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Hyper–Detour Index of Unicyclic Graphs

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Abstract

We determine the n-vertex unicyclic graphs with the smallest, the second and the third smallest hyper–detour indices for $n \geq 5$, and the n-vertex unicyclic graphs with the k-th largest hyper–detour indices for all k up to $\lfloor \frac{n}{2} \rfloor + 4$ for $n \geq 6$ (and to five if $n = 5$). To obtain these results, we also determine the n-vertex unicyclic graphs of cycle length r, $3 \leq r \leq n$, with the smallest and the largest hyper–detour indices.

1. INTRODUCTION

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. For $u, v \in V(G)$, the (graph–theoretical) distance d_{uv} between u and v in G is the length of a shortest path connecting them, and the detour distance l_{uv} is between u and v in G the length of a longest path connecting them. Note that $l_{uu} = d_{uu} = 0$ for any $u \in V(G)$.

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The oldest graph–theoretical molecular descriptor is the Wiener index introduced in 1947 [1, 2]. The hyper–Wiener index was introduced by Randić [3] in 1993 for trees, which was extended to all connected graphs by Klein et al. [4]. The Wiener index of the graph G is defined as [2]

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

The hyper–Wiener index of the graph G is defined as [4]

$$WW(G) = \sum_{\{u,v\} \subseteq V(G)} \binom{d_{uv}+1}{2} = \frac{1}{4} \sum_{u \in V(G)} \sum_{v \in V(G)} \left(d_{uv}^2 + d_{uv}\right) .$$

If the distance used in the definitions of the Wiener and the hyper–Wiener indices is replaced by the detour distance, then the resulting quantities are called the detour and the hyper–detour indices, respectively. The detour index was named so by Lukovits [5] in 1996, which was also introduced by Amić and Trinajstić [6] earlier as the Wiener–like index. The hyper–detour index of the graph G, denoted by $\omega\omega(G)$, was proposed by Lukovits [5], see also [7]. It is defined as [5, 7, 8]

$$\omega\omega(G) = \sum_{\{u,v\} \subseteq V(G)} \binom{l_{uv}+1}{2} = \frac{1}{4} \sum_{u \in V(G)} \sum_{v \in V(G)} \left(l_{uv}^2 + l_{uv}\right) .$$

Let $V(G) = \{u_1, u_2, \ldots, u_n\}$. The detour–path matrix [9, 10] of G is an $n \times n$ symmetric matrix whose off–diagonal (i, j)-entry is the count of all paths of any length (at least one) that are included within a longest path between vertex u_i and vertex u_j, i.e., $\binom{l_{u_i u_j}+1}{2}$, and whose diagonal entries are all equal to 0. Then the hyper–detour index is calculated as the half–sum of the entries of the detour–path matrix [11]. Note that $\omega\omega(G) = WW(G)$ if G is a tree.

Intercorrelation between hyper–detour index and other molecular descriptors such as the Wiener index, the hyper–Wiener index, the Harary index, the hyper–Harary index, and the detour index was studied in [12] on three sets of branched and unbranched alkanes and cycloalkanes with up to eight carbon atoms, and the hyper–detour index has been tested in structure–property modeling, see, e.g., [13]. Recent applications of the hyper–detour index may be found in, e.g., [14].

Xing et al. [15] studied the properties of the hyper–Wiener index of unicyclic graphs. Zhou and Cai [16] began the study of the mathematical properties of the detour index. In this paper, we investigate the hyper–detour index of unicyclic graphs. We determine the n-vertex unicyclic graphs with the smallest, the second and the third smallest hyper–detour indices for $n \geq 5$, and the n-vertex unicyclic graphs with the k-th largest hyper–detour indices for all k up to $\lfloor \frac{n}{2} \rfloor + 4$ for $n \geq 6$ (and to five if $n = 5$). To obtain these results, we also determine the n-vertex unicyclic graphs of cycle length r, $3 \leq r \leq n$, with the smallest and the largest hyper–detour indices.

2. PRELIMINARIES

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

Lemma 2.1. [17] *Let T be an n-vertex tree different from S_n and P_n. Then* $\frac{1}{2}(n-1)(3n-4) = WW(S_n) < WW(T) < WW(P_n) = \frac{1}{24}n(n-1)(n+1)(n+2)$.

For a connected graph G with $u \in V(G)$, let $W_u(G) = \sum\limits_{v \in V(G)} d_{uv}$ and $WW_u(G) = \frac{1}{2} \sum\limits_{v \in V(G)} (d_{uv}^2 + d_{uv})$. The following lemma is easy to check.

Lemma 2.2. *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*

$$n - 1 = W_x(S_n) \leq W_u(T) \leq W_y(P_n) = \binom{n}{2},$$

$$n - 1 = WW_x(S_n) \leq WW_u(T) \leq WW_y(P_n) = \binom{n+1}{3}.$$

In either case, 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.

For $n \geq 5$, let S_n' be the tree formed by attaching a pendent vertex to a pendent vertex of the star S_{n-1}, and for $n \geq 6$, let S_n'' be the tree formed by attaching two pendent vertices to a pendent vertex of the star S_{n-2}.

Lemma 2.3. [17] *Among the n-vertex trees, S_n' for $n \geq 5$ is the unique tree with the second smallest hyper–Wiener index, which is equal to $\frac{1}{2}(3n^2 - n - 14)$, and S_n'' for $n \geq 6$ is the unique tree with the third smallest hyper–Wiener index, which is equal to* $\frac{1}{2}(3n^2 + 5n - 44)$.

For a connected graph G with u, $v \in V(G)$, let L_{uv} denote $\binom{l_{uv}+1}{2} = \frac{1}{2}(l_{uv}^2 + l_{uv})$. Let $\omega_u(G) = \sum_{v\in V(G)} l_{uv}$ and $\omega\omega_u(G) = \sum_{v\in V(G)} L_{uv}$. Let C_n be the n-vertex cycle with $n \geq 3$.

Lemma 2.4. [5] *Let v be a vertex on the cycle C_r with $r \geq 3$. Then $\omega_v(C_r) = \frac{1}{4}(3r^2 - 4r + \varepsilon_r)$ where $\varepsilon_r = 1$ if r is odd and $\varepsilon_r = 0$ if r is even,*

$$\omega\omega_v(C_r) = \begin{cases} \frac{(r-1)(r+1)(7r-3)}{24} & \text{if } r \text{ is odd,} \\ \frac{r(r+1)(7r-10)}{24} & \text{if } r \text{ is even,} \end{cases}$$

$$\omega\omega(C_r) = \begin{cases} \frac{r(r-1)(r+1)(7r-3)}{48} & \text{if } r \text{ is odd,} \\ \frac{r^2(r+1)(7r-10)}{48} & \text{if } r \text{ is even.} \end{cases}$$

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 have exactly one vertex v_i in common 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 $\sum_{i=1}^{r} |T_i| = n$, and $|H| = |V(H)|$ for a graph H.

Proposition 2.1. *For $r \geq 3$, let $G = C_r(T_1, T_2, \ldots, T_r)$. Then*

$$\begin{aligned} \omega\omega(G) &= \sum_{i=1}^{r} WW(T_i) + \sum_{i=1}^{r}(|G| - |T_i|)WW_{v_i}(T_i) + \sum_{i=1}^{r}\sum_{j\neq i} |T_i| l_{v_i v_j} W_{v_j}(T_j) \\ &\quad + \sum_{1\leq i<j\leq r} [|T_i||T_j| L_{v_i v_j} + W_{v_i}(T_i) W_{v_j}(T_j)]\,. \end{aligned}$$

Proof. For $a \in V(T_i)$ and $b \in V(T_j)$ with $1 \leq i < j \leq r$, we have

$$\begin{aligned} L_{ab} &= \frac{1}{2}\left(l_{ab}^2 + l_{ab}\right) \\ &= \frac{1}{2}\left[(d_{av_i} + d_{bv_j} + l_{v_i v_j})^2 + d_{av_i} + d_{bv_j} + l_{v_i v_j}\right] \\ &= \frac{1}{2}\left(d_{av_i}^2 + d_{av_i} + d_{bv_j}^2 + d_{bv_j} + l_{v_i v_j}^2 + l_{v_i v_j} + 2d_{av_i}d_{bv_j} + 2d_{av_i}l_{v_i v_j} + 2d_{bv_j}l_{v_i v_j}\right) \\ &= \frac{1}{2}\left(d_{av_i}^2 + d_{av_i}\right) + \frac{1}{2}\left(d_{bv_j}^2 + d_{bv_j}\right) + L_{v_i v_j} + d_{av_i}d_{bv_j} + d_{av_i}l_{v_i v_j} + d_{bv_j}l_{v_i v_j}\,. \end{aligned}$$

Thus, we have

$$\omega\omega(G) - \sum_{i=1}^{r} WW(T_i) = \sum_{1\leq i<j\leq r} \sum_{a\in V(T_i)} \sum_{b\in V(T_j)} L_{ab}$$

$$
\begin{aligned}
&= \sum_{1\le i<j\le r} \Big[|T_j|WW_{v_i}(T_i) + |T_i|WW_{v_j}(T_j) + |T_i||T_j|L_{v_iv_j} \\
&\quad +W_{v_i}(T_i)W_{v_j}(T_j) + |T_j|l_{v_iv_j}W_{v_i}(T_i) + |T_i|l_{v_iv_j}W_{v_j}(T_j)\Big] \\
&= \sum_{i=1}^{r}(|G|-|T_i|)WW_{v_i}(T_i) \\
&\quad + \sum_{1\le i<j\le r} \Big[|T_i||T_j|L_{v_iv_j} + W_{v_i}(T_i)W_{v_j}(T_j)\Big] \\
&\quad + \sum_{i=1}^{r}\sum_{j\ne i} |T_i|l_{v_iv_j}W_{v_j}(T_j)\,.
\end{aligned}
$$

The result follows. ■

For an edge e of the graph G, $G-e$ denotes the graph obtained from G by deleting the edge e, and for an edge of the complement of G, $G+e$ denotes the graph obtained from G by adding the edge e.

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

3. UNICYCLIC GRAPHS WITH SMALL HYPER–DETOUR INDICES

In this section, we determine the n-vertex unicyclic graph(s) of cycle length r, $3 \le r \le n$, with the smallest hyper–detour index and n-vertex unicyclic graphs with the smallest, the second and the third smallest hyper–detour indices.

Let $S_{n,r} = C_r(T_1, T_2, \ldots, T_r)$, where $|T_1| = n-r+1$, $|T_2| = \cdots = |T_r| = 1$, and T_1 is a star with center v_1. In particular, $S_{n,n} = C_n$.

Lemma 3.1. *For $3 \le r \le n$,*

$$
\omega\omega(S_{n,r}) = \begin{cases} \frac{3n^2}{2} + \frac{(7r^3+15r^2-79r-27)n}{24} + \frac{-7r^4-33r^3+79r^2+57r}{48} & \text{if } r \text{ is odd,} \\ \frac{3n^2}{2} + \frac{(7r^3+15r^2-82r-36)n}{24} + \frac{-7r^4-33r^3+82r^2+72r}{48} & \text{if } r \text{ is even.} \end{cases}
$$

Proof. To compute $\omega\omega(S_{n,r})$, consider the contributions of the pairs of vertices in the star $T_1 = S_{n-r-1}$, the pairs of vertices in the cycle, and the pairs with one vertex in T_1 and the other vertex in the cycle both different from v_1. It is easily seen that

$$
\omega\omega(S_{n,r}) \;=\; WW(S_{n-r+1}) + \omega\omega(C_r) + \frac{1}{2}\sum_{i=2}^{r}\left[(1+l_{v_1v_i})^2 + 1 + l_{v_1v_i}\right](n-r)
$$

$$
\begin{aligned}
&= WW(S_{n-r+1}) + \omega\omega(C_r) + (n-r)\sum_{i=2}^{r}\left(\frac{1}{2}l_{v_1v_i}^2 + \frac{3}{2}l_{v_1v_i} + 1\right) \\
&= WW(S_{n-r+1}) + \omega\omega(C_r) \\
&\quad +(n-r)\left[\omega\omega_{v_1}(C_r) + \omega_{v_1}(C_r)\right] + (n-r)(r-1)\,.
\end{aligned}
$$

Now the result follows from Lemmas 2.1 and 2.4. ■

Proposition 3.1. *Let $G \in \mathbb{U}_{n,r}$, where $3 \le r \le n$. Then $\omega\omega(G) \ge \omega\omega(S_{n,r})$ with equality if and only if $G = S_{n,r}$.*

Proof. It is obvious for $r = n-1,\ n$. Suppose that $r \le n-2$. Let $G = C_r(T_1, T_2, \ldots, T_r)$ be a graph with the smallest hyper–detour index in $\mathbb{U}_{n,r}$. By Proposition 2.1 and Lemmas 2.1 and 2.2, T_i is a star with center v_i for each $i = 1, 2, \ldots, r$. Suppose that there exist j and k with $1 \le j < k \le r$ such that $|T_j|,\ |T_k| \ge 2$. Let $a \in V(T_j)$, $b \in V(T_k)$ with $a \ne v_j$ and $b \ne v_k$. Suppose without loss of generality that $\omega\omega_a(G) \le \omega\omega_b(G)$. Then for $G' = G - v_kb + v_jb \in \mathbb{U}_{n,r}$, we have $\omega\omega_a(G) - \omega\omega_a(G') = L(a,b) - \frac{1}{2}(2^2+2) = L_{ab} - 3$ and then

$$
\begin{aligned}
\omega\omega(G') - \omega\omega(G) &= \omega\omega_b(G') - \omega\omega_b(G) = \omega\omega_a(G') - \omega\omega_b(G) \\
&= \omega\omega_a(G) + 3 - L_{ab} - \omega\omega_b(G) \\
&= \omega\omega_a(G) - \omega\omega_b(G) + 3 - \frac{1}{2}\left[\left(2 + l_{v_jv_k}\right)^2 + 2 + l_{v_jv_k}\right] \\
&= \omega\omega_a(G) - \omega\omega_b(G) - \frac{1}{2}\left(l_{v_jv_k}^2 + 5l_{v_jv_k}\right) < 0,
\end{aligned}
$$

which is a contradiction to the choice of G. Thus $r-1$ of $|T_1|, |T_2|, \ldots, |T_r|$ are equal to 1 and the remaining one is equal to $n-(r-1)$, i.e., $G = S_{n,r}$. ■

Let Γ_n be the set of n-vertex unicyclic graphs $C_3(T_1, T_2, T_3)$ with $|T_2| = |T_3| = 1$. Let Ψ_n be the set of n-vertex unicyclic graphs $C_3(T_1, T_2, T_3)$ with $|T_1| \ge |T_2| \ge \max\{|T_3|, 2\}$. Let Φ_n be the set of n-vertex unicyclic graphs with cycle length at least four. Then, $\mathcal{U}_n = \Gamma_n \cup \Psi_n \cup \Phi_n$.

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

Lemma 3.2. *Among the graphs in Γ_n, B'_n for $n \geq 5$ is the unique graph with the second smallest hyper–detour index, which is equal to $\frac{1}{2}(3n^2 + 11n - 38)$, and B''_n for $n \geq 6$ is the unique graph with the third smallest hyper–detour index, which is equal to $\frac{1}{2}(3n^2 + 17n - 64)$.*

Proof. The case $n = 5$ is trivial. Let $G = C_3(T_1, T_2, T_3) \in \Gamma_n$ with $n \geq 6$. Note that $\omega\omega(C_3) = 9$. Then

$$\omega\omega(G) = 9 + WW(T_1) + 2 \sum_{u \in V(T_1) \setminus \{v_1\}} \binom{l_{uv_2} + 1}{2},$$

which, together with Lemma 2.3, implies that B'_n and B''_n are the unique graphs with respectively the second and the third smallest hyper–detour indices, which are equal to $\frac{1}{2}(3n^2 + 11n - 38)$ and $\frac{1}{2}(3n^2 + 17n - 64)$, respectively. This proves the lemma. ■

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, b, $c \geq 1$ and $a + b + c = n$.

Lemma 3.3. *Among the graphs in Ψ_n with $n \geq 5$, $S_n(n-3, 2, 1)$ is the unique graph with the smallest hyper–detour index, which is equal to $\frac{1}{2}(3n^2 + 19n - 80)$.*

Proof. Let $G = C_3(T_1, T_2, T_3) \in \Psi_n$ with $a \geq b \geq \max\{c, 2\}$ and $a + b + c = n$, where $a = |T_1|$, $b = |T_2|$ and $c = |T_3|$.

If $G = S_n(a, b, c)$ and $G \neq S_n(n - 3, 2, 1)$, then it is easily seen that $\omega\omega_x(G) \leq \omega\omega_y(G)$ for pendent vertices $x \in V(T_1)$ and $y \in V(T_2) \cup V(T_3)$, and by the proof of Proposition 3.1, we have

$$\omega\omega(S_n(a, b, c)) \geq \omega\omega(S_n(a + c - 1, b, 1)) \geq \omega\omega(S_n(n - 3, 2, 1))$$

and at least one of the two inequalities is strict. If $G \neq S_n(a, b, c)$, then by Proposition 2.1, we have $\omega\omega(G) > \omega\omega(S_n(a, b, c)) \geq \omega\omega(S_n(n-3, 2, 1)) = \frac{1}{2}(3n^2+19n-80)$. Then the result follows. ■

Proposition 3.2. *Among the graphs in $\mathcal{U}_n$,*

(i) $S_{n,3}$ for $n \geq 3$ is the unique graph with the smallest hyper–detour index, which is

equal to $\frac{1}{2}(3n^2+5n-24)$;

(ii) C_4 *for* $n=4$, $S_5(2,2,1)$ *for* $n=5$ *and* B'_n *for* $n\geq 6$ *are the unique graphs with the second smallest hyper–detour index, which is equal to* 30 *for* $n=4$, 45 *for* $n=5$, *and* $\frac{1}{2}(3n^2+11n-38)$ *for* $n\geq 6$;

(iii) B'_5 *for* $n=5$, $S_n(n-3,2,1)$ *for* $n=6,7$, B''_8 *and* $S_8(5,2,1)$ *for* $n=8$, *and* B''_n *for* $n\geq 9$ *are the unique graphs with the third smallest hyper–detour index, which is equal to* 46 *for* $n=5$, 71 *for* $n=6$, 100 *for* $n=7$, 132 *for* $n=8$, *and* $\frac{1}{2}(3n^2+17n-64)$ *for* $n\geq 9$.

Proof. By Lemma 3.1, if r is odd with $3\leq r\leq n-1$, then

$$\begin{aligned}24\left[\omega\omega(S_{n,r+1})-\omega\omega(S_{n,r})\right] &= (21r^2+48r-69)n-14r^3-69r^2+26r+57\\ &\geq (21r^2+48r-69)(r+1)-14r^3-69r^2+26r+57\\ &= 7r^3+5r-12>0,\end{aligned}$$

and if r is even with $4\leq r\leq n-1$, then

$$\begin{aligned}24\left[\omega\omega(S_{n,r+1})-\omega\omega(S_{n,r})\right] &= (21r^2+54r-48)n-14r^3-72r^2+8r+48\\ &\geq (21r^2+54r-48)(r+1)-14r^3-72r^2+8r+48\\ &= r(7r^2+3r+14)>0\,.\end{aligned}$$

It follows that $\omega\omega(S_{n,r})$ is increasing with respect to $r\in\{3,4,\ldots,n\}$. Thus, by Proposition 3.1 and Lemma 3.1, $S_{n,3}$ is the unique graph in $\mathcal{U}_n$ with the smallest hyper–detour index, which is equal to $\frac{1}{2}(3n^2+5n-24)$, proving (i). Moreover, $S_{n,4}$ is the unique graph in Φ_n with the smallest hyper–detour index, which is equal to $\frac{1}{2}(3n^2+27n-96)$.

Now we prove (ii). The case $n=4$ is trivial. For $n\geq 5$, the graphs in $\mathcal{U}_n$ with the second smallest hyper–detour index are just the graphs in $\mathcal{U}_n\setminus\{S_{n,3}\}=(\Gamma_n\setminus\{S_{n,3}\})\cup\Psi_n\cup\Phi_n$ with the smallest hyper–detour index, which, by Lemmas 3.2 and 3.3, is equal to $\min\{\frac{1}{2}(3n^2+11n-38),\frac{1}{2}(3n^2+19n-80),\frac{1}{2}(3n^2+27n-96)\}$. It is equal to $\frac{1}{2}(3n^2+19n-80)=45$ for $n=5$ and $\frac{1}{2}(3n^2+11n-38)$ for $n\geq 6$. Then (ii) follows.

¿From (i) and (ii) and by Lemmas 3.2 and 3.3, we find that the graphs in $\mathcal{U}_5$ with the third smallest hyper–detour index are just the graphs in $\mathcal{U}_5\setminus\{S_{5,3},S_5(2,2,1)\}=$

$(\Gamma_5 \setminus \{S_{5,3}\}) \cup \Phi_5$ with the smallest hyper–detour index, which is equal to $\min\{\frac{1}{2}(3 \times 5^2 + 11 \times 5 - 38), \frac{1}{2}(3 \times 5^2 + 27 \times 5 - 96)\} = \min\{46, 57\} = 46$, and for $n \geq 6$, the graphs in $\mathcal{U}_n$ with the third smallest hyper–detour index are just the graphs in $\mathcal{U}_n \setminus \{S_{n,3}, B'_n\} = (\Gamma_n \setminus \{S_{n,3}, B'_n\}) \cup \Psi_n \cup \Phi_n$ with the smallest hyper–detour index, which is equal to $\min\{\frac{1}{2}(3n^2 + 17n - 64), \frac{1}{2}(3n^2 + 19n - 80), \frac{1}{2}(3n^2 + 27n - 96)\}$. For $n \geq 9$,

$$\frac{1}{2}(3n^2 + 17n - 64) < \frac{1}{2}(3n^2 + 19n - 80) < \frac{1}{2}(3n^2 + 27n - 96)$$

and for $n = 6, 7, 8$, the corresponding values are listed in Table 1. Now (iii) follows easily. ■

Table 1: Some graphs and their hyper–detour indices.

graph	hyper–detour indices			
	n	6	7	8
B''_n	$\frac{1}{2}(3n^2 + 17n - 64)$	73	101	132
$S_n(n-3, 2, 1)$	$\frac{1}{2}(3n^2 + 19n - 80)$	71	100	132
$S_{n,4}$	$\frac{1}{2}(3n^2 + 27n - 96)$	87	120	156

4. UNICYCLIC GRAPHS WITH LARGE HYPER–DETOUR INDICES

In this section, we determine the n-vertex unicyclic graph(s) of cycle length r, $3 \leq r \leq n$, with the largest hyper–detour index and the n-vertex unicyclic graphs with the k-th largest hyper–detour indices for all k up to $\lfloor \frac{n}{2} \rfloor + 4$ for $n \geq 6$ (and to five if $n = 5$).

Let $P_{n,r} = C_r(T_1, T_2, \ldots, T_r)$, where $|T_1| = n - r + 1$, $|T_2| = \cdots = |T_r| = 1$, and T_1 is a path with a terminal vertex v_1. In particular, $P_{n,n} = C_n$.

Lemma 4.1. *For $3 \leq r \leq n$,*

$$\omega\omega(P_{n,r}) = \begin{cases} \frac{n^4+2n^3+(3r^2-6r+2)n^2+(-3r^3+12r^2-15r+4)n}{24} + \frac{5r^4-19r^3+19r^2-5r}{48} & \text{if } r \text{ is odd}, \\ \frac{n^4+2n^3+(3r^2-6r-1)n^2+(-3r^3+12r^2-12r-2)n}{24} + \frac{5r^4-19r^3+16r^2+4r}{48} & \text{if } r \text{ is even}. \end{cases}$$

Proof. To compute $\omega\omega(P_{n,r})$, consider the contributions of the pairs of vertices in the path $T_1 = P_{n-r+1}$, the pairs of vertices in the cycle, and the pairs with one vertex in T_1 and the other vertex in the cycle both different from v_1. It is easily seen that

$$\begin{aligned}
\omega\omega(P_{n,r}) &= WW(P_{n-r+1}) + \omega\omega(C_r) + \frac{1}{2}\sum_{i=2}^{r}\sum_{j=1}^{n-r}\left[(j + l_{v_1v_i})^2 + j + l_{v_1v_i}\right] \\
&= WW(P_{n-r+1}) + \omega\omega(C_r) \\
&\quad + \frac{1}{2}(r-1)\sum_{j=1}^{n-r}(j^2 + j) + \sum_{i=2}^{r}\sum_{j=1}^{n-r} j l_{v_1v_i} + \frac{1}{2}(n-r)\sum_{i=2}^{r}(l_{v_1v_i}^2 + l_{v_1v_i}) \\
&= WW(P_{n-r+1}) + \omega\omega(C_r) \\
&\quad + (r-1)\binom{n-r+2}{3} + \binom{n-r+1}{2}\omega_{v_1}(C_r) + (n-r)\omega\omega_{v_1}(C_r)\,.
\end{aligned}$$

Now the result follows from Lemmas 2.1 and 2.4. ■

Proposition 4.1. *Let $G \in \mathbb{U}_{n,r}$, where $3 \le r \le n$. Then $\omega\omega(G) \le \omega\omega(P_{n,r})$ with equality if and only if $G = P_{n,r}$.*

Proof. It is obvious for $r = n-1,\, n$. Suppose that $r \le n-2$. Let $G = C_r(T_1, T_2, \ldots, T_r)$ be a graph with the largest hyper–detour index in $\mathbb{U}_{n,r}$. By Proposition 2.1 and Lemmas 2.1 and 2.2, T_i is a path with v_i as one of its end vertices for each $i = 1, 2, \ldots, r$. Suppose that there exist j and k with $1 \le j < k \le r$ such that $|T_j|,\ |T_k| \ge 2$. Let $a \ne v_j$ and $b \ne v_k$ be terminal vertices of T_j and T_k, respectively. Suppose without loss of generality that $\omega\omega_a(G) \ge \omega\omega_b(G)$. Let c be the neighbor of b in G. Then for $G' = G - cb + ab \in \mathbb{U}_{n,r}$, we have

$$\begin{aligned}
\omega\omega(G') - \omega\omega(G) &= \omega\omega_b(G') - \omega\omega_b(G) \\
&= \sum_{u\in V(G)\setminus\{b\}}\binom{1 + l_{au} + 1}{2} - \omega\omega_b(G) \\
&= \sum_{u\in V(G)\setminus\{b\}}\binom{l_{au} + 1}{2} + \sum_{u\in V(G)\setminus\{b\}}(l_{au} + 1) - \omega\omega_b(G) \\
&= \omega\omega_a(G) - L_{ab} + \sum_{u\in V(G)\setminus\{a,b\}}(l_{au} + 1) + 1 - \omega\omega_b(G) \\
&= \omega\omega_a(G) - \omega\omega_b(G) + n - 1 + \sum_{u\in V(G)\setminus\{a,b\}} l_{au} - L_{ab}\,.
\end{aligned}$$

Let $z_0z_1\ldots z_s$ be the longest path from $z_0 = a$ to $z_s = b$ in G, where $s = l_{ab} \ge |T_j| - 1 + |T_k| - 1 + \lceil\frac{r}{2}\rceil \ge |T_j| + |T_k|$. Thus $1 < |T_j| < l_{ab} - 1$. Obviously, $l_{az_i} \ge i$ for

$i = 1, 2, \ldots, s-1$ and $l_{az_{|T_j|}} = |T_j| - 1 + r - 1 = |T_j| + r - 2 > |T_j|$. Then $\sum\limits_{u \in V(G) \setminus \{a,b\}} l_{au} \geq \sum\limits_{i=1}^{s-1} l_{az_i} > \sum\limits_{i=1}^{l_{ab}-1} i = \frac{1}{2}\,(l_{ab}^2 - l_{ab})$, and thus $n - 1 + \sum\limits_{u \in V(G) \setminus \{a,b\}} l_{au} - L_{ab} > n - 1 - l_{ab} \geq 0$. We have $\omega\omega(G') > \omega\omega(G)$, which is a contradiction to the choice of G. It follows that $G = P_{n,r}$. ■

For integer i with $i = 2, 3, \ldots, \lfloor \frac{n}{2} \rfloor$, let $Q_{n,n-2}(1, i)$ be the unicyclic graph obtained by attaching a pendent vertex to v_1 and a pendent vertex to v_i of the cycle C_{n-2}.

Proposition 4.2. *Among the graphs in $\mathcal{U}_n$ with $n \geq 5$, C_n, $P_{n,n-1}$ and $P_{n,n-2}$ are the unique graphs with respectively the largest, the second and the third largest hyper–detour indices, which are respectively equal to $\frac{1}{48}n(n-1)(n+1)(7n-3)$, $\frac{1}{48}(7n^4 - 17n^3 + 29n^2 - 55n + 36)$ and $\frac{1}{48}(7n^4 - 31n^3 + 107n^2 - 257n + 318)$ for odd n, $\frac{1}{48}n^2(n+1)(7n-10)$, $\frac{1}{48}(7n^4 - 17n^3 + 32n^2 - 52n + 48)$ and $\frac{1}{48}(7n^4 - 31n^3 + 104n^2 - 260n + 288)$ for even n, $Q_{n,n-2}(1, k-2)$ is the unique graph with the k-th largest hyper–detour index for $k = 4, 5, \ldots, \lfloor \frac{n}{2} \rfloor + 2$, which is equal to $\frac{1}{48}(7n^4 - 31n^3 + 71n^2 - 161n + 210) + \frac{1}{2}(n - k + 4)(n - k + 3)$ for odd n, and $\frac{1}{48}(7n^4 - 31n^3 + 68n^2 - 164n + 192) + \frac{1}{2}(n - k + 4)(n - k + 3)$ for even n, $S_{n,n-2}$ is the unique graph with the $\left(\lfloor \frac{n}{2} \rfloor + 3\right)$-th largest hyper–detour index, which is equal to $\frac{1}{48}(7n^4 - 31n^3 + 71n^2 - 161n + 354)$ for odd n, and $\frac{1}{48}(7n^4 - 31n^3 + 68n^2 - 164n + 336)$ for even n, and if $n \geq 6$, then $P_{n,n-3}$ is the unique graph with the $\left(\lfloor \frac{n}{2} \rfloor + 4\right)$-th largest hyper–detour index, which is equal to $\frac{1}{48}(7n^4 - 45n^3 + 215n^2 - 699n + 1050)$ for odd n, and $\frac{1}{48}(7n^4 - 45n^3 + 218n^2 - 696n + 1104)$ for even n.*

Proof. Suppose that $3 \leq r \leq n-1$. If r is odd, then by Lemma 4.1, we have

$$\begin{aligned} & 24\left[\omega\omega(P_{n,r+1}) - \omega\omega(P_{n,r})\right] \\ = \; & 6(r-1)n^2 + 9(-r^2 + 2r - 1)n + 10r^3 - 15r^2 + 2r + 3\,. \end{aligned}$$

Let $f_1(n)$ be the expression in the right–hand side of the above equation. Since $n \geq r+1$, the derivative $f_1'(x)$ satisfies

$$\begin{aligned} f_1'(n) &= 12(r-1)n + 9(-r^2 + 2r - 1) \\ &\geq 12(r-1)(r+1) + 9(-r^2 + 2r - 1) \\ &= 3(r-1)(r+7) > 0, \end{aligned}$$

and then $f_1(n)$ is increasing for $n \geq r+1$. It follows that $24\,[\omega\omega(P_{n,r+1}) - \omega\omega(P_{n,r})] = f_1(n) \geq f_1(r+1) = 7r^3 + 5r - 12 > 0$. Then we have $\omega\omega(P_{n,r+1}) > \omega\omega(P_{n,r})$ for odd $r \geq 3$. If r is even, then by Lemma 4.1, we have

$$24\,[\omega\omega(P_{n,r+1}) - \omega\omega(P_{n,r})] = 6rn^2 + 3(-3r^2 + 4r)n + 10r^3 - 12r^2 - 4r\,.$$

Let $f_2(n)$ be the expression in the right–hand side of the above equation. Since $n \geq r+1$, the derivative $f_2'(x)$ satisfies

$$f_2'(n) = 12rn + 3(-3r^2 + 4r) \geq 12r(r+1) + 3(-3r^2 + 4r) = 3r(r+8) > 0,$$

and then $f_2(n)$ is increasing for $n \geq r+1$. It follows that $24\,[\omega\omega(P_{n,r+1}) - \omega\omega(P_{n,r})] = f_2(n) \geq f_2(r+1) = r(7r^2+3r+14) > 0$. Then we have $\omega\omega(P_{n,r+1}) > \omega\omega(P_{n,r})$ for even $r \geq 4$. Thus, $\omega\omega(P_{n,r})$ is increasing with respect to $r \in \{3, 4, \ldots, n\}$. By Proposition 4.1 and Lemma 4.1, C_n, $P_{n,n-1}$ and $P_{n,n-2}$ are the unique graphs with respectively the largest, the second largest, and the third largest hyper–detour indices.

It is easily seen that

$$\begin{aligned}
\omega\omega(Q_{n,n-2}(1,i)) &= \omega\omega(C_{n-2}) + 2\sum_{j=1}^{n-2} \frac{1}{2}\left[\left(1 + l_{v_1v_j}\right)^2 + 1 + l_{v_1v_j}\right] + \binom{2 + l_{v_1v_i} + 1}{2} \\
&= \omega\omega(C_{n-2}) + 2\omega\omega_{v_1}(C_{n-2}) + 2\omega_{v_1}(C_{n-2}) \\
&\quad +2(n-2) + \binom{l_{v_1v_i} + 3}{2}.
\end{aligned}$$

Note that $\omega\omega(Q_{n,n-2}(1,i))$ is increasing for $\lceil \frac{n-2}{2} \rceil \leq l_{v_1v_i} \leq n-3$. By Propositions 3.1 and 4.1, the hyper–detour indices of graphs in $\mathbb{U}_{n,n-2}$ for $n \geq 5$ can be ordered as:

$$\begin{aligned}
&\omega\omega(P_{n,n-2}) > \omega\omega(Q_{n,n-2}(1,2)) > \omega\omega(Q_{n,n-2}(1,3)) \\
&\quad > \cdots > \omega\omega\left(Q_{n,n-2}\left(1, \left\lfloor \frac{n}{2} \right\rfloor\right)\right) > \omega\omega(S_{n,n-2})\,.
\end{aligned}$$

By Lemma 3.1, we have

$$\omega\omega(S_{n,n-2}) = \begin{cases} \frac{1}{48}(7n^4 - 31n^3 + 71n^2 - 161n + 354) & \text{if } n \text{ is odd,} \\ \frac{1}{48}(7n^4 - 31n^3 + 68n^2 - 164n + 336) & \text{if } n \text{ is even.} \end{cases}$$

By Lemma 4.1, we have

$$\omega\omega(P_{n,n-3}) = \begin{cases} \frac{1}{48}(7n^4 - 45n^3 + 215n^2 - 699n + 1050) & \text{if } n \text{ is odd,} \\ \frac{1}{48}(7n^4 - 45n^3 + 218n^2 - 696n + 1104) & \text{if } n \text{ is even.} \end{cases}$$

It follows that the hyper–detour indices of graphs in $\mathcal{U}_5$ can be ordered as: $\omega\omega(C_5) > \omega\omega(P_{5,4}) > \omega\omega(P_{5,3}) > \omega\omega(Q_{5,3}(1,2)) > \omega\omega(S_{5,3})$. Suppose that $n \geq 6$. If n is odd, then

$$\omega\omega(S_{n,n-2}) - \omega\omega(P_{n,n-3}) = 2n(7n^2 - 72n + 269) - 696 > 0,$$

and if n is even, then

$$\omega\omega(S_{n,n-2}) - \omega\omega(P_{n,n-3}) = 2n(7n^2 - 75n + 266) - 768 > 0\,.$$

Thus among the graphs in $\mathcal{U}_n$ for $n \geq 6$, the first a few largest hyper–detour indices can be ordered as:

$$\begin{aligned}\omega\omega(C_n) > \omega\omega(P_{n,n-1}) > \omega\omega(P_{n,n-2}) > \omega\omega(Q_{n,n-2}(1,2)) > \omega\omega(Q_{n,n-2}(1,3))\\ > \cdots > \omega\omega\left(Q_{n,n-2}\left(1, \left\lfloor \frac{n}{2} \right\rfloor\right)\right) > \omega\omega(S_{n,n-2}) > \omega\omega(P_{n,n-3})\,.\end{aligned}$$

Note that $\omega\omega(Q_{n-2}(1,i))$ is equal to $\frac{1}{48}(7n^4 - 31n^3 + 71n^2 - 161n + 210) + \frac{1}{2}(n - i + 2)(n-i+1)$ if n is odd, and $\frac{1}{48}(7n^4 - 31n^3 + 68n^2 - 164n + 192) + \frac{1}{2}(n-i+2)(n-i+1)$ if n is even. The result follows easily. ■

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