Hindawi
Journal of Mathematics
Volume 2021, Article ID 8722383, 11 pages
https://doi.org/10.1155/2021/8722383

Research Article

Bicyclic Graphs with the Second-Maximum and Third-Maximum Degree Resistance Distance

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Received 7 August 2021; Accepted 14 September 2021; Published 10 November 2021

Academic Editor: Francisco Balibrea

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Let $G = (V, E)$ be a connected graph. The resistance distance between two vertices u and v in G, denoted by $R_G(u, v)$, is the effective resistance between them if each edge of G is assumed to be a unit resistor. The degree resistance distance of G is defined as $D_R(G) = \sum_{\{u,v\}\subseteq V(G)} (d_G(u) + d_G(v))R_G(u, v)$, where $d_G(u)$ is the degree of a vertex u in G and $R_G(u, v)$ is the resistance distance between u and v in G. A bicyclic graph is a connected graph $G = (V, E)$ with $|E| = |V| + 1$. This paper completely characterizes the graphs with the second-maximum and third-maximum degree resistance distance among all bicyclic graphs with $n \geq 6$ vertices.

1. Introduction

All graphs considered in this paper are simple and undirected. Let $G = (V, E)$ be a graph with n vertices and m edges. Let $N_G(v)$ be the set of vertices adjacent to v in G. The *degree* of v in G, denoted by $d_G(v)$, is equal to $|N_G(v)|$. Denote the minimum degree of vertices in G by $\delta(G)$. A vertex of degree one is called a *pendant vertex*, and the edge incident with a pendant vertex is called a *pendant edge*. The *distance* between two vertices u and v of G, denoted by $d_G(u, v)$ or $d(u, v)$, is the length of a shortest path connecting u and v in G. For a subset S of V, denote by $G[S]$, the subgraph induced by S and $G - S$ the graph $G[V(G)\setminus S]$. We use $G - v$ instead of $G - \{v\}$ if $S = \{v\}$ for simplicity. Let P_n and C_n be the path and the cycle graphs on n vertices, respectively.

A topological index or a graph-theoretic index is a real number related to a graph. Topological indices of molecular graphs are one of the oldest and most widely used descriptors in quantitative structure-activity relationships [1, 2]. One of the most exhaustively studied [3, 4] topological indices is the *Wiener index*. The Wiener index was introduced in 1947 [5] and defined as $W(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u, v)$. It is well correlated with many physical and chemical properties of organic molecules and chemical compounds.

Based on the electrical network theory, Klein and Randić [6] proposed a novel distance function called *resistance distance* in 1993. They treated a graph G as an electric network by considering each edge of G as a unit resistor. Then, the resistance distance between two vertices u and v in G, denoted by $R_G(u, v)$, is defined as the effective resistance between them. Klein and Randić [6] also proved that $R_G(u, v) \leq d_G(u, v)$, with equality if and only if there is a unique path connecting u and v in G. In recent years, this new type of distance between vertices in a graph has attracted prominent attention in mathematics and chemistry [6–11].

Similar to the Wiener index, the *Kirchhoff index* of a graph G is defined as

$$Kf(G) = \sum_{\{u,v\}\subseteq V(G)} R_G(u, v). \tag{1}$$

This invariant has wide applications in electric circuit, physical interpretations, chemistry, and graph theory [12–16].

In 2012, Gutman et al. [17] introduced the concept of the *degree resistance distance* defined as

$$D_R(G) = \sum_{\{u,v\}\subseteq V(G)} (d_G(u) + d_G(v))R_G(u,v). \quad (2)$$

Palacios called it as *additive degree-Kirchhoff index* in [18]. In [17], Gutman et al. [17] presented some properties of $D_R(G)$ and characterized the unicyclic graphs with the minimum and second-minimum $D_R(G)$. Later, the unicyclic graphs with the maximum and second-maximum D_R-value were considered in [19, 20]. In [21, 22], the cactus graphs with the minimum, the second-minimum, and the third-minimum D_R-values were also completely characterized. Recently, the bicyclic graphs with maximum and minimum D_R-values were determined in [23, 24], respectively.

A *bicyclic graph* $G = (V, E)$ is a connected graph such that $|E| = |V| + 1$. The *kernel* of G, denoted by $\hat{G}$, is the unique bicyclic subgraph of G with no pendant vertices. Any bicyclic graph G is obtained from its kernel $\hat{G}$ by attaching trees to some vertices in $\hat{G}$. Given a family of graphs $\mathscr{G}$, the graphs with the maximum and second maximum values of topological indices among $\mathscr{G}$ are examined widely, see in [25–29]. Motivated by this, in this paper, we determine the graphs with the second-maximum and third-maximum degree resistance distance among all bicyclic graphs with $n \geq 6$ vertices.

2. Preliminaries

Let $\mathscr{B}_n$ be the set of bicyclic graphs of order n, $\mathscr{B}_n^{\infty}$ be the set of bicyclic graphs of order n with exactly two cycles, and $\mathscr{B}_n^{\theta} = \mathscr{B}_n \setminus \mathscr{B}_n^{\infty}$. Let $B(p,q)$ be obtained from two vertex-disjoint cycles C_p and C_q by identifying a vertex $u \in V(C_p)$ and a vertex $v \in V(C_q)$, $B(p,l,q)$ be obtained from two vertex-disjoint cycles C_p and C_q by connecting a vertex $u \in V(C_p)$ and a vertex $v \in V(C_q)$ by a path $uv_1v_2 \ldots v_{l-1}v$ of length $l\,(l \geq 1)$, and $B(P_r, P_s, P_t)$ be the union of three internally disjoint paths P_r, P_s, and P_t, respectively, with common end vertices, where $r, s, t \geq 2$ and at most one of them is 2.

Let G be a graph and v be a vertex in G. Define $Kf_v(G) = \sum_{u\in V(G)} R_G(u,v)$ and $D_v(G) = \sum_{u\in V(G)} d_G(u)R_G(u,v)$.

We present a few lemmas which will be employed later to establish our main results.

Lemma 1 (see [13]). *Let G be a connected graph with a pendant vertex v with its unique neighbor w. Then, $Kf_v(G) = Kf_w(G - v) + n - 1$.*

Lemma 2 (see [13]). *Let G be a bicyclic graph of order n and $v \in V(G)$. Then, $Kf_v(G) \leq n^2/2 - n/2 - 15/4$. Moreover, if $d_G(v) \geq 2$, then $Kf_v(G) \leq n^2/2 - 3n/2 + 1/3$.*

The following remark can be obtained from the proof of Lemma 2.

Remark 1. Let G be a graph in $\mathscr{B}_n^{\infty}$ and $v \in V(G)$. Then, $Kf_v(G) \leq n^2/2 - n/2 - 6$.

Lemma 3 (see [17]). *Let G be a connected graph with a cut vertex v such that G_1 and G_2 are two connected subgraphs of G having v as the only common vertex and $V(G_1) \bigcup V(G_2) = V(G)$. Let $n_1 = |V(G_1)|, n_2 = |V(G_2)|$, $m_1 = |E(G_1)|$, and $m_2 = |E(G_2)|$. Then, $D_R(G) = D_R(G_1) + D_R(G_2) + 2m_2Kf_v(G_1) + 2m_1Kf_v(G_2) + (n_2 - 1)D_v(G_1) + (n_1 - 1)D_v(G_2)$.*

Lemma 4 (see [17]). *Let C_k be a cycle with length k and $v \in C_k$. Then, $Kf(C_k) = (k^3 - k)/12, D_R(C_k) = (k^3 - k)/3$, $Kf_v(C_k) = (k^2 - 1)/6$, and $D_v(C_k) = (k^2 - 1)/3$.*

Lemma 5 (see [23]). *Let H be a connected graph of order $h > 2$ and C_k be a cycle of order $k \geq 4$. Let F be the graph of order k obtained from C_3 by attaching one pendant path of order $k - 3$ to one vertex of C_3. Further suppose G_1 is the graph obtained from H and C_k by identifying one vertex in H and one vertex in C_k; G_2 is the graph obtained from H and F by identifying one vertex in H and the pendant vertex in F. Then, we have $D_R(G_1) < D_R(G_2)$.*

By an argument similar to that of Lemma 5, we easily get the following result.

Lemma 6. *Let G be a connected graph of order $n > 2$ and C_k be a cycle of order $k \geq 5$. Let F be obtained by identifying a pendant vertex of P_{k-3} with any vertex of C_4. Suppose G_1 is the graph obtained from G and C_k by identifying one vertex in G and one vertex in C_k; G_2 is obtained from G and F by identifying one vertex in G and the pendant vertex in F. Then, $D_R(G_1) < D_R(G_2)$.*

In [23], Du and Tu characterized the unique bicyclic graph with maximum degree resistance distance. They also presented two significant lemmas in [23].

Theorem 1 (see [23]). *Let G be a bicyclic graph of order $n \geq 6$; then, $D_R(G) \leq 2n^3/3 + n^2 - 19n + 88/3$, with equality if and only if $G \cong B(3, n-5, 3)$.*

Lemma 7 (see [23]). *Let G be a bicyclic graph of order n and $v \in V(G)$. Then, $D_v(G) \leq n^2 + 2n - 73/4$.*

Lemma 8 (see [23]). *Let G be a bicyclic graph of order n, v be a pendant vertex of G, and w be its neighbor. Then, $D_R(G) = D_R(G - v) + D_w(G - v) + 2Kf_w(G - v) + 3n$.*

3. Bicyclic Graphs with the Second-Maximum Degree Resistance Distance

In this section, we will determine the bicyclic graphs with the second-maximum degree resistance distance.

Suppose $n \geq 6$. Let $B(3, n-5, 3)$ be obtained from two 3-cycles $v_1v_2v_3v_1$ and $v_{n-2}v_{n-1}v_nv_{n-2}$ by connecting v_3 and v_{n-2} by a path $v_3v_4 \cdots v_{n-3}v_{n-2}$. Define $G_n^1 = B(3, n-5, 3) - v_{n-1}v_n + v_{n-1}v_{n-3}$ and $G_n^{2,i} = G_n^1 - v_{n-2}v_n + v_iv_n$, where $3 \leq i \leq n-3$. Let $G_n^3\,(G_n^5)$ be obtained from a 4-cycle $C_4 = v_1v_2v_3v_4v_1$ and a path $P = v_5 \ldots v_n$ by adding the edges v_1v_3 (v_2v_4, resp.) and v_4v_5. Let $G_n^4 \cong B(4, n-6, 3)$ be obtained from a 4-cycle $v_1v_2v_3v_4v_1$ and a 3-cycle $v_{n-2}v_{n-1}v_nv_{n-2}$ by connecting v_4 and v_{n-2} by a path $v_4v_5\ldots v_{n-3}v_{n-2}$ (see Figure 1). Then, we have the following lemma.

Lemma 9. *Let G_n^1, $G_n^{2,i}$, G_n^3, G_n^4, and G_n^5 be defined as above. Then, $D_R(G_n^1) = 2/3n^3 + n^2 - 79/3n + 56$, $D_R(G_n^{2,i}) = 2/3n^3 + n^2 - 17n + 4i^2 - 4ni + 88/3$, $D_R(G_n^3) = 2/3n^3 + n^2 - 293/12n + 117/2$, $D_R(G_n^4) = 2/3n^3 + n^2 - 82/3n + 167/3$, and $D_R(G_n^5) = 2/3n^3 + n^2 - 163/6n + 139/2$.*

Proof. By Lemma 8 and Theorem 1, we easily obtain

$$
\begin{aligned}
D_R(G_n^1) &= D_R(G_n^1 - v_n) + D_{v_{n-2}}(G_n^1 - v_n) + 2Kf_{v_{n-2}}(G_n^1 - v_n) + 3n\\
&= \left[\frac{2}{3}(n-1)^3 + (n-1)^2 - 19(n-1) + \frac{88}{3}\right]\\
&\quad + \left[2\cdot\frac{2}{3} + 3\cdot\frac{2}{3} + 2\cdot\left(\frac{2}{3}+1\right) + 2\cdot\left(\frac{2}{3}+2\right) + \cdots + 2\cdot\left(\frac{2}{3}+n-7\right) + 3\cdot\left(\frac{2}{3}+n-6\right)\right.\\
&\quad \left. + 2\cdot\left(\frac{4}{3}+n-6\right) + 2\cdot\left(\frac{4}{3}+n-6\right)\right] + 2\cdot\left[\frac{2}{3}+\frac{2}{3}+\left(\frac{2}{3}+1\right)\right.\\
&\quad \left. + \left(\frac{2}{3}+2\right) + \cdots + \left(\frac{2}{3}+n-6\right) + 2\left(\frac{4}{3}+n-6\right)\right] + 3n\\
&= \left[\frac{2}{3}(n-1)^3 + (n-1)^2 - 19(n-1) + \frac{88}{3}\right]\\
&\quad + \left(n^2 - \frac{14}{3}n + \frac{4}{3}\right) + 2\cdot\left(\frac{n^2}{2} - \frac{17}{6}n + 3\right) + 3n\\
&= \frac{2}{3}n^3 + n^2 - \frac{79}{3}n + 56,\\
D_R(G_n^{2,i}) &= D_R(G_n^{2,i} - v_n) + D_{v_i}(G_n^{2,i} - v_n) + 2Kf_{v_i}(G_n^{2,i} - v_n) + 3n\\
&= \left[\frac{2}{3}(n-1)^3 + (n-1)^2 - 19(n-1) + \frac{88}{3}\right] + [2\cdot 1 + 2\cdot 2\\
&\quad + \cdots + 2\cdot(i-4) + 3\cdot(i-3) + 4\cdot\left(i-3+\frac{2}{3}\right) + 2\cdot 1 + 2\cdot 2\\
&\quad + \cdots + 2\cdot(n-4-i) + 3\cdot(n-3-i) + 4\cdot\left(n-3-i+\frac{2}{3}\right)]\\
&\quad + 2\cdot[1 + 2 + \cdots + (i-3) + 2\cdot\left(i-3+\frac{2}{3}\right) + 1 + 2 + \cdots\\
&\quad + (n-3-i) + 2\cdot\left(n-3-i+\frac{2}{3}\right)] + 3n\\
&= \left(\frac{2}{3}n^3 - n^2 - 19n + \frac{146}{3}\right) + \left(n^2 + 2i^2 - 2ni - \frac{38}{3}\right)\\
&\quad + 2\cdot\frac{3n^2 - 3n + 6i^2 - 6ni - 20}{6} + 3n\\
&= \frac{2}{3}n^3 + n^2 - 17n + 4i^2 - 4ni + \frac{88}{3}.
\end{aligned}
\tag{3}
$$

Let $H = G_n^3[\{v_1, v_2, v_3, v_4\}]$. By Lemma 3,

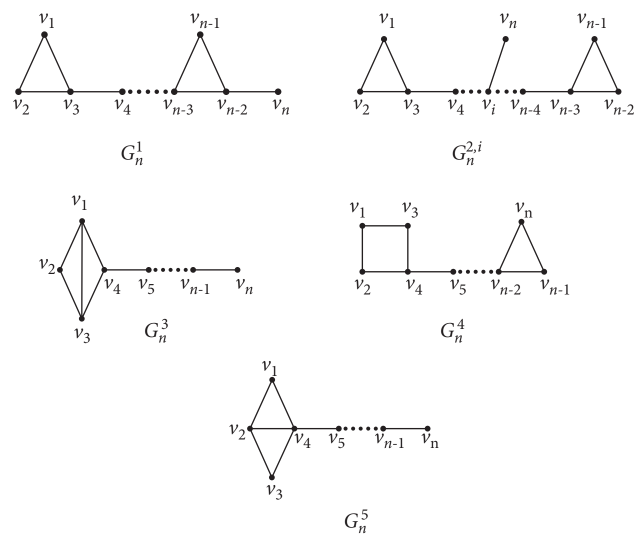

FIGURE 1: Graphs $G_n^1, G_n^{2,i}, G_n^3, G_n^4$, and G_n^5.

$$\begin{aligned}
D_R\left(G_n^3\right) &= D_R(H) + D_R(P_{n-3}) + 2(n-4)Kf_{v_4}(H) + 10Kf_{v_4}(P_{n-3}) \\
&\quad + (n-4)D_{v_4}(H) + 3D_{v_4}(P_{n-3}) \\
&= \frac{39}{2} + \left[\frac{2}{3}(n-3)^3 - (n-3)^2 + \frac{1}{3}(n-3)\right] + 2\cdot(n-4)\cdot\frac{9}{4} \\
&\quad + 10\cdot\frac{(n-3)(n-4)}{2} + (n-4)\cdot\frac{23}{4} + 3\cdot(n-4)^2 \\
&= \frac{2}{3}n^3 + n^2 - \frac{293}{12}n + \frac{117}{2}.
\end{aligned} \tag{4}$$

Let $F = G_n^4 - \{v_{n-1}, v_n\}$. By Lemmas 3 and 6,

$$\begin{aligned}
D_R\left(G_n^4\right) &= D_R(C_3) + D_R(F) + 2(n-2)Kf_{v_{n-2}}(C_3) + 6Kf_{v_{n-2}}(F) \\
&\quad + (n-3)D_{v_{n-2}}(C_3) + 2D_{v_{n-2}}(F) \\
&= 8 + \left[\frac{2}{3}(n-2)^3 - \frac{53}{3}(n-2) + 48\right] + \frac{8}{3}(n-2) + 6\left[\frac{(n-2)^2}{2}\right. \\
&\quad \left. - \frac{n-2}{2} - \frac{7}{2}\right] + \frac{8}{3}(n-3) + 2\left[(n-2)^2 - 11\right] \\
&= \frac{2}{3}n^3 + n^2 - \frac{82}{3}n + \frac{167}{3}.
\end{aligned} \tag{5}$$

Let $S = G_n^5[\{v_1, v_2, v_3, v_4\}]$. By Lemma 3,

$$
\begin{aligned}
D_R\left(G_n^5\right) &= D_R(S) + D_R(P_{n-3}) + 2(n-4)Kf_{v_4}(S) + 10Kf_{v_4}(P_{n-3}) \\
&\quad + (n-4)D_{v_4}(S) + 3D_{v_4}(P_{n-3}) \\
&= \frac{39}{2} + \left[\frac{2}{3}(n-4)^3 + (n-4)^2 + \frac{1}{3}(n-4)\right] + 2(n-4)\cdot\frac{7}{4} \\
&\quad + 10\cdot\frac{(n-3)(n-4)}{2} + 4(n-4) + 3(n-4)^2 \\
&= \frac{2}{3}n^3 + n^2 - \frac{163}{6}n + \frac{139}{2}.
\end{aligned} \tag{6}
$$

□

Theorem 2. *Suppose G is a graph in $\mathscr{B}_n^{\infty}$ with $G \not\cong B(3, n-5, 3)$ and $n \geq 6$. Then, $D_R(G) \leq 2/3n^3 + n^2 - 79/3n + 56$, with equality if and only if $G \cong G_n^1$, where G_n^1 is defined as in Lemma 9.*

Proof. It is easy to verify that, for any graph G in $\mathscr{B}_6^{\infty}$ with $G \not\cong B(3,1,3)$, $D_R(G) \leq 78 = 2/3\cdot 6^3 + 6^2 - 79/3\cdot 6 + 56$, with equality if and only if $G \cong G_6^1$.

Now, we assume $n \geq 7$ and consider the following two cases.

Case 1 $\delta(G) = 1$: let v be a pendant vertex in G. If $G - v \cong B(3, n-6, 3)$, then either $G \cong G_n^1$, or $G \cong G_n^{2,i}$, where G_n^1 and $G \cong G_n^{2,i}$ are defined as in Lemma 9. By Lemma 9,

$$
\begin{aligned}
D_R\left(G_n^{2,i}\right) &= \frac{2}{3}n^3 + n^2 - 17n + 4i^2 - 4ni + \frac{88}{3} \\
&\leq \frac{2}{3}n^3 + n^2 - 17n + 4\cdot 3^2 - 4n\cdot 3 + \frac{88}{3} \\
&< \frac{2}{3}n^3 + n^2 - \frac{79}{3}n + 56.
\end{aligned} \tag{7}
$$

If $G - v \not\cong B(3, n-6, 3)$, we prove it by induction on n. Let w be the neighbor of v. By the inductive hypothesis, Remark 1, and Lemmas 7–9

$$
\begin{aligned}
D_R(G) &= D_R(G-v) + D_w(G-v) + 2Kf_w(G-v) + 3n \\
&\leq \frac{2}{3}(n-1)^3 + (n-1)^2 - \frac{79}{3}(n-1) \\
&\quad + 56 + \left[(n-1)^2 + 2(n-1)\right. \\
&\quad \left. - \frac{73}{4}\right] + 2\left(\frac{(n-1)^2}{2} - \frac{n-1}{2} - 6\right) + 3n \\
&= \frac{2}{3}n^3 + n^2 - \frac{79}{3}n + \frac{641}{12} \\
&< \frac{2}{3}n^3 + n^2 - \frac{79}{3}n + 56.
\end{aligned} \tag{8}
$$

Case 2 ($\delta(G) \geq 2$): in this case, G is of the form $B(p,q)$ or $B(p,l,q)$. By Lemmas 5 and 6, we have $D_R(G) \leq D_R(G_n^4)$, with equality if and only if $G \cong G_n^4$.

Note that $D_R(G_n^4) < D_R(G_n^1)$ by Lemma 9. Therefore, the proof is complete. □

Theorem 3. *Suppose G is a graph of order $n \geq 4$ in $\mathscr{B}_n^{\theta}$. Then, $D_R(G) \leq 2/3n^3 + n^2 - 293/12n + 117/2$, with equality if and only if $G \cong G_n^3$, where G_n^3 is defined in Lemma 9.*

Proof. It is easy to verify that the only graph in $\mathscr{B}_4^{\theta}$ is G_4^3 and $D_R(G_4^3) = 2/3\cdot 4^3 + 4^2 - 293/12\cdot 4 + 117/2$. We assume $n \geq 5$ next, and consider the following two cases.

Case 1 ($\delta(G) = 1$): let v be a pendant vertex in G and w be the neighbor of v. We prove it by induction on n. By the inductive hypothesis, Lemma 2, and Lemmas 7–9,

$$
\begin{aligned}
D_R(G) &= D_R(G-v) + D_w(G-v) + 2Kf_w(G-v) + 3n \\
&\leq \frac{2}{3}(n-1)^3 + (n-1)^2 - \frac{293}{12}(n-1) \\
&\quad + \frac{117}{2} + \left[(n-1)^2 + 2(n-1)\right. \\
&\quad \left. - \frac{73}{4}\right] + 2\cdot\left(\frac{(n-1)^2}{2} - \frac{n-1}{2} - \frac{15}{4}\right) + 3n \\
&= \frac{2}{3}n^3 + n^2 - \frac{293}{12}n + \frac{117}{2}.
\end{aligned} \tag{9}
$$

The equality $D_R(G-v) = 2/3n^3 + n^2 - 293/12n + 117/2$ holds if and only if $D_R(G-v) = 2/3(n-1)^3 + (n-1)^2 - 293/12(n-1) + 117/2$, $D_w(G-v) = (n-1)^2 + 2\cdot(n-1) - 73/4$, and $Kf_w(G-v) = (n-1)^2/2 - (n-1)/2 - 15/4 = n^2/2 - 3/2n - 11/4$. By the inductive hypothesis, $G - v \cong G_{n-1}^3$, which is obtained from a 4-cycle $C_4 = v_1v_2v_3v_4v_1$ and a path $P = v_5 \ldots v_{n-1}$ by adding the edges v_1v_3 and v_4v_5. We show that $w = v_{n-1}$, i.e., $G \cong G_n^3$. By direct calculation, we have $Kf_{v_{n-1}}(G_{n-1}^3) = n^2/2 - 3/2n - 11/4$, $Kf_{v_1}(G_{n-1}^3) = Kf_{v_3}(G_{n-1}^3) = n^2/2 - 31/8n + 69/8 < n^2/2 - 3/2n - 11/4$, and $Kf_{v_2}(G_{n-1}^3) = n^2/2 - 7/2n + 29/4 < n^2/2 - 3/2n - 11/4$. Obviously, $Kf_u(G_{n-1}^3) < Kf_{v_{n-1}}(G_{n-1}^3)$ if $u \in V(G_{n-1}^3) \setminus \{v_1, v_2, v_3, v_{n-1}\}$. Therefore, $w = v_{n-1}$, i.e., $G \cong G_n^3$.

Case 2 ($\delta(G) \geq 2$): then, G is of the form $B(P_k, P_l, P_m)$. Suppose x and y are the only two vertices of degree 3. Since $Kf(G) \leq 1/8n^3$ (see [13]), we have

$$\begin{aligned} D_R(G) &= \sum_{\{u,v\}\subseteq V(G)} (d(u) + d(v))R(u,v) \\ &= 4Kf(G) + Kf_x(G) + Kf_y(G) \\ &\leq 4 \cdot \frac{1}{8}n^3 + 2 \cdot \left(\frac{1}{2}n^2 - \frac{3}{2}n + \frac{1}{3}\right) (\text{by Lemma 2}) \\ &= \frac{1}{2}n^3 + n^2 - 3n + \frac{2}{3}. \end{aligned} \tag{10}$$

If $n \geq 10$, then $1/2n^3 + n^2 - 3n + 2/3 < 2/3n^3 + n^2 - 293/12n + 117/2$. For any graph $G \cong B(P_k, P_l, P_m)$ when $n = 5, 6, 7, 8, 9$, we have calculated $D_R(G)$ and found that $D_R(G) < 2/3n^3 + n^2 - 293/12n + 117/2$.

Combining Theorems 1–3, we can obtain the first main result of our paper. □

Theorem 4. *Suppose G is a bicyclic graph of order $n \geq 6$ with $G \not\cong B(3, n-5, 3)$. Then, $D_R(G) \leq 2/3n^3 + n^2 - 293/12n + 117/2$, with equality if and only if $G \cong G_n^3$, where G_n^3 is defined as in Lemma 9.*

4. Bicyclic Graphs with the Third-Maximum Degree Resistance Distance

In this section, we will determine the bicyclic graphs with the third-maximum degree resistance distance.

Lemma 10. *Let $G_n^{3,i}$ be obtained from a 4-cycle $C_4 = v_1v_2v_3v_4v_1$, a path $P = v_5 \ldots v_{n-1}$ and an isolated vertex v_n by adding the edges v_1v_3, v_4v_5, and v_iv_n, where $1 \leq i \leq n-2$ and $n \geq 6$. Then, $D_R(G_n^{3,1}) = D_R(G_n^{3,3}) = 2/3n^3 + n^2 - 455/12n + 493/4$, $D_R(G_n^{3,2}) = 2/3n^3 + n^2 - 437/12n + 237/2$, $D_R(G_n^{3,4}) = 2/3n^3 + n^2 - 485/12n + 277/2$, and $D_R(G_n^{3,i}) = 2/3n^3 + n^2 - 293/12n - 4ni + 4i^2 + 4i + 117/2$, for $5 \leq i \leq n-2$.*

Proof. By Lemmas 8 and 9, we easily obtain

$$\begin{aligned} D_R\left(G_n^{3,1}\right) &= D_R\left(G_n^{3,3}\right) = D_R\left(G_{n-1}^3\right) + D_{v_1}\left(G_{n-1}^3\right) + 2Kf_{v_1}\left(G_{n-1}^3\right) + 3n \\ &= \left[\frac{2}{3}(n-1)^3 + (n-1)^2 - \frac{293}{12}(n-1) + \frac{117}{2}\right] \\ &\quad + 2 \cdot \frac{5}{8} + 3 \cdot \frac{5}{8} + 3 \cdot \frac{1}{2} + 2 \cdot \left(\frac{5}{8} + 1\right) + \cdots + 2 \cdot \left(\frac{5}{8} + n - 6\right) + \left(n - 5 + \frac{5}{8}\right) \\ &\quad + 2 \cdot \left[\frac{5}{8} + \frac{5}{8} + \frac{1}{2} + \left(\frac{5}{8} + 1\right) + \cdots + \left(\frac{5}{8} + n - 5\right)\right] + 3n \\ &= \left[\frac{2}{3}(n-1)^3 + (n-1)^2 - \frac{293}{12}(n-1) + \frac{117}{2}\right] + \left(n^2 - \frac{35}{4}n + \frac{91}{4}\right) \\ &\quad + \left(n^2 - \frac{31}{4}n + \frac{69}{4}\right) + 3n = \frac{2}{3}n^3 + n^2 - \frac{455}{12}n + \frac{493}{4}, \end{aligned}$$

$$\begin{aligned} D_R\left(G_n^{3,2}\right) &= D_R\left(G_{n-1}^3\right) + D_{v_2}\left(G_{n-1}^3\right) + 2Kf_{v_2}\left(G_{n-1}^3\right) + 3n \\ &= \left[\frac{2}{3}(n-1)^3 + (n-1)^2 - \frac{293}{12}(n-1) + \frac{117}{2}\right] \\ &\quad + 3 \cdot \frac{5}{8} + 3 \cdot \frac{5}{8} + 3 \cdot 1 + 2 \cdot 2 + \cdots + 2 \cdot (n-5) + (n-4) + 2 \cdot \left(\frac{5}{8} + \frac{5}{8} + 1\right. \\ &\quad \left. + \cdots + n - 4\right) + 3n \end{aligned}$$

$$
\begin{aligned}
&= \left[\frac{2}{3}(n-1)^3 + (n-1)^2 - \frac{293}{12}(n-1) + \frac{117}{2}\right] \\
&\quad + \left(n^2 - 8n + \frac{83}{4}\right) \\
&\quad + \left(n^2 - 7n + \frac{29}{2}\right) + 3 \\
&= \left[\frac{2}{3}n^3 + n^2 - \frac{437}{12}n + \frac{237}{2},\right. \\
&D_R\left(G_n^{3,4}\right) = D_R\left(G_{n-1}^3\right) + D_{v_4}\left(G_{n-1}^3\right) + 2Kf_{v_4}\left(G_{n-1}^3\right) + 3n \\
&= \left[\frac{2}{3}(n-1)^3 + (n-1)^2 - \frac{293}{12}(n-1) + \frac{117}{2}\right] \\
&\left[+ 2\cdot 3\cdot\frac{5}{8} + 2\cdot 1 + 2\cdot 1 + 2\cdot 2 + \cdots + 2\cdot(n-6) + (n-5)\right] + 2\cdot\left(2\cdot\frac{5}{8} + 1 + 1\right. \\
&\quad + \cdots + n - 5 + 3n = \left[\frac{2}{3}(n-1)^3 + (n-1)^2 - \frac{293}{12}(n-1) + \frac{117}{2}\right] + \left(n^2 - 10n + \frac{123}{4}\right) \\
&\quad + \left(n^2 - 9n + \frac{49}{2}\right) + 3n = \frac{2}{3}n^3 + n^2 - \frac{485}{12}n + \frac{277}{2},
\end{aligned}
\tag{11}
$$

and for $5 \le i \le n-2$,

$$
\begin{aligned}
D_R\left(G_n^{3,i}\right) &= D_R\left(G_{n-1}^3\right) + D_{v_i}\left(G_{n-1}^3\right) + 2Kf_{v_i}\left(G_{n-1}^3\right) + 3n \\
&= \left[\frac{2}{3}(n-1)^3 + (n-1)^2 - \frac{293}{12}(n-1) + \frac{117}{2}\right] \\
&\quad + 2\cdot 1 + 2\cdot 2 + \cdots \\
&\quad + 2\cdot(n-2-i) + (n-1-i) + 2\cdot\left[1 + 2\cdot 2 + \cdots + 2\cdot(i-5)\right. \\
&\quad + 3\cdot(i-4) + 2\cdot 3\cdot\left(i - 4 + \frac{5}{8}\right) + 2\cdot(i-3) + 2\cdot 1 + 2 + \cdots \\
&\quad \left. + (n-1-i) + 1 + 2 + \cdots + i - 3 + 2\cdot\left(i - 4 + \frac{5}{8}\right)\right] + 3n \\
&= \left[\frac{2}{3}(n-1)^3 + (n-1)^2 - \frac{293}{12}(n-1) + \frac{117}{2}\right] \\
&\quad + \left(n^2 - 2ni - 2n + 2i^2 + 4i - \frac{69}{4} + n^2 - 2ni - n + 2i^2 - \frac{15}{2}\right) + 3n \\
&= \frac{2}{3}n^3 + n^2 - \frac{293}{12}n - 4ni + 4i^2 + 4i + \frac{117}{2}.
\end{aligned}
\tag{12}
$$

Proposition 1. *Suppose $G \not\cong G_n^3$ is a bicyclic graph of order $n \ge 5$ and $v \in V(G)$, where G_n^3 is defined as in Lemma 9. Then, $Kf_v(G) \le n^2/2 - n/2 - 17/4$.*

Proof. It is not hard to verify that, for any bicyclic graph $G \not\cong G_5^3$ of order 5 and $v \in V(G)$, $Kf_v(G) \le 5^2/2 - 5/2 - 17/4$. Thus, we assume $n \ge 6$ in the following cases.

Case 1 ($d(v) = 1$): let w be the neighbor of v.

Suppose $G - v \cong G_{n-1}^3$, where G_{n-1}^3 is obtained from a 4-cycle $C_4 = v_1v_2v_3v_4v_1$ and a path $P = v_5 \ldots v_{n-1}$ by adding the edges v_1v_3 and v_4v_5. Then, $w \neq v_{n-1}$ since $G \not\cong G_n^3$. By Lemma 1,

$$\begin{aligned} Kf_v(G) &= Kf_w(G - v) + n - 1 \\ &\leq \max\left\{Kf_{v_{n-2}}\left(G_{n-1}^3\right), Kf_{v_2}\left(G_{n-1}^3\right)\right\} + n - 1 \\ &= \max\left\{\frac{n^2}{2} - \frac{5}{2}n + \frac{1}{4}, \frac{n^2}{2} - \frac{7}{2}n + \frac{29}{4}\right\} + n - 1 \\ &= \max\left\{\frac{n^2}{2} - \frac{3}{2}n - \frac{3}{4}, \frac{n^2}{2} - \frac{5}{2}n + \frac{25}{4}\right\} \\ &< \frac{n^2}{2} - \frac{n}{2} - \frac{17}{4}. \end{aligned} \tag{13}$$

If $G - v \not\cong G_{n-1}^3$, we shall prove it by induction on n. By the inductive hypothesis, $Kf_v(G) = Kf_w(G - v) + n - 1 \leq (n-1)^2/2 - (n-1)/2 - 17/4 + n - 1 = n^2/2 - n/2 - 17/4$.

Case 2: $d(v) \geq 2$.

By Lemma 2, $Kf_v(G) \leq n^2/2 - 3n/2 + 1/3 < n^2/2 - n/2 - 17/4$. □

Lemma 11 (see [23]). *Let G be a bicyclic graph of order n, v be a pendant vertex of G, and w be its neighbor. Then,* $D_v(G) = D_w(G - v) + 2n + 1$.

Proposition 2. *Let* $G \not\cong G_n^3$ *be a graph in* $\mathscr{B}_n^\theta$ *of order* $n \geq 5$ *and* $v \in V(G)$, *where* G_n^3 *is defined as in Lemma 9. Then,* $D_v(G) \leq n^2 + 2n - 20$.

Proof. It is easy to verify that for any graph $G \in \mathscr{B}_5^\theta$ with $G \not\cong G_5^3$ and $v \in V(G)$, $D_v(G) \leq 15 = 5^2 + 2 \cdot 5 - 20$. Thus, we assume $n \geq 6$ in the following cases.

Case 1 ($d_G(v) = 1$): let w be the neighbor of v.

Suppose $G - v \cong G_{n-1}^3$, where G_{n-1}^3 is obtained from a 4-cycle $C_4 = v_1v_2v_3v_4v_1$ and a path $P = v_5 \ldots v_{n-1}$ by adding the edges v_1v_3 and v_4v_5. Then, $w \neq v_{n-1}$ since $G \not\cong G_n^3$. Moreover, $D_v(G) = D_w(G_{n-1}^3) + 2n + 1$ by Lemma 11. By direct calculation, we get $D_{v_1}(G_{n-1}^3) = D_{v_3}(G_{n-1}^3) = n^2 - 35/4n + 91/4$, $D_{v_2}(G_{n-1}^3) = n^2 - 8n + 83/4$, $D_{v_4}(G_{n-1}^3) = n^2 - 10n + 123/4$, and

$$\begin{aligned} D_{v_i}\left(G_{n-1}^3\right) &= n^2 - 2n + 2i^2 + (4 - 2n)i - \frac{69}{4} \\ &\leq n^2 - 2n + 2(n-2)^2 + (4 - 2n)(n-2) - \frac{69}{4} \\ &= n^2 - 2n - \frac{69}{4}\left(= D_{v_{n-2}}\left(G_{n-1}^3\right)\right), \end{aligned} \tag{14}$$

if $5 \leq i \leq n - 2$. Thus, $D_w(G_{n-1}^3) \leq D_{v_{n-2}}(G_{n-1}^3)$ and $D_v(G) \leq D_{v_{n-2}}(G_{n-1}^3) + 2n + 1 = n^2 - 65/4 < n^2 + 2n - 20$.

If $G - v \not\cong G_{n-1}^3$, we prove it by induction on n. By the inductive hypothesis, $D_v(G) = D_w(G) + 2n + 1 \leq (n-1)^2 + 2(n-1) - 20 + 2n + 1 = n^2 + 2n - 20$.

Case 2: $d_G(v) \geq 2$.

Subcase 1: v is not contained by any cycle of G.

By the same argument as that of Case 2 of Lemma 2.6 in [23], we can construct a series of bicyclic graphs $G_1, G_2, \ldots, G_{k-1}$ in $\mathscr{B}_n^\theta$ such that $D_v(G) < D_v(G_1) < \cdots < D_v(G_{k-1})$ and v is a pendant vertex in G_{k-1}, where $k = d_G(v) \geq 2$.

Suppose $G_{k-1} \cong G_n^3$. Then, G_{k-1} is obtained from a 4-cycle $C_4 = v_1v_2v_3v_4v_1$ and a path $P = v_5 \cdots v_{n-1}v$ by adding the edges v_1v_3 and v_4v_5. By the transformation from G_{k-2} to G_{k-1}, we can conclude that $G_{k-2} = G_{k-1} - v_{n-2}v_{n-1} + v_{n-2}v$, i.e., $G_{k-2} \cong G_{k-1}$. Note that $D_v(G_{k-2}) = n^2 - 73/4$. We have $D_v(G) \leq D_v(G_{k-2}) < n^2 + 2n - 20$.

If $G_{k-1} \not\cong G_n^3$, then, by Case 1, $D_v(G) < D_v(G_{k-1}) \leq n^2 + 2n - 20$.

Subcase 2: v is in a cycle of G.

Let $\hat{G}$ be the kernel of G. By Claims 1 and 2 of Lemma 2.6 in [23], we can construct a graph G'' in $\mathscr{B}_n^\theta$ having $\hat{G}$ as its kernel and $D_v(G) \leq D_v(G'')$. Moreover, G'' is obtained from $\hat{G}$ by attaching a pendant path to the vertex u, where u is a vertex of $\hat{G}$ such that $R_G(u, v) = \max_{w \in V(\hat{G})} R_G(w, v)$.

Suppose G'' has only two vertices of degree three, say w_1 and w_2. Without loss of generality, we assume that $v \neq w_1$, and $v \neq w_2$. Then, by Lemma 2,

$$\begin{aligned} D_v(G'') &= 3\left(R_{G''}(w_1, v) + R_{G''}(w_2, v)\right) + \sum_{w \neq w_1, w_2} 2R_{G''}(w, v) \\ &= R_{G''}(w_1, v) + R_{G''}(w_2, v) + 2Kf_v(G'') \\ &< d_{G''}(w_1, v) + d_{G''}(w_2, v) + 2Kf_v(G'') \\ &\leq n + 2\left(\frac{n^2}{2} - \frac{3}{2}n + \frac{1}{3}\right) \\ &< n^2 + 2n - 20. \end{aligned} \tag{15}$$

Suppose G'' has exactly three vertices of degree three, say w_1, w_2, and w_3. Let w_4 be the pendant vertex of G''. Without loss of generality, we assume that $v \neq w_1, w_2, w_3$. Then, by Lemma 2,

$$\begin{aligned} D_v(G'') &= 3\left(R_{G''}(w_1, v) + R_{G''}(w_2, v) + R_{G''}(w_3, v)\right) + R_{G''}(w_4, v) \\ &\quad + \sum_{w \neq w_1, w_2, w_3, w_4} 2R_{G''}(w, v) \\ &< R_{G''}(w_1, v) + R_{G''}(w_2, v) + R_{G''}(w_3, v) + 2Kf_v(G'') \\ &< d_{G''}(w_1, v) + d_{G''}(w_2, v) + d_{G''}(w_3, v) + 2Kf_v(G'') \end{aligned}$$

$$\leq \frac{3(n-1)}{2} + 2\cdot\left(\frac{n^2}{2} - \frac{3}{2}n + \frac{1}{3}\right) \leq n^2 + 2n - 20. \tag{16}$$

Suppose G'' has a vertex of degree four, say w_1, and a vertex of degree three, say w_2. Let w_3 be the pendant vertex of G''. Without loss of generality, we assume that $v \neq w_1, w_2$. Then, by Lemma 2,

$$\begin{aligned} D_v(G'') &= 4R_{G''}(w_1, v) + 3R_{G''}(w_2, v) + R_{G''}(w_3, v) + \sum_{w \neq w_1,w_2,w_3} 2R_{G''}(w, v) \\ &< 2R_{G''}(w_1, v) + R_{G''}(w_2, v) + 2Kf_v(G'') \\ &< 2d_{G''}(w_1, v) + d_{G''}(w_2, v) + 2Kf_v(G'') \\ &\leq \frac{3(n-1)}{2} + 2\cdot\left(\frac{n^2}{2} - \frac{3}{2}n + \frac{1}{3}\right) \\ &\leq n^2 + 2n - 20, \end{aligned} \tag{17}$$

which completes the proof. □

Theorem 5. *Suppose G is a graph of order $n \geq 5$ in $\mathscr{B}_n^{\theta}\backslash\{G_n^3\}$. Then, $D_R(G) \leq 2/3n^3 + n^2 - 163/6n + 139/2$, with equality if and only if $G \cong G_n^5$, where G_n^3 and G_n^5 are defined as in Lemma 9.*

Proof. It is not hard to verify that, for any graph G in $\mathscr{B}_5^{\theta}\backslash\{G_5^3\}$, $D_R(G) \leq 42 = 2/3 \cdot 5^3 + 5^2 - 163/6 \cdot 5 + 139/2$, with equality if and only if $G \cong G_5^5$.

We assume that $n \geq 6$, and consider the following two cases.

Case 1: $\delta(G) = 1$.

Let v_n be a pendant vertex of G. Suppose $G - v_n \cong G_{n-1}^3$, where G_{n-1}^3 is obtained from a 4-cycle $C_4 = v_1v_2v_3v_4v_1$, and a path $P = v_5 \cdots v_{n-1}$ by adding the edges v_1v_3 and v_4v_5. Then, $G \cong G_n^{3,i}$, where $1 \leq i \leq n-2$, and $G_n^{3,i}$ is defined in the Lemmas 10. By Lemma 10,

$$\begin{aligned} D_R(G_n^{3,1}) &= D_R(G_n^{3,3}) = \frac{2}{3}n^3 + n^2 - \frac{455}{12}n + \frac{493}{4} < \frac{2}{3}n^3 + n^2 - \frac{163}{6}n + \frac{139}{2}, \\ D_R(G_n^{3,2}) &= \frac{2}{3}n^3 + n^2 - \frac{437}{12}n + \frac{237}{2} < \frac{2}{3}n^3 + n^2 - \frac{163}{6}n + \frac{139}{2}, \\ D_R(G_n^{3,4}) &= \frac{2}{3}n^3 + n^2 - \frac{485}{12}n + \frac{277}{2} < \frac{2}{3}n^3 + n^2 - \frac{163}{6}n + \frac{139}{2}, \\ D_R(G_n^{3,i}) &= \frac{2}{3}n^3 + n^2 - \frac{293}{12}n - 4ni + 4i^2 + 4i + \frac{117}{2} \\ &\leq \frac{2}{3}n^3 + n^2 - \frac{293}{12}n - 4n(n-2) + 4(n-2)^2 + 4(n-2) + \frac{117}{2} \\ &= \frac{2}{3}n^3 + n^2 - \frac{341}{12}n + \frac{133}{2} \\ &< \frac{2}{3}n^3 + n^2 - \frac{163}{6}n + \frac{139}{2}, \end{aligned} \tag{18}$$

for $5 \leq i \leq n-2$.

If $G - v_n \not\cong G_{n-1}^3$, we prove it by induction on n. Let w be the neighbor of v_n. By the inductive hypothesis, Lemma 8, and Propositions 1 and 2,

$$D_R(G) = D_R(G-v_n) + D_w(G-v_n) + 2Kf_w(G-v_n) + 3n$$
$$\leq \left[\frac{2}{3}(n-1)^3 + (n-1)^2 - \frac{163}{6}(n-1) + \frac{139}{2}\right] + (n-1)^2 + 2(n-1)$$
$$- 20 + 2\cdot\left(\frac{(n-1)^2}{2} - \frac{n-1}{2} - \frac{17}{4}\right) + 3n$$
$$= \frac{2}{3}n^3 + n^2 - \frac{163}{6}n + \frac{139}{2}. \quad (19)$$

The equality $D_R(G) = 2/3n^3 + n^2 - 163/6n + 139/2$ holds if and only if $D_R(G-v_n) = 2/3(n-1)^3 + (n-1)^2 - 163/6(n-1) + 139/2$, $D_w(G-v_n) = (n-1)^2 + 2(n-1) -20$, and $Kf_w(G-v_n) = (n-1)^2/2- (n-1)/2- 17/4 = n^2/2 - 3/2n - 13/4$. By the inductive hypothesis, $G - v_n \cong G^5_{n-1}$, where G^5_{n-1} is obtained from a 4-cycle $C_4 = v_1v_2v_3v_4v_1$ and a path $P = v_5 \ldots v_{n-1}$ by adding the edges v_2v_4 and v_4v_5. We show that $w = v_{n-1}$, i.e., $G \cong G^5_n$.

By direct calculation, we have $Kf_{v_{n-1}}(G^5_{n-1}) = n^2/2 - 3/2n - 13/4$, $Kf_{v_2}(G^5_{n-1}) = n^2/2 - 4n + 37/4 < n^2/2 - 3/2n - 13/4$, and $Kf_{v_1}(G^5_{n-1}) = Kf_{v_3}(G^5_{n-1}) = n^2/2 - 31/8n + 73/8 < n^2/2 -3/2n - 13/4$. Obviously, $Kf_v(G^5_{n-1}) < Kf_{v_{n-1}}(G^5_{n-1})$ if $v \in V(G^5_{n-1}) \setminus \{v_1, v_2, v_3, v_{n-1}\}$. Therefore, $w = v_{n-1}$, i.e., $G \cong G^5_n$.

Case 2: $\delta(G) \geq 2$.

By a similar argument to that of Case 2 in Theorem 3, we obtain

$$D_R(G) \leq \frac{1}{2}n^3 + n^2 - 3n + \frac{2}{3}. \quad (20)$$

If $n \geq 11$, then $1/2n^3 + n^2 - 3n + 2/3 < 2/3n^3 + n^2 - 163/6n + 139/2$. For any graph of the form $B(P_k, P_l, P_m)$ when $n = 6, 7, 8, 9, 10$, we have calculated $D_R(G)$ and found that $D_R(G) \leq 2/3n^3 + n^2 - 163/6n + 139/2$.

From Theorems 2 and 4, we obtain the following result. □

Theorem 6. *Let G^1_n and G^5_n be defined as in Lemma 9. Then, among all bicyclic graphs of order n,*

(i) If $6 \leq n \leq 16$, the graph G^5_n is the unique graph with the third-maximum degree resistance distance of value $2/3n^3 + n^2 - 163/6n + 139/2$

(ii) If $n \geq 17$, the graph G^1_n is the unique graph with the third-maximum degree resistance distance of value $2/3n^3 + n^2 - 79/3n + 56$

5. Conclusion

As a molecular structure descriptor, the Wiener index is one of the widely employed topological indices, as it is well correlated with many physical and chemical properties of a variety of classes of chemical compounds. A weighted version of the Wiener index is the degree resistance distance. In this paper, we characterize the graphs with the second-maximum and third-maximum degree resistance distance among all bicyclic graphs with fixed order. Furthermore, we present an open problem.

Problem 1. Characterize the tricyclic graphs of order n with the maximum and second-maximum degree resistance distance.

Data Availability

All the proofs and exemplary data of this study are included within the article.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Acknowledgments

The research of the first author was supported by National Natural Science Foundation of China (no. 11801568).

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