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Minimum Detour Index of Bicyclic Graphs

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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 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 $3 \le r \le n - 2$, and determined the graphs with the first three smallest and largest detour indices respectively in the class of n-vertex unicyclic graphs for $n \ge 5$. 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 $n \ge 5$. 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 $n \ge 6$. 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 $n \ge 5$.

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 $n \ge 3$. 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 pendent 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 $\mathcal{B}_n$ be the set of n-vertex bicyclic graphs. Let $\mathcal{B}_n^1$ and $\mathcal{B}_n^2$ be the sets of n-vertex bicyclic graphs respectively with two cycles and with three cycles. Then, $\mathcal{B}_n = \mathcal{B}_n^1 \cup \mathcal{B}_n^2$. Let $\mathbf{G}_n^{p,q}$ and $\mathbf{G}_n^{p,r,q}$ 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 $G_n^{p,r,q}(T_{u_1}T_{u_2}\ldots T_{u_p}, T_{v_1}T_{v_2}\ldots T_{v_q}, T_{w_1}T_{w_2}\ldots T_{w_r})$, where $\sum_{i=1}^{p} |T_{u_i}| + \sum_{j=2}^{q-1} |T_{v_j}| + \sum_{k=2}^{r-1} |T_{w_k}| = n$. 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 $S_n^{p,r,q}$ (see Figure 1). Let us define an n-vertex graph $\Theta_n^{p,r,q}$ in $\mathbf{G}_n^{p,r,q}$ 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 $G \in \mathbf{G}_n^{p,r,q}$, where $p, q \geq 3, r \geq 2$ and $p + q + r - 4 \leq n$. Then $\omega(G) \geq \omega(S_n^{p,r,q})$ with equality if and only if $G = S_n^{p,r,q}$.*

Proof. Let G_0 be a graph with the smallest detour index among graphs $\mathbf{G}_n^{p,r,q}$. We need only to show that $G_0 = S_n^{p,r,q}$.

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.

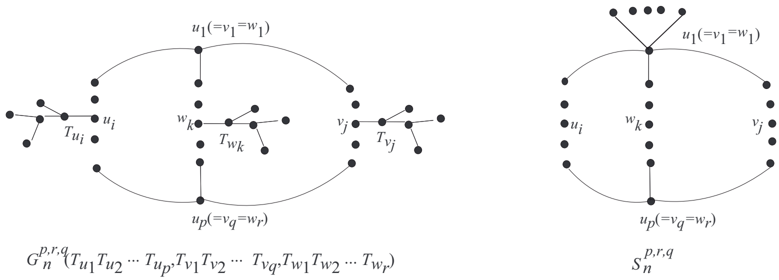

Figure 1: The graphs $G_n^{p,r,q}(T_{u_1}T_{u_2}\ldots T_{u_p}, T_{v_1}T_{v_2}\ldots T_{v_q}, T_{w_1}T_{w_2}\ldots T_{w_r})$ and $S_n^{p,r,q}$

Suppose without loss of generality that the tree T_{u_i} is not a star. Let G_1 be obtained from G_0 by deleting all edges of T_{u_i} and connected all isolated vertices to u_i; that is, the tree rooted at u_i in G_1 and T'_{u_i} is a star with its center at u_i. For G_0, u_i is a cut vertex, and T_{u_i} and $G_0 - (V(T_{u_i}) \setminus \{u_i\})$ are two induced subgraphs. By Lemma 1, $\omega(T'_{u_i}) < \omega(T_{u_i})$. On the other hand, it is easily seen that $L(u_i|T'_{u_i}) < L(u_i|T_{u_i})$. 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 pendent 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 $L(u_b|G_2) = L(u_b|G_0)-[l(u_b, u_a)+1]+1 = L(u_b|G_0)-l(u_b, u_a)$, $\omega(G_0) - \omega(G_2) = L(u_a|G_0) - L(u_b|G_0) + l(u_b, u_a) > 0$. If $L(u_a|G_0) < L(u_b|G_0)$, let G_2 be obtained from G_0 by deleting a pendent 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 $|T_{u_i}| = \alpha$. Let G_3 be the graph constructed from G_0 by deleting all pendent vertices of T_{u_i} 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 pendent vertices of T_{u_i}, that is, $G = \Theta^{p,r,q}_{n-|T_{u_i}|+1}$. It follows that $\omega(G_0)-\omega(G_3)$=$[L(u_i|G)-L(u_1|G)](\alpha - 1)$ by Lemma 4. By the definition of detour distance, we know $L(u_i|G) > L(u_1|G)$. 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 $\omega(G) = \frac{1}{2}\sum_{u\in V(G)} L(u|G) = L(w|G) + \sum\limits_{\{u,v\}\subseteq V(G)\setminus\{w\}} l(u,v|G)$

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 Θ' be constructed from Θ 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 Θ to Θ', we found that only the detour distance between x and any other vertex has the possibility of increasing, the increment is denoted by integer λ_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 $\sum\limits_{\{u,v\}\subseteq V(\Theta')\setminus\{x\}} l(u,v|\Theta') - \sum\limits_{\{u,v\}\subseteq V(\Theta)\setminus\{x\}} l(u,v|\Theta) \leq 0$. 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 $\sum\limits_{y\in V(P_p)\cup V(P_q)\setminus\{w_r\}} l_{\Theta'}(u_1,y) = \sum\limits_{y\in V(P_p)\cup V(P_q)\setminus\{w_r\}} l_{\Theta}(u_1,y)$, denoted by m (integer). Thus $L(u_1|\Theta') = \sum\limits_{k=2}^{r-1} l_{\Theta'}(u_1,w_k) + m + l_{\Theta'}(u_1,x) = \frac{1}{2}(r-2)(2q+r-5) + m + 1$ and $L(x|\Theta) = L(w_{r-1}|\Theta) \geq L(w_r|\Theta) + n - 2 = L(u_1|\Theta) + n - 2 = \sum\limits_{k=2}^{r} l_{\Theta}(u_1,w_k) + m + n - 2 = \frac{1}{2}(r-1)(2q+r-4) + m + n - 2$. 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 Θ'' from Θ 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* $q \geq 4$.

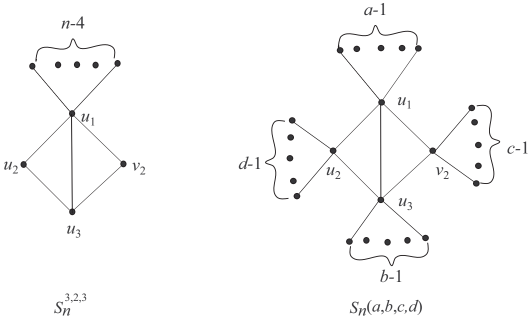

Figure 2: The graphs $S_n^{3,2,3}$ and $S_n(a,b,c,d)$

Proof. Let $\Theta = \Theta_n^{3,2,q}$, where $q+1=n$. We constructed the graph Θ''' from Θ 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 pendent vertex. It implies that $\Theta''' = S_n^{3,2,q-1}$.

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 $L(h|\Theta''') - L(h|\Theta) = L(u_1|C_{n-1}) - L(h|C_n) + n - 2 = -\lceil \frac{n}{2} \rceil < 0$. Hence, Lemma 7 holds. □

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

Proof. At first, we will prove that $\omega(S_n^{p,r,q}) > \omega(S_n^{p,r-1,q})$ for $r \geq 3$. For $S_n^{p,r,q}$, 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 pendent vertex. Then we obtain a graph $S_n^{p,r-1,q}$. Since u_1 is a cut-vertex of $S_n^{p,r,q}$, T_{u_1} and G' are two induced subgraphs of $S_n^{p,r,q}$ by $V(T_{u_1})$ and $V(S_n^{p,r,q} \setminus T_{u_1}) \cup \{u_1\}$. u_1 is also a cut-vertex of $S_n^{p,r-1,q}$, and T_{u_1} and G'' are two induced subgraphs of $S_n^{p,r-1,q}$ by $V(T_{u_1})$ and $V(S_n^{p,r-1,q} \setminus T_{u_1}) \cup \{y\} \cup \{u_1\}$. Here, $G' = \Theta_{n-|T_{u_1}|+1}^{p,r,q}$ and $G'' = S_{n-|T_{u_1}|+1}^{p,r-1,q}$. Then $\omega(G') > \omega(G'')$ by Lemma 5. Since

$$\begin{aligned} L(u_1|G') - L(u_1|G'') &= \sum_{k=2}^{r-1} l_{G'}(u_1, w_k) - [\sum_{k=2}^{r-2} l_{G''}(u_1, w_k) + l_{G''}(u_1, y)] \\ &= (r-2)(\frac{r-3}{2} + q) - (r-3)(\frac{r-4}{2} + q) - 1 \\ &= q + r - 4 > 0 \end{aligned}$$

and by Lemma 4, we have

$$\omega(S_n^{p,r,q}) - \omega(S_n^{p,r-1,q}) = \omega(G') + |T_{u_1}|L(u_1|G') - \omega(G'') - |T_{u_1}|L(u_1|G'') > 0,$$

which implies that $\omega(S_n^{p,r,q}) > \omega(S_n^{p,r-1,q})$. The rest may be deduced by analogy, then

$$\omega(S_n^{p,r,q}) > \omega(S_n^{p,r-1,q}) > \omega(S_n^{p,r-2,q}) > \ldots > \omega(S_n^{p,2,q}). \tag{1}$$

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. □

For positive integers a, b, c, d, let $S_n(a,b,c,d) \in \mathbf{G}_n^{3,2,3}$, 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 $\Gamma_n^1 \subseteq \mathbf{G}_n^{3,2,3}$, and for any graph $G \in \Gamma_n^1$, $|T_{u_1}| = n-3$ $(u_1 = v_1 = w_1)$, $|T_{u_i}| = |T_{v_j}| = |T_{w_k}| = 1$ for $i, j, k \neq 1$. Let $\Gamma_n^2 \subseteq \mathbf{G}_n^{3,2,3}$, and for any graph $G \in \Gamma_n^2$, $|T_{u_2}| = n-3$, $|T_{u_i}| = |T_{v_j}| = |T_{w_k}| = 1$ 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 $\Delta_n = \{G \in \mathbf{G_n^{p,r,q}} | 8 < p+q+r \leq n+4\}$. Since $\mathbf{G_n^{3,2,3}} = \{G \in \mathbf{G_n^{p,r,q}} | p+q+r = 8\}$ and $p+q+r \geq 8$ for any $G \in \mathcal{B}_n^2$, obviously, $\mathcal{B}_n^2 = \mathbf{G_n^{3,2,3}} \cup \Delta_n$.

Lemma 8 *Among the graphs in Δ_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:

$$\omega(S_n^{p,3,q}) > \omega(S_n^{p-1,3,q}) > \omega(S_n^{p-2,3,q}) > \ldots > \omega(S_n^{3,3,q}) \tag{4}$$

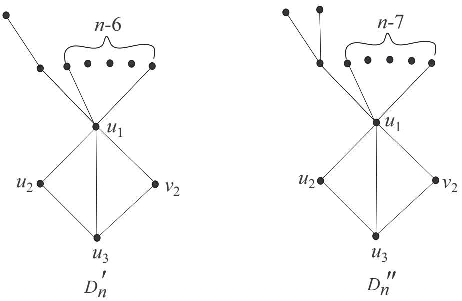

Figure 3: The graphs D'_n and D''_n

and

$$\omega(S_n^{3,3,q}) > \omega(S_n^{3,3,q-1}) > \omega(S_n^{3,3,q-2}) > \ldots > \omega(S_n^{3,3,3}). \quad (5)$$

Combining Theorem 1 and inequality sequences (1)∼(5), it follows that the graph with the smallest detour index among Δ_n is from $\{S_n^{3,3,3}, S_n^{3,2,4}\}$. By lemma 4, we compute that $\omega(S_n^{3,3,3}) = n^2 + 5n - 18 < \omega(S_n^{3,2,4}) = n^2 + 8n - 28$. Hence, the result holds. □

Lemma 9 *Among the graphs in Γ_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 $G \in \Gamma_n^1 \setminus \{S_n^{3,2,3}, D'_n, D''_n\}$. Note that $|T_{u_1}| = n-3$, $|T_{u_i}| = |T_{v_j}| = |T_{w_k}| = 1$, for $i, j, k \neq 1$. Let $G_1 = \Theta_4^{3,2,3}$ 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-3} or S''_{n-3}. By Lemma 3 of [23], we have $\omega(G_2) > \omega(S''_{n-3}) > \omega(S'_{n-3})$ for $n \geq 7$. Then, $L(u_1|G_2) > L(u_1|S''_{n-3}) > L(u_1|S'_{n-3})$ together with Lemma 4, we obtain that D'_n and D''_n are respectively the unique graphs in Γ_n^1 with the second and third smallest detour indices, where $\omega(D'_n) = \omega(S'_{n-3}) + \omega(\Theta_4^{3,2,3}) + 3L(u_1|S'_{n-3}) + 8(n-4) = n^2 + 4n - 14$ and $\omega(D''_n) = \omega(S''_{n-3}) + \omega(\Theta_4^{3,2,3}) + 3L(u_1|S''_{n-3}) + 8(n-4) = n^2 + 5n - 19$. This proves the result. □

Also, the following lemma is obvious.

Lemma 10 *Among the graphs in Γ_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* $\Lambda_n \setminus \{S_n^{3,2,3}\}$ *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 $\Lambda_n \setminus \{S_n^{3,2,3}\}$. 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 $S_n(a,1,1,1) = S_n^{3,2,3}$, 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. $\omega(S_n(n-4,1,2,1)) = n^2+6n-25 < \omega(S_n(2,1,n-4,1)) = n^2+7n-31 < \omega(S_n(n-5,1,3,1)) = n^2+9n-45 < \ldots$. 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 $\omega(S_n(n-4,2,1,1)) = n^2+5n-21 < \omega(S_n(n-5,3,1,1)) = n^2+7n-35 < \omega(S_n(n-6,4,1,1)) = n^2+9n-53 < \ldots < \omega(S_n(n-2-\lfloor \frac{n-2}{2} \rfloor, \lfloor \frac{n-2}{2} \rfloor, 1,1) = \begin{cases} \frac{3}{2}n^2-n-3 & : \ for\ even\ n \\ \frac{3}{2}n^2-n-\frac{7}{2} & : \ for\ odd\ n \end{cases}$.
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 $\omega(S_n(1,1,n-4,2)) = n^2+7n-30 < \omega(S_n(1,1,n-5,3)) = n^2+10n-51 < \ldots < \omega(S_n(1,1,n-2-\lfloor \frac{n-2}{2} \rfloor, \lfloor \frac{n-2}{2} \rfloor) = \begin{cases} \frac{7n^2-8n-12}{4} & : \ for\ even\ n \\ \frac{7n^2-8n-15}{4} & : \ for\ odd\ n \end{cases}$.
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

$G = S_6(1,1,3,1)$ or $S_6(2,2,1,1)$. Furthermore, it is easy to know that $G_0 \in \{D'_6, E'_6\}$. 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 $G \in \Gamma_n^1 \cup \Lambda_n \setminus S_n^{3,2,3}$ 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 $S_n^{p,q} \in \mathcal{B}_n^1$ 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 $B'_n \in \mathcal{B}_n^1$ 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 $B''_n \in \mathcal{B}_n^1$ 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 $\phi_n(a,b,c) \in \mathcal{B}_n^1$ 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 $\psi_n(a,b,c) \in \mathcal{B}_n^1$ 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 $\mathcal{B}_n^1$ 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, 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* $\mathcal{B}_n$ *with* $n \geq 5$*, the following holds:*

(i) For $n \geq 5$*,* $S_n^{3,3}$ *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*.* $S_5^{3,3,3}$ *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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