Minimum Detour Index of Bicyclic Graphs

Chunjuan Du

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. A graph with \(n\) vertices and \(n+1\) edges is called a bicyclic graph. In this paper, we consider the detour indices of bicyclic graphs with two cycles or three cycles and determine the graphs with the first four smallest detour indices in the class of \(n\)-vertex bicyclic graphs for \(n \geq 5\).

1 Introduction and Preliminaries

Let \(G\) be a connected graph with the vertex set \(V(G)\) and edge set \(E(G)\). The distance between vertices \(u\) and \(v\) in \(G\) is the length (number of edges) of a shortest path between them, denoted by \(d(u, v|G)\) [1, 2]. The Wiener index of the graph \(G\) is defined as [3, 4]

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

As one of the oldest topological indices, the Wiener index has found various applications in chemical research [5–7] and has also been studied extensively in mathematics [7–10]. See [11–13] for more new results on the Wiener index. The detour distance [14, 15] (also
known under the name elongation) between vertices $u$ and $v$ in $G$ is the length of a longest path between them, denoted by $l(u,v|G)$. The detour index of the graph $G$ is defined as [14–17]

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

The detour index has been applied to chemistry, especially in quantitative structure-activity relationship (QSAR) studies, see [14–19] for more details.

For the computation aspect of the detour index, some computer methods were discussed in [16,20–22]. Recently, Zhou and Cai [23] established some basic mathematical properties of the detour index, especially, they gave bounds for the detour index, determined the graphs with minimum and maximum detour indices respectively in the class of $n$-vertex unicyclic graphs with cycle length $r$, where $3 \leq r \leq n-2$, and determined the graphs with the first three smallest and largest detour indices respectively in the class of $n$-vertex unicyclic graphs for $n \geq 5$. Then in [24, 25] Qi and Zhou studied the detour index of unicyclic graphs whose vertices on the unique cycle have degree at least three and the unicyclic graphs with given maximum degree, respectively. In [26], they also studied the Hyper-detour index of unicyclic graphs. Qi [27] determined the graphs with the smallest and largest detour indices respectively in the class of $n$-vertex bicyclic graphs with exactly two cycles for $n \geq 5$. Du [28] determined the graphs with the second and the third smallest and largest detour indices in the class of $n$-vertex bicyclic graphs with exactly two cycles for $n \geq 6$. In this paper, we consider the detour indices of bicyclic graphs with two cycles or three cycles and determine the graphs with the first four smallest detour indices in the class of $n$-vertex bicyclic graphs for $n \geq 5$.

Let $S_n$, $P_n$ and $C_n$ be respectively the $n$-vertex star, path and cycle. A connected graph $G$ with $n$ vertices is a unicyclic graph if $|E(G)| = n$ and is a bicyclic graph if $|E(G)| = n + 1$. Obviously a bicyclic graph contains either two or three cycles.

**Lemma 1** ([8]) Let $T$ be an $n$-vertex tree different from $S_n$ and $P_n$. Then $(n - 1)^2 = W(S_n) < W(T) < W(P_n) = \frac{n^3 - n}{6}$.

For a connected graph $G$ with $u \in V(G)$, let $D(u|G) = \sum_{v \in V(G)} d(u, v|G)$ and let $L(u|G) = \sum_{v \in V(G)} l(u, v|G)$. Then $W(G) = \frac{1}{2} \sum_{u \in V(G)} D(u|G)$, $\omega(G) = \frac{1}{2} \sum_{u \in V(G)} L(u|G)$.

**Lemma 2** ([23]) Let $v$ be a vertex on the cycle $C_n$ with $n \geq 3$. Then $L(v|C_n) = \frac{1}{4}(3n^2 - 4n + n_0)$ and $\omega(C_n) = \frac{1}{8}n(3n^2 - 4n + n_0)$ where $n_0 = 1$ if $n_0$ is odd and $n_0 = 0$ if $n_0$ is
even.

**Lemma 3 ([27])** Let $x$ be a cut-vertex of a connected graph $G$, and let $u$ and $v$ be vertices occurring in different components which arise upon the deletion of $x$. Then

$$l(u, v|G) = l(u, x|G) + l(x, v|G)$$

Obviously, if $w$ is a pendant vertex of a connected graph $G$ order $n$ and $y$ is the unique neighbor of $w$, then $L(w|G) = L(y|G) + n - 2$.

For a graph $G$, let $|G| = |V(G)|$.

**Lemma 4 ([25])** Let $x$ be a cut vertex of a connected graph $G$ and $G - x$ consists of two vertex-disjoint subgraphs $G'_1$ and $G'_2$. Let $G_i$ be the subgraph of $G$ induced by $V(G'_i) \cup \{x\}$, $i = 1, 2$. Then $\omega(G) = \omega(G_1) + \omega(G_2) + (|G_1| - 1)L(x|G_2) + (|G_2| - 1)L(x|G_1)$.

## 2 Bicyclic Graphs with Small Detour Indices

Let $B_n$ be the set of $n$-vertex bicyclic graphs. Let $B^1_n$ and $B^2_n$ be the sets of $n$-vertex bicyclic graphs respectively with two cycles and with three cycles. Then, $B_n = B^1_n \cup B^2_n$.

Let $G_{p,q}^n$ and $G_{p,r,q}^n$ be the sets of $n$-vertex bicyclic graphs respectively with two cycles $C_p$ and $C_q$ without common path, and with three cycles $C_{p+r-2}$, $C_{q+r-2}$ and $C_{p+q-2}$, where $2 \leq r \leq p \leq q$ are all integers and $C_{p+r-2}$, $C_{q+r-2}$ have a common path $P_r$.

For integers $1 \leq i \leq p$, $1 \leq j \leq q$, $1 \leq k \leq r$, $T_{u_i}$, $T_{v_j}$, $T_{w_k}$ are trees attached at $u_i$, $v_j$, $w_k$ vertices of $P_p$, $P_q$ and $P_r$ respectively. We denote a bicyclic graph with three cycles by $G_{p,r,q}^n(T_{u_1}T_{u_2} \ldots T_{u_p}, T_{v_1}T_{v_2} \ldots T_{v_q}, T_{w_1}T_{w_2} \ldots T_{w_r})$, where $\sum_{i=1}^p |T_{u_i}| + \sum_{j=2}^q |T_{v_j}| + \sum_{k=2}^r |T_{w_k}| = n$. In particular, if only one tree $T_{u_1}(= T_{v_1} = T_{w_1})$ is a star with center vertex $u_1$, and the other trees $T_{u_i}, T_{v_j}, T_{w_k}(i, j, k \neq 1)$ are all trivial, the graph is denoted by $S_{p,r,q}$ (see Figure 1). Let us define an $n$-vertex graph $\Theta_{p,r,q}^n$ in $G_{p,r,q}^n$ to be a graph with all trees are trivial, i.e., $|T(u_i)| = |T(v_j)| = |T(w_k)| = 1$ for each $i, j, k$. Obviously, $p+r+q-4 = n$.

**Theorem 1** Let $G \in G_{p,r,q}^n$, where $p,q \geq 3, r \geq 2$ and $p + q + r - 4 \leq n$. Then $\omega(G) \geq \omega(S_{p,r,q}^n)$ with equality if and only if $G = S_{p,r,q}^n$.

**Proof.** Let $G_0$ be a graph with the smallest detour index among graphs $G_{p,r,q}^n$. We need only to show that $G_0 = S_{p,r,q}^n$.

Claim 1. $T_{u_i}, T_{v_j}, T_{w_k}$ are all stars with their centers at $u_i, v_j, w_k$ for each $i, j, k$. 


Suppose without loss of generality that the tree $T_{u_1}$ is not a star. Let $G_1$ be obtained from $G_0$ by deleting all edges of $T_{u_1}$ and connected all isolated vertices to $u_1$; that is, the tree rooted at $u_1$ in $G_1$ and $T'_{u_1}$ is a star with its center at $u_1$. For $G_0$, $u_1$ is a cut vertex, and $T_{u_1}$ and $G_0 - (V(T_{u_1}) \setminus \{u_1\})$ are two induced subgraphs. By Lemma 1, $\omega(T'_{u_1}) < \omega(T_{u_1})$. On the other hand, it is easily seen that $L(u_1|T'_{u_1}) < L(u_1|T_{u_1})$. Then $\omega(G_1) < \omega(G_0)$ from Lemma 4, which is a contradiction to the choice of $G_0$. Hence, Claim 1 follows.

Claim 2. Only one tree of $T_{u_i}, T_{v_j}, T_{w_k}$ is nontrivial for all $i,j,k$.

Without loss of generality, suppose that $T_{u_a}$ and $T_{u_b}$ are nontrivial. By Claim 1, we know that $T_{u_a}$ and $T_{u_b}$ are both stars. If $L(u_a|G_0) \geq L(u_b|G_0)$, let $G_2$ be obtained from $G_0$ by deleting a pendant vertex $x$ of $T_{u_a}$ and attaching it to $u_b$. By Lemmas 3 and 4, it follows that $\omega(G_0) - \omega(G_2) = L(x|G_0) - L(x|G_2) = [L(u_a|G_0) + n - 2] - [L(u_b|G_2) + n - 2] = L(u_a|G_0) - L(u_b|G_2)$. Since $L(u_b|G_2) = L(u_b|G_0) - |l(u_b, u_a)| + 1 = L(u_b|G_0) - l(u_b, u_a)$, $\omega(G_0) - \omega(G_2) = L(u_a|G_0) - L(u_b|G_0) + l(u_a, u_b) > 0$. If $L(u_a|G_0) < L(u_b|G_0)$, let $G_2$ be obtained from $G_0$ by deleting a pendant vertex $y$ of $T_{u_b}$ and attaching it to $u_a$. Similarly, we have $\omega(G_0) - \omega(G_2) > 0$. This contradicts the choice of $G_0$. Hence, Claim 2 follows.

Claim 3. Only one tree of $T_{u_1}$ and $T_{u_p}$ is nontrivial.

For $G_0$, suppose that only $T_{u_i}(i \neq 1, p)$ is nontrivial and $|T_{u_1}| = \alpha$. Let $G_3$ be the graph constructed from $G_0$ by deleting all pendant vertices of $T_{u_1}$ and connecting all isolated vertices to $u_1$, that is, $G_3 = S_{n}^{p,r,q}$. Let $G$ be constructed from $G_0$ by deleting all pendant vertices of $T_{u_1}$, that is, $G = \Theta_{n}^{p,r,q}_{|T_{u_1}| + 1}$. It follows that $\omega(G_0) - \omega(G_3) = [L(u_1|G) - L(u_1|G)](\alpha - 1)$ by Lemma 4. By the definition of detour distance, we know $L(u_1|G) > L(u_1|G)$. It implies that $\omega(G_0) > \omega(G_3)$, which is a contradiction to the choice of $G_0$. Hence, Claim 3 follows.
Claim 1, 2, 3 yield Theorem 1.

We need the following three Lemmas to prove the Theorem 2. Note that \( \omega(G) = \frac{1}{2} \sum_{u \in V(G)} L(u|G) = L(w|G) + \sum_{\{u,v\} \subseteq V(G) \setminus \{w\}} l(u,v|G) \)

**Lemma 5** \( \omega(\Theta_n^{p,r,q}) > \omega(S_n^{p,r-1,q}) \) for \( r \geq 3 \).

**Proof.** Let \( \Theta = \Theta_n^{p,r,q} \), where \( p + q + r - 4 = n \). Let \( \Theta' \) be constructed from \( \Theta \) by deleting the vertex \( w_{r-1} \), adding edge \( w_{r-2}w_r \), and attaching the isolated vertex \( x \) to \( u_1 \) as a pendent vertex. It implies that \( \Theta' = S_n^{p,r-1,q} \). Considered the transformation from \( \Theta \) to \( \Theta' \), we found that only the detour distance between \( x \) and any other vertex has the possibility of increasing, the increment is denoted by integer \( \lambda_1 \). That is \( \lambda_1 = L(x|\Theta') - L(x|\Theta) \).

The detour distance between any other two vertices will reduce or keep to be unchanged. That is \( \sum_{\{u,v\} \subseteq V(\Theta') \setminus \{x\}} l(u,v|\Theta') - \sum_{\{u,v\} \subseteq V(\Theta) \setminus \{x\}} l(u,v|\Theta) \leq 0 \). Now we will to show that \( \lambda_1 < 0 \), which will lead to \( \omega(\Theta') < \omega(\Theta) \).

\[
\lambda_1 = L(x|\Theta') - L(x|\Theta) = L(u_1|\Theta') + n - 2 - L(x|\Theta). \]

It is easy to know that \( \sum_{y \in V(P_2) \cup V(P_3) \setminus \{w_r\}} l_{\Theta'}(u_1,y) = \sum_{y \in V(P_2) \cup V(P_3) \setminus \{w_r\}} l_{\Theta}(u_1,y) \), denoted by \( m \) (integer). Thus \( L(u_1|\Theta') = \sum_{k=2}^{r-1} l_{\Theta'}(u_1,w_k) + m + l_{\Theta'}(u_1,x) = \frac{1}{2}(r - 2)(2q + r - 5) + m + 1 \) and \( L(x|\Theta) = L(w_{r-1}|\Theta) \geq L(w_r|\Theta) + n - 2 = L(u_1|\Theta) + n - 2 = \sum_{k=2}^{r} l_{\Theta}(u_1,w_k) + m + n - 2 = \frac{1}{2}(r - 1)(2q + r - 4) + m + n - 2. \) Since \( n = p + q + r - 4, \) we obtained \( \lambda_1 \leq p - n < 0. \)

Therefore, Lemma 5 holds.

In the following Lemmas 6 and 7, we consider the cases of \( r = 2, p \geq 4 \) and \( r = 2, p = 3, q \geq 4 \). The proofs of them are similar to that of Lemma 5.

**Lemma 6** \( \omega(\Theta_n^{p,2,q}) > \omega(S_n^{p-1,2,q}) \) for \( p \geq 4 \).

**Proof.** Let \( \Theta = \Theta_n^{p,2,q} \), where \( p + q - 2 = n \). We construct the graph \( \Theta'' \) from \( \Theta \) by deleting the vertex \( u_{p-1} \), adding edge \( u_{p-2}u_p \), and attaching the isolated vertex \( z \) to \( u_1 \) as a pendent vertex. This implies that \( \Theta'' = S_n^{p-1,2,q} \). Since \( L(z|\Theta'') = L(u_1|\Theta'') + n - 2 = L(u_1|C_{n-1}) + n - 1 \) and \( L(z|\Theta) > L(u_{p-1}|C_n) = L(u_1|C_n) \), by Lemma 2 we obtain \( L(z|\Theta'') - L(z|\Theta) < L(u_1|C_{n-1}) - L(u_1|C_n) + n - 1 = \frac{1}{4}(-2n + 3 - r_n + r_{n-1}) < 0 \), where \( r_n = 1 \) for odd \( n \) and \( r_n = 0 \) for even \( n \). Thus, \( \omega(\Theta'') < \omega(\Theta) \). Hence Lemma 6 holds.

**Lemma 7** \( \omega(\Theta_n^{3,2,q}) > \omega(S_n^{3,2,q-1}) \) for \( q \geq 4 \).
Proof. Let $\Theta = \Theta^{3,2,q}_n$, where $q + 1 = n$. We constructed the graph $\Theta''$ from $\Theta$ by deleting the vertex $v_{q-1}$, adding edge $v_{q-2}v_q$, and attaching the isolated vertex $h$ to $u_1$ as a pendant vertex. It implies that $\Theta'' = S^{3,2,q}_n$.

We will show that $L(h|\Theta'') - L(h|\Theta) < 0$. In fact, since $L(h|\Theta'') = L(u_1|\Theta'') + n - 2 = L(u_1|C_{n-1}) + n - 1$ and $L(h|\Theta) = L(h|C_n) + 1$, we have $L(h|\Theta'') - L(h|\Theta) = L(u_1|C_{n-1}) - L(h|C_n) + n - 2 = -[\frac{n}{2}] < 0$. Hence, Lemma 7 holds.

Theorem 2 Among graphs of $B^2_n$ for $n \geq 4$, $S^{3,2,3}_n$ is the graph with the smallest detour index, which is equal to $n^2 + 3n - 11$.

Proof. At first, we will prove that $\omega(S^{p,r,q}_n) > \omega(S^{p,r-1,q}_n)$ for $r \geq 3$. For $S^{p,r,q}_n$, let us delete the vertex $w_{r-1}$, connect $w_{r-2}$ and $w_r$, and attach the isolate vertex $y$ to $u_1$ as a pendant vertex. Then we obtain a graph $S^{p,r-1,q}_n$. Since $u_1$ is a cut-vertex of $S^{p,r,q}_n$, $T_{u_1}$ and $G'$ are two induced subgraphs of $S^{p,r,q}_n$ by $V(T_{u_1})$ and $V(S^{p,r,q}_n \setminus T_{u_1}) \cup \{u_1\}$. $u_1$ is also a cut-vertex of $S^{p,r-1,q}_n$, and $T_{u_1}$ and $G''$ are two induced subgraphs of $S^{p,r-1,q}_n$ by $V(T_{u_1})$ and $V(S^{p,r-1,q}_n \setminus T_{u_1}) \cup \{y\} \cup \{u_1\}$. Here, $G' = \Theta^{p,r,q}_{n-|T_{u_1}|+1}$ and $G'' = S^{p,r-1,q}_{n-|T_{u_1}|+1}$. Then $\omega(G') > \omega(G'')$ by Lemma 5. Since

$$L(u_1|G') - L(u_1|G'') = \sum_{k=2}^{r-1} l_{G'}(u_1, w_k) - [\sum_{k=2}^{r-2} l_{G'}(u_1, w_k) + l_{G'}(u_1, y)]$$

$$= (r - 2)(\frac{r - 3}{2} + q) - (r - 3)(\frac{r - 4}{2} + q) - 1$$

$$= q + r - 4 > 0$$

and by Lemma 4, we have

$$\omega(S^{p,r,q}_n) - \omega(S^{p,r-1,q}_n) = \omega(G') + |T_{u_1}|L(u_1|G') - \omega(G'') - |T_{u_1}|L(u_1|G'') > 0,$$
which implies that \( \omega(S_{n}^{p,q}) > \omega(S_{n}^{p,1,q}) \). The rest may be deduced by analogy, then
\[
\omega(S_{n}^{p,q}) > \omega(S_{n}^{p,1,q}) > \omega(S_{n}^{p,2,q}) > \ldots > \omega(S_{n}^{p,2,q}). \tag{1}
\]

Secondly, by Lemmas 4 and 6 we obtain
\[
\omega(S_{n}^{p,2,q}) > \omega(S_{n}^{p-1,2,q}) > \omega(S_{n}^{p-2,r,q}) > \ldots > \omega(S_{n}^{3,2,q}). \tag{2}
\]

By Lemmas 4 and 7, we have
\[
\omega(S_{n}^{3,2,q}) > \omega(S_{n}^{3,2,q-1}) > \omega(S_{n}^{3,2,q-2}) > \ldots > \omega(S_{n}^{3,2,3}). \tag{3}
\]

Hence, the result holds. \(\square\)

For positive integers \(a, b, c, d\), let \(S_{n}(a,b,c,d) \in G_{n}^{3,2,3}\), formed by attaching \(a - 1, b - 1, c - 1\) and \(d - 1\) pendent vertices to \(u_{1}, u_{3}, v_{2}\), and \(u_{2}\) of \(\Theta_{4}^{3,2,3}\) respectively, where \(a \geq b, c \geq d\) and \(a + b + c + d = n\) (see Figure 2). Let \(\Lambda_{n} = \{S_{n}(a,b,c,d)|a+b+c+d=n\}\).

Let \(\Gamma_{n}^{1} \subseteq G_{n}^{3,2,3}\), and for any graph \(G \in \Gamma_{n}^{1}, |T_{u_{1}}| = n - 3, |T_{u_{1}}| = |T_{v_{j}}| = |T_{w_{k}}| = 1\) for \(i, j, k \neq 1\). Let \(\Gamma_{n}^{2} \subseteq G_{n}^{3,2,3}\), and for any graph \(G \in \Gamma_{n}^{2}, |T_{u_{2}}| = n - 3, |T_{u_{1}}| = |T_{v_{j}}| = |T_{w_{k}}| = 1\) for other \(i, j, k\).

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 \(S''_{n} = T_{n:n-4,2}\) for \(n \geq 5\). For \(n \geq 6\), let \(D'_{n}\) and \(E'_{n}\) respectively be the \(n\)-vertex bicyclic graphs formed by attaching \(n - 6\) pendent vertices and a path \(P_{2}\) to \(u_{1}\) for \(D'_{n}\) and to \(u_{2}\) for \(E'_{n}\) of \(\Theta_{4}^{3,2,3}\). For \(n \geq 7\), let \(D''_{n}\) and \(E''_{n}\) be the \(n\)-vertex bicyclic graphs formed by attaching \(n - 7\) pendent vertices and the star \(S_{3}\) at its center vertex to \(u_{1}\) for \(D''_{n}\) and to \(u_{2}\) for \(E''_{n}\) of \(\Theta_{4}^{3,2,3}\). Obviously, \(D'_{n}, D''_{n} \in \Gamma_{n}^{1}\) and \(E'_{n}, E''_{n} \in \Gamma_{n}^{2}\) (see Figure 3).

Let \(\Delta_{n} = \{G \in G_{n}^{p,r,q}|8 < p+q+r \leq n+4\}\). Since \(G_{n}^{3,2,3} = \{G \in G_{n}^{p,r,q}|p+q+r = 8\}\) and \(p+q+r \geq 8\) for any \(G \in B_{n}^{2}\), obviously, \(B_{n}^{2} = G_{n}^{3,2,3} \cup \Delta_{n}\).

**Lemma 8** Among the graphs in \(\Delta_{n}\) with \(n \geq 5\), \(S_{n}^{3,3,3}\) is the unique graph with the smallest detour index, which is equal to \(n^{2} + 5n - 18\).

**Proof.** Without loss of generality, let \(r \leq p \leq q\). By the proof of Theorem 2, we have the inequality sequences:
\[
\omega(S_{n}^{p,q}) > \omega(S_{n}^{p-1,q}) > \omega(S_{n}^{p-2,3,q}) > \ldots > \omega(S_{n}^{3,3,q}) \tag{4}
\]
Combining Theorem 1 and inequality sequences (1)\textasciitilde(5), it follows that the graph with the smallest detour index among \( \Delta_n \) is from \( \{ S_{n-3}, S_n', S_n'' \} \). By Lemma 4, we compute that 

\[
\omega(S_{n-3}) = n^2 + 5n - 18 < \omega(S_n') = n^2 + 8n - 28.
\]

Hence, the result holds.

\( \square \)

**Lemma 9** Among the graphs in \( \Gamma_n^1 \) with \( n \geq 7 \), the \( D_n' \) and \( D_n'' \) are the graphs with the second and third smallest detour index, which is equal to \( n^2 + 4n - 14 \) and \( n^2 + 5n - 19 \), respectively.

**Proof.** For any \( n \)-vertex bicyclic graph \( G \in \Gamma_n^1 \setminus \{ S_{n-3}, S_n', S_n'' \} \). Note that \( |T_{u_1}| = n - 3 \), \( |T_{u_i}| = |T_{v_j}| = |T_{w_k}| = 1 \), for \( i, j, k \neq 1 \). Let \( G_1 = \Theta_3^{2,3} \) and \( G_2 \) be an induced subgraph of \( G \) by \( V(G \setminus G_1) \cup \{ u_1 \} \). Obviously, \( G_2 \) is a tree not \( S_{n-3}, S_n', S_n'' \). By Lemma 3 of [23], we have \( \omega(G_2) > \omega(S_n'') > \omega(S_n') \) for \( n \geq 7 \). Then, \( L(u_1|G_2) > L(u_1|S_n'') > L(u_1|S_n') \) together with Lemma 4, we obtain that \( D_n' \) and \( D_n'' \) are respectively the unique graphs in \( \Gamma_n^1 \) with the second and third smallest detour indices, where \( \omega(D_n') = \omega(S_n') + \omega(\Theta_3^{2,3}) + 3L(u_1|S_n') + 8(n - 4) = n^2 + 4n - 14 \) and \( \omega(D_n'') = \omega(S_n'') + \omega(\Theta_3^{2,3}) + 3L(u_1|S_n'') + 8(n - 4) = n^2 + 5n - 19 \). This proves the result.

\( \square \)

Also, the following lemma is obvious.

**Lemma 10** Among the graphs in \( \Gamma_n^2 \) with \( n \geq 7 \), the \( E_n' \) and \( E_n'' \) are the graphs with the second and third smallest detour index, which is equal to \( n^2 + 5n - 18 \) and \( n^2 + 6n - 23 \), respectively.
Lemma 11 Among the graphs in $\Lambda_n \setminus \{S_n^{3,3}\}$ with $n \geq 7$, $S_n(1,1,n-3,1)$ is the unique graph with the smallest detour index, which is equal to $n^2 + 4n - 15$. $S_n(n-4, 2, 1, 1)$ is the unique graph with the second smallest detour index, which is equal to $n^2 + 5n - 21$.

Proof. Suppose that $G$ is the graph with the smallest detour index of $\Lambda_n \setminus \{S_n^{3,3}\}$. The proof of Theorem 1 Claim 2 implies that there are at most two trees of $T_{u_i}, T_{v_j}, T_{w_k}$ for $1 \leq i, j \leq 3$ and $1 \leq k \leq 2$ to be nontrivial.

If only one tree is nontrivial, $G \in \{S_n(a,1,1,1), S_n(1,1,c,1)\}$ for $a, c \geq 2$. Since $S_n(a,1,1,1) = S_n^{3,3}$, then $G = S_n(1,1,c,1)$, i.e. $G = S_n(1,1,n-3,1)$ and $\omega(G) = n^2 + 4n - 15$.

If the two trees are nontrivial, $G \in \{S_n(a,1,c,1), S_n(a,b,1,1), S_n(1,1,c,d)\}$ for $a, b, c, d \geq 2$. We consider the following three cases.

Case 1. $G \in \{S_n(a,1,c,1)|a + c + 2 = n\}$. For $2 \leq c \leq n - 4$ and $a = n - 2 - c$, we have $\omega(S_n(a,1,c,1)) = \omega(S_n(n - 2 - c, 1, c, 1)) = -3c^2 + (3n - 5)c + n^2 - 3$. Let $f(c) = -3c^2 + (3n - 5)c + n^2 - 3$, then $f'(c) = -6c + 3n - 5$. $f(c)$ is an increasing function if $2 \leq c \leq \lfloor \frac{3n-5}{6} \rfloor$ and $f(c)$ is a decreasing function if $\lceil \frac{3n-5}{6} \rceil \leq c \leq n - 4$. So, we have the sequences: $f(2) < \ldots < f(\lfloor \frac{3n-5}{6} \rfloor)$ and $f(\lceil \frac{3n-5}{6} \rceil) > \ldots > f(n - 4)$. By direct computation, we have $f(2) < f(n - 4) < f(3) < \ldots$, i.e. $\omega(S_n(n - 4, 1, 2, 1)) = n^2 + 3n - 25 < \omega(S_n(2,1,n-4,1)) = n^2 + 7n - 31 < \omega(S_n(n-5,1,3,1)) = n^2 + 9n - 45 < \ldots$. Then $G = S_n(n-4,1,2,1)$ and $\omega(G) = f(2) = n^2 + 6n - 25$.

Case 2. $G \in \{S_n(a,b,1,1)|a + b + 2 = n\}$. Without loss of generality, let $a \geq b \geq 2$. Thus $2 \leq b \leq \lfloor \frac{n-2}{2} \rfloor$. Analogous to the proof of Case 1 given above, we deduce $\omega(S_n(a,b,1,1)) = \omega(S_n(n - 2 - b, b, 1, 1)) = -2b^2 + 2(n - 2)b + n^2 + n - 5$. It implies that the sequence $\omega(S_n(n - 4, 2, 1, 1)) = n^2 + 5n - 21 < \omega(S_n(n-5,3,1,1)) = n^2 + 7n - 35 < \omega(S_n(n-6,4,1,1)) = n^2 + 9n - 53 < \ldots < \omega(S_n(n-2-\lceil \frac{n-2}{2} \rceil, \lceil \frac{n-2}{2} \rceil, 1, 1)) = \begin{cases} \frac{3}{2}n^2 - n - 3 & : \text{for even } n \\ \frac{3}{2}n^2 - n - \frac{7}{2} & : \text{for odd } n \end{cases}$.

Then $G = S_n(n-4,2,1,1)$ and $\omega(G) = n^2 + 5n - 21$.

Case 3. If $G \in \{S_n(1,1,c,d)|c + d + 2 = n\}$. Without loss of generality, let $c \geq d \geq 2$. Thus $2 \leq d \leq \lfloor \frac{n-2}{2} \rfloor$. Also analogous to the proof of Case 1 given above, we deduce $\omega(S_n(1,1,c,d)) = \omega(S_n(1,1,n - 2 - d, d)) = -3d^2 + 3(n - 2)d + n^2 + n - 6$. It implies that the sequence $\omega(S_n(1,1,n-4,2)) = n^2 + 7n - 30 < \omega(S_n(1,1,n-5,3)) = n^2 + 10n - 51 < \ldots < \omega(S_n(1,1,n-2-\lfloor \frac{n-2}{2} \rfloor, \lfloor \frac{n-2}{2} \rfloor)) = \begin{cases} \frac{7n^2 - 8n - 12}{4} & : \text{for even } n \\ \frac{7n^2 - 8n - 15}{4} & : \text{for odd } n \end{cases}$.

Then $G = S_n(1,1,n-4,2)$ and $\omega(G) = n^2 + 7n - 30$. 
In conclusion, \( G \in \{ S_n(1,1,n-3,1), S_n(n-4,1,2,1), S_n(n-4,2,1,1), S_n(1,1,n-4,2) \} \). Together with their detour indices, we obtain \( G = S_n(1,1,n-3,1) \). Furthermore, it is easy to know that \( S_n(n-4,2,1,1) \) is the unique graph with the second smallest detour index in \( \Lambda_n \setminus \{ S_n^{3,2,3} \} \) with \( n \geq 7 \), which is equal to \( n^2 + 5n - 21 \). Hence, the result holds.

The main results of this paper are Theorems 3 and 4.

**Theorem 3** Among the graphs in \( \mathcal{B}_n^2 \) with \( n \geq 5 \), the following holds:

(i) For \( n = 5 \), \( S_5^{3,2,3} \) is the unique graph with the smallest detour index, which is equal to 29; \( S_5(1,1,2,1) \) is the unique graph with the second smallest detour index, which is equal to 30; \( S_5^{3,3,3} \) is the unique graph with the third smallest detour index, which is equal to 32;

(ii) For \( n = 6 \), \( S_6^{3,2,3} \) is the unique graph with the smallest detour index, which is equal to 43; \( S_6(1,1,3,1) \) and \( S_6(2,2,1,1) \) are the graphs with the second smallest detour index, which is equal to 45; \( D'_6 \) is the graph with the third smallest detour index, which is equal to 46.

(iii) For \( n \geq 7 \), \( S_n^{3,2,3} \) is the unique graph with the smallest detour index, which is equal to \( n^2 + 3n - 11 \); \( S_n(1,1,n-3,1) \) is the graph with the second smallest detour index, which is equal to \( n^2 + 4n - 15 \). For \( n \geq 8 \), \( D'_n \) is the graph with the third smallest detour index, which is equal to \( n^2 + 4n - 14 \). For \( n = 7 \), \( D'_n \) and \( S_n(n-4,2,1,1) \) are the graphs with the third smallest detour index, which is equal to 63.

**Proof.** Among the graphs in \( \mathcal{B}_n^2 \) with \( n \geq 4 \), by Theorem 2, we know \( S_n^{3,2,3} \) is the unique graph with the smallest detour index, which is equal to \( n^2 + 3n - 11 \).

Let \( G \) and \( G_0 \) be the graphs with the second and third smallest detour index respectively.

For \( n = 5 \), there are only four graphs \( S_5^{3,2,3}, S_5(1,1,2,1), S_5^{3,3,3} \) and \( S_5^{3,2,4} \) in \( \mathcal{B}_n^2 \). By directed computation, the result holds.

For \( n = 6 \), if \( p+q+r > 8 \), we have \( G = S_6^{3,3,3} \) by Lemma 8; if \( p+q+r = 8 \), then \( G \neq E'_6 \) by the Claim 1 of Theorem 1. Thus \( G \in \{ D'_6, S_6(1,1,3,1), S_6(2,1,2,1), S_6(2,2,1,1), S_6(1,1,2,2) \} \). By the proof of Lemma 11 and a little computation, \( \omega(S_6^{3,3,3}) = \omega(S_6(1,1,2,2)) = 48 > \omega(S_6(2,1,2,1)) = 47 > \omega(D'_6) = 46 > \omega(S_6(1,1,3,1)) = \omega(S_6(2,2,1,1)) = 45 \). Thus
$G = S_b(1, 1, 3, 1)$ or $S_b(2, 2, 1, 1)$. Furthermore, it is easy to know that $G_0 \in \{D'_n, E'_n\}$. Since $\omega(E'_6) = 48 > \omega(D'_6)$, then $G_0 = D'_6$.

For $n \geq 7$, if $p + q + r > 8$, $G \in \Delta_n$. Thus by Lemma 8, $G = S_n^{3,3,3}$; If $p + q + r = 8$, we know that $G \in \Gamma_n \cup \Lambda_n \setminus S_n^{3,2,3}$ by the proof of Theorem 1. By Lemmas 9 and 11, $G \in \{D'_n, S_n(1, 1, n - 3, 1)\}$. Since $\omega(S_n^{3,3,3}) = n^2 + 5n - 18 > \omega(D'_n) = n^2 + 4n - 14 > \omega(S_n(1, 1, n - 3, 1)) = n^2 + 4n - 15$, we have $G = S_n(1, 1, n - 3, 1)$. Then combining Lemmas 10 and 11, $G_0 \in \{D'_n, E'_n, S_n(n - 4, 2, 1, 1)\}$ and $\omega(D'_n) = n^2 + 4n - 14 \leq \omega(S_n(n - 4, 2, 1, 1)) = n^2 + 5n - 21 < \omega(E'_n) = n^2 + 5n - 18$ with the second equality if and only if $n = 7$. Thus $G_0 = D'_n$ for $n \geq 8$ and $G_0 = D'_n$ or $S_n(n - 4, 2, 1, 1)$ for $n = 7$.

Hence, the proof of theorem is completed. □

We will recall the conclusion of bicyclic graph with exactly two cycles in Lemma 12. Let $S_n^{a,q} \in B_n^1$ be the graph formed by attaching $n + 1 - p - q$ pendent vertices to the unique common vertex of the two cycles $C_p$ and $C_q$. Let $B'_n \in B_n^1$ be the $n$-vertex bicyclic graph with two 3-cycles sharing a common vertex $u_1(v_1)$, and attaching a path $P_2$ and $n - 7$ pendent vertices to the vertex $u_1$. Let $B''_n \in B_n^1$ be the $n$-vertex bicyclic graph with two 3-cycles sharing a common vertex $u_1(v_1)$, and attaching a star $S_3$ at its center and $n - 7$ pendent vertices to the vertex $u_1$. Let $\phi_n(a, b, c) \in B_n^1$ be a bicyclic graph with two triangles having a common vertex $u_1(v_1)$ formed by attaching $a - 1$ pendent vertices to $u_1$, and attaching $b - 1$ and $c - 1$ pendent vertices to the two neighbors of $u_1$ in the same triangle respectively. Let $\psi_n(a, b, c) \in B_n^1$ be a bicyclic graph with two triangles having a path $P_2$ formed by attaching $a - 1$ pendent vertices to $u_1$ which is one of the common vertices of triangles and terminal vertices of $P_2$, and attaching $b - 1$ and $c - 1$ pendent vertices to the two neighbors of $u_1$ in the same triangle respectively.

Lemma 12 ([27, 28]) Among the graphs in $B_n^1$ with $n \geq 5$, the following holds:

(i) For $n \geq 5$, $S_n^{3,3}$ is the unique graph with the smallest detour index, which is equal to $n^2 + 2n - 7$;

(ii) For $n = 6$, $\phi_6(1, 2, 1)$ and $\psi_6(1, 1, 1)$ are the unique graphs with the second smallest detour index, which is equal to 45; $S_6^{3,4}$ is the unique graph with the third smallest detour index, which is equal to 50.

(iii) For $n \geq 7$, $B'_n$ is the second smallest detour index, which is equal to $n^2 + 3n - 10$; For $n = 7$, $\phi_7(2, 2, 1)$ and $\psi_7(2, 1, 1)$ are the unique graphs with the third smallest detour index.
index, which is equal to 62. For \( n \geq 8 \), \( B_n'' \), \( \phi_n(n-5, 2, 1) \) and \( \psi_n(n-5, 1, 1) \) are the unique graphs with the third smallest detour index, which is equal to \( n^2 + 4n - 15 \).

The following Theorem 4 is obvious from the Theorem 3 and Lemma 12.

**Theorem 4** Among graphs of \( B_n \) with \( n \geq 5 \), the following holds:

(i) For \( n \geq 5 \), \( S_n^{3, n} \) is the graph with the smallest detour index, which is equal to \( n^2 + 2n - 7 \). \( S_n^{3, 2, 3} \) is the graph with the second smallest detour index, which is equal to \( n^2 + 3n - 11 \).

(ii) For \( n = 5 \), \( S_5(1, 1, 2, 1) \) is the third smallest detour index, which is equal to 30. \( S_5^{3, 3} \) is the forth smallest detour index, which is equal to 32.

(iii) For \( n = 6 \), \( S_6(1, 1, 3, 1) \), \( S_6(2, 2, 1, 1) \), \( \phi_6(1, 2, 1) \) and \( \psi_6(1, 1, 1) \) are the third smallest detour index, which is equal to 45. \( D_6' \) is the forth smallest detour index, which is equal to 46.

(iv) For \( n \geq 7 \), \( B_n' \) is the third smallest detour index, which is equal to \( n^2 + 3n - 10 \). \( \phi_n(n-5, 2, 1) \), \( \psi_n(n-5, 1, 1) \), \( S_n(1, 1, n-3, 1) \) and \( B_n'' \) (for \( n \geq 8 \)) are the unique graphs with the forth smallest detour index, which is equal to \( n^2 + 4n - 15 \).

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**References**


