detour index.

By Lemmas 1, 2 and 5, T_i is a path with one terminal vertex v_i for $i = 1, 2, \dots, r$.

If $r-1$ of $|T_1|, \dots, |T_r|$ are equal to one, then $G = Q_{n,r}(n-r, 0)$. Otherwise, suppose that $|T_i|, |T_j| \ge 2$ with $i \ne j$. Let $x \in V(T_i), y \in V(T_j)$ be the terminal vertices with $x \ne v_i$ and $y \ne v_j$, and suppose without loss of generality that $L(x|G) \ge L(y|G)$. Consider $G' = G - zy + xy \in \mathbb{U}_{n,r}$, where z is the (unique) neighbor of y in G. It is easily seen that

$$\begin{aligned} \omega(G') - \omega(G) &= L(y|G') - L(y|G) \\ &= L(x|G') + n - 2 - L(y|G) \\ &= [L(x|G) + 1 - l(x, y|G)] + n - 2 - L(y|G) \\ &= L(x|G) - L(y|G) + n - 1 - l(x, y|G). \end{aligned}$$

If v_i and v_j are not adjacent, or there is another tree T_k, besides T_i and T_j, with at least two vertices, then $l(x, y|G) < n-1$, and thus $\omega(G') > \omega(G)$, a contradiction. It follows that $G = Q_{n,r}(a, b)$ with $a \ge b \ge 0$. If $b \ge 1$, then $G' = Q_{n,r}(a+1, b-1)$ and $\omega(Q_{n,r}(a+1, b-1)) - \omega(Q_{n,r}(a, b)) = L(x|G) - L(y|G)$.

For the terminal vertex x of G, the contributions to $L(x|G)$ of the vertices of the path P_a, the cycle C_r and the path P_b are respectively $\frac{(a-1)a}{2}$, $a + a(r-1) + L(v_i|C_r)$ and $b(a+r-1) + \frac{b(b+1)}{2}$. Thus $L(x|G) = \frac{(a-1)a}{2} + [a + a(r-1) + L(v_i|C_r)] + \left[b(a+r-1) + \frac{b(b+1)}{2}\right] = \frac{1}{2}(n-r)(n+r-1) + L(v_i|C_r)$ is a constant. The same is true, by symmetry, for vertex y. Then $\omega(Q_{n,r}(a+1, b-1)) = \omega(Q_{n,r}(a, b))$ for $a \ge b \ge 1$. Thus $\omega(Q_{n,r}(a, b))$ is independent of the values of a and b. ■

Though graphs in $\mathcal{Q}_{n,r}$ where $3 \le r \le n-2$ have equal detour index, they obviously have different detour matrices.

For $3 \le r \le n$, setting T_1 to be a path with one terminal vertex v_1, $n_1 = |T_1| = n - r + 1$, $n_i = |T_i| = 1$ for $i = 2, \dots, r$ in $C_r(T_1, T_2, \dots, T_r)$, we get $Q_{n,r}(n-r, 0)$. Let $H \in \mathcal{Q}_{n,r}$. By Lemmas 5 and 6,

$$\begin{aligned} \omega(H) &= \omega\left(Q_{n,r}(n-r, 0)\right) \\ &= \sum_{i=1}^{r} \frac{n_i^3 - n_i}{6} + \sum_{1 \le i < j \le r} \left[\frac{(n_i - 1)n_i}{2} + n_i n_j l(v_i, v_j|C_r)\right] \end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{6}\left[(n-r+1)^3-(n-r+1)\right]+\frac{1}{2}(r-1)(n-r)(n-r+1)\\
&\quad + \sum_{1\le i<j\le r} |T_i||T_j| l(v_i,v_j|C_r)\\
&= \frac{1}{6}(n-r)(n-r+1)(n+2r-1)+\left(\frac{2n}{r}-1\right)\omega(C_r)\\
&= \frac{1}{6}(n-r)(n-r+1)(n+2r-1)+\frac{1}{8}(2n-r)(3r^2-4r+r_0).
\end{aligned}
$$

Proposition 6. *Among graphs in $\mathcal{U}_n$, C_n, $Q_{n,n-1}(1,0)$ $(= S_{n,n-1})$, and $Q_{n,n-2}(2,0)$ and $Q_{n,n-2}(1,1)$ are respectively the unique graphs with the first, the second, and the third largest detour indices, which are equal to $\frac{1}{8}n(3n^2-4n+n_0)$, $n-1+\frac{1}{8}(n+1)(3n^2-10n+8-n_0)$, and $3n-5+\frac{1}{8}(n+2)(3n^2-16n+20+n_0)$, respectively, where $n_0=1$ if n is odd and $n_0=0$ if n is even.*

Proof. For $3\le r\le n$, let $h(r)=\frac{1}{6}(n-r)(n-r+1)(n+2r-1)+\frac{1}{8}(2n-r)(3r^2-4r+r_0)$, where $r_0=1$ if r is odd and $r_0=0$ if r is even. If r is even with $r\le n-1$, then

$$h(r+1)-h(r)=-\frac{1}{8}\left[r^2-(4n-2)r\right]>0$$

and if r is odd with $r\le n-1$, then

$$h(r+1)-h(r)=-\frac{1}{8}\left[r^2-4nr+4n-1\right]>0.$$

Thus, $h(r)$ is increasing for $r\in\{3,4,\ldots,n\}$. Note that for any $H\in\mathcal{Q}_{n,r}$, $\omega(H)=h(r)$. Then $\omega\left(Q_{n,r}(a,b)\right)<\omega(C_n)$ if $3\le r\le n-1$ and $\omega\left(Q_{n,r}(a,b)\right)<\omega\left(Q_{n,n-2}(2,0)\right)$ $=\omega\left(Q_{n,n-2}(1,1)\right)<\omega\left(Q_{n,n-1}(1,0)\right)$ if $3\le r\le n-2$ and $G\ne Q_{n,n-2}(2,0), Q_{n,n-2}(1,1)$. By Proposition 5 and the expression $h(r)$ for the detour index of graphs in $\mathcal{Q}_{n,r}$, the result follows. ■

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