

Maximal Degree Resistance Distance of Unicyclic Graphs

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Abstract

The resistance distance $r(u, v)$ between two vertices u, v of a connected graph G is defined as the effective resistance between them in the corresponding electrical network constructed from G by replacing each edge of G with a unit resistor. Let G be a connected graph, the degree resistance distance of G is defined as $D_R(G) = \sum_{\{u,v\} \subseteq V(G)} [d(u) + d(v)]r(u, v)$, where $d(u)$ is the degree of the vertex u . In this paper, we firstly characterize n -vertex unicyclic graphs with given girth having maximum and second maximum degree resistance distance, then give n -vertex unicyclic graphs with the maximum and second maximum degree resistance distance.

1 Introduction

All graphs considered here are both connected and simple if not stated in particular. The distance between vertices u and v of graph G , denoted by $d(u, v) = d(u, v|G)$, is the length of a shortest path between them. The degree of the vertex u is $d(u)$ (or $d_G(u)$), if the underlying graph needs to be specified, then we shall write the degree as $d(u|G)$. n, m are the number of vertices and edges of G . The famous Wiener index was introduced by Harold Wiener in 1947, defined as [1]

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u, v) \quad (1)$$

The concept of resistance distance was introduced by Klein and Randić [2] in 1993, on the basis of electrical network theory. They viewed a graph G as an electrical network N such that each edge of G is assumed to be a unit resistor. The resistance distance between

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the vertices u and v of a graph G , denoted by $r(u, v) = r(u, v|G)$, is defined to be the effective resistance between nodes $u, v \in N$. Analogous to the definition of the Wiener index, the Kirchhoff index $Kf(G)$ of a graph G is defined as [2,3]

$$Kf(G) = \sum_{\{u,v\} \subseteq V(G)} r(u, v) \tag{2}$$

If G is a tree, then $r(u, v) = d(u, v)$ for any two vertices u and v , the Kirchhoff and Wiener indices of trees coincide.

The Kirchhoff index is an important molecular structure descriptor [4], it has been well studied in both mathematical and chemical literatures. For a general graph G , I. Lukovits et al. [5] showed that $Kf(G) \geq n - 1$ with equality if and only if G is complete graph K_n , and P_n has maximal Kirchhoff index. Palacios [6] showed that $Kf(G) \leq \frac{1}{6}(n^3 - n)$ with equality if and only if G is a path. For a circulant graph G , Ref. [7] showed that

$$n - 1 \leq Kf(G) \leq \frac{1}{12}(n^3 - n),$$

the first equality holds if and only if G is K_n and the second does if and only if G is C_n . For more information on the Kirchhoff index, see the recent surveys [8–12].

A modified version of the Wiener index is the degree distance, was introduced by A. A. Dobrynin and A. A. Kochetova [13], defined as

$$D(G) = \sum_{\{u,v\} \subseteq V(G)} [d(u) + d(v)]d(u, v) \tag{3}$$

If G is a tree on n vertices, then the Wiener index and the degree distance are related as $D(G) = 4W(G) - n(n - 1)$ (for details see [13]).

The degree resistance distance was introduced by I. Gutman, L. Feng and G. Yu in [14]:

$$D_R(G) = \sum_{\{u,v\} \subseteq V(G)} [d(u) + d(v)]r(u, v) \tag{4}$$

They investigated the degree resistance distance of unicyclic graphs, determined the unicyclic graphs with minimum and second minimum D_R -value. J. L. Palacios in [15] renamed degree resistance distance as *additive degree-Kirchhoff index* and gave tight upper and lower bounds for the degree resistance distance of a connected undirected graph by using Markov chain theory.

If G is a tree, then $r(u, v) = d(u, v)$ for any two vertices u and v . Consequently, the degree distances and degree resistance distances coincide as well, i.e.,

$$D_R(G) = 4W(G) - n(n - 1). \tag{5}$$

In this paper, we concentrate still on unicyclic graphs. A graph G is called a unicyclic graph if it contains exactly one cycle. Let $G = U(C_l; T_1, T_2, \dots, T_l)$ be the unicyclic graph with $C_l = v_1 v_2 \dots v_l v_1$ as the unique cycle in G , and for each $i (1 \leq i \leq l)$, let T_i be the component of $G - (V(C_l) - v_i)$. Obviously, T_i is a tree.

For convenience, let $\mathcal{U}(n, l)$ be the set of all unicyclic graphs on n vertices containing cycle C_l , S_n^l denotes the graph obtained from cycle C_l by adding $n - l$ pendant edges to one vertex of C_l , P_n^l denotes the graph obtained by identifying one end-vertex of P_{n-l+1} with any vertex of C_l , $\mathcal{W}(n)$ be the unicyclic graph with n vertices. Let P_{k-1} be the path with the vertices v_1, v_2, \dots, v_{k-1} , the graph $T(k, i, 1)$ is construct from P_{k-1} by adding one pendant edge to the vertex $v_i (2 \leq i \leq k - 2)$, the unicyclic graph $U(C_l; T(k, i, 1)) (l \geq 3, 2 \leq i \leq k - 2, k + l = n + 1)$ is the graph obtained from cycle C_l by joining v_1 of $T(k, i, 1)$ to a vertex of C_l , see Figure 1(2).

The paper is organized as follows. In Section 2 we state some preparatory results, whereas in Section 3 we investigated the degree resistance distance of $\mathcal{U}(n, l)$, and give the maximum and second maximum degree resistance distance of $\mathcal{U}(n, l)$. In Section 4, we give the maximum and second maximum degree resistance distance of $\mathcal{W}(n)$.

2 Preliminary Results

For a graph G with $v \in V(G)$, $G - v$ denotes the graph obtained from G by deleting v (and its incident edges). For an edge uv of the graph G (the complement of G , respectively), $G - uv (G + uv, respectively)$ denotes the graph resulting from G by deleting (adding, respectively) the edge uv .

Let H be a subgraph of graph G , for a vertex $u \in V(H)$, let

$$r(u|H) = \sum_{v \in V(H)} r(v, u|H), \quad S'(u|H) = \sum_{v \in V(H)} d_H(v)r(v, u|H)$$

Let C_n be the cycle on $n \geq 3$ vertices, for any two vertices $v_i, v_j \in V(C_n)$ with $i < j$, by Ohm's law, we have

$$r_{C_n}(v_i, v_j) = \frac{(j - i)(n + i - j)}{n}$$

For any vertex $u \in V(C_n)$, we are readily to have $r(u|C_n) = \frac{n^2 - 1}{6}$, $S'(u|C_n) = \frac{n^2 - 1}{3}$.

Lemma 2.1([16]). Let T be any n vertices trees different from path P_n and S_n . Then

$$(n - 1)^2 \leq W(T) \leq \frac{1}{6}(n^3 - n), \tag{6}$$

the left equality holds if and only if $G \cong S_n$ and the right holds if and only if $G \cong P_n$.

Lemma 2.2[2]. Let x be a cut vertex of a connected graph and a and b be vertices occurring in different components which arise upon deletion of x , then $r_G(a, b) = r_G(a, x) + r_G(x, b)$.

Lemma 2.3[14]. Let G_1 and G_2 be connected graphs with disjoint vertex sets, with n_1 and n_2 vertices, and with m_1 and m_2 edges, respectively. Let $u_1 \in V(G_1)$; $u_2 \in V(G_2)$. Constructing the graph G by identifying the vertices u_1 and u_2 , and denote the so obtained vertex by u . Then

$$D_R(G) = D_R(G_1) + D_R(G_2) + 2m_2r(u_1|G_1) + 2m_1r(u_2|G_2) + (n_2 - 1)S'(u_1|G_1) \\ + (n_1 - 1)S'(u_2|G_2)$$

Let v be a vertex of degree $p + 1$ in a graph G , such that vv_1, vv_2, \dots, vv_p are pendant edges incident with v , and u is the neighbor of v distinct from v_1, v_2, \dots, v_p , and $G' = \sigma(G, v)$ by removing the edges vv_1, vv_2, \dots, vv_p and adding new edges uv_1, uv_2, \dots, uv_p . From the reference [14], one has

Lemma 2.4[14]. Let $G' = \sigma(G, v)$ be a graph transformed from the graph G , $d(u) \geq 1$ described above. Then $D_R(G) \geq D_R(G')$, with equality holds if and only if G is a star with v as its center.

Lemma 2.5. Let G_0 be a connected graphs with $m_0 > 1$ edges, and $u, v \in V(G_0)$ be two distinct vertices with degree at least 3 in G_0 such that $r(u, v) = l$. Let $P_s = u_1u_2 \dots u_s$ and $P_t = v_1v_2 \dots v_t$ be two paths of order $s \geq 1$ and $t \geq 1$, respectively. Let $G_{s,t}$ be the graph obtained from G_0 , P_s and P_t by adding edges uu_1, vv_1 . Suppose that $G_{s-1,t+1} = G_{s,t} - u_r u_{r-1} + v_t u_r$ and $G_{s+1,t-1} = G_{s,t} - v_{t-1} v_t + u_s v_t$. Then either $D_R(G_{s,t}) < D_R(G_{s-1,t+1})$ or $D_R(G_{s,t}) < D_R(G_{s+1,t-1})$.

Proof. Let H be the graph induced by $V(G_0) \cup V(P_t)$. By Lemma 2.3, one has

$$D_R(G_{s,t}) = D_R(H) + D_R(P_{s+1}) + 2(m_0 + t)r(u|P_{s+1}) + 2sr(u|H) \\ + (n_0 + t - 1)S'(u|P_{s+1}) + sS'(u|H)$$

On one hand,

$$D_R(H) = D_R(G_0) + D_R(P_{t+1}) + 2tr(v|G_0) + 2m_0r(v|P_{t+1}) + tS'(v|G_0) \\ + (n_0 - 1)S'(v|P_{t+1}) \\ = D_R(G_0) + 2tr(v|G_0) + tS'(v|G_0) + m_0t(t + 1) + D_R(P_{t+1}) + (n_0 - 1)t^2 \\ + \frac{2}{3}t^3 + t^2 + \frac{1}{3}t$$

Further, from equation (5), one arrives at

$$D_R(P_{s+1}) = 4W(P_{s+1}) - s(s+1) = \frac{2}{3}s^3 + s^2 + \frac{1}{3}s,$$

and analogously, $D_R(P_{t+1}) = \frac{2}{3}t^3 + t^2 + \frac{1}{3}t$.

On the other hand,

$$r(u|H) = \sum_{z \in V(G_0)} r(z, u) + \sum_{z \in V(H-G_0)} r(z, u) = r(u|G_0) + lt + \frac{1}{2}t(t+1),$$

$$r(u|P_{s+1}) = \frac{1}{2}s(s+1), \quad S'(u|P_{s+1}) = \sum_{z \in V(P_{s+1})} d_H(z)r(z, u) = s^2,$$

and analogously,

$$\begin{aligned} S'(u|H) &= \sum_{z \in V(H)} d_H(z)r(z, u) \\ &= \sum_{z \in V(G_0)} d_{G_0}(z)r(z, u) + 2l + t + 2 \sum_{i=1}^{t-1} (2+i) \\ &= S'(u|G_0) + 2lt + t^2 \end{aligned}$$

Finally,

$$\begin{aligned} D_R(G_{s,t}) &= D_R(G_0) + 2sr(u|G_0) + 2tr(v|G_0) + sS'(u|G_0) + tS'(v|G_0) \\ &\quad + m_0[s(s+1) + t(t+1)] + (n_0 - 1)(s^2 + t^2) + \frac{2}{3}(s^3 + t^3) \\ &\quad + 2st(s+t) + (s+t)^2 + \frac{1}{3}(s+t) + 4lst \end{aligned}$$

Similarly,

$$\begin{aligned} D_R(G_{s-1,t+1}) &= D_R(G_0) + 2(s-1)r(u|G_0) + 2(t+1)r(v|G_0) + (s-1)S'(u|G_0) \\ &\quad + (t+1)S'(v|G_0) + m_0[s(s-1) + (t+1)(t+2)] + (n_0 - 1)[(s-1)^2 \\ &\quad + (t+1)^2] + \frac{2}{3}[(s-1)^3 + (t+1)^3] + 2(s-1)(t+1)(s+t) \\ &\quad + (s+t)^2 + \frac{1}{3}(s+t) + 4l(s-1)(t+1) \end{aligned}$$

and

$$\begin{aligned} D_R(G_{s+1,t-1}) &= D_R(G_0) + 2(s+1)r(u|G_0) + 2(t-1)r(v|G_0) + (s+1)S'(u|G_0) \\ &\quad + (t-1)S'(v|G_0) + m_0[(s+1)(s+2) + t(t-1)] + (n_0 - 1)[(s+1)^2 \\ &\quad + (t-1)^2] + \frac{2}{3}[(s+1)^3 + (t-1)^3] + 2(s+1)(t-1)(s+t) \\ &\quad + (s+t)^2 + \frac{1}{3}(s+t) + 4l(s+1)(t-1) \end{aligned}$$

So we get

$$\begin{aligned} & D_R(G_{s-1,t+1}) - D_R(G_{s,t}) \\ &= 2[r(v|G_0) - r(u|G_0)] + S'(v|G_0) - S'(u|G_0) + 2(m_0 + n_0 - 1 - 2l)(-s + t + 1) \end{aligned}$$

By a similar reasoning, one has

$$\begin{aligned} & D_R(G_{s+1,t-1}) - D_R(G_{s,t}) \\ &= 2[r(u|G_0) - r(v|G_0)] + S'(u|G_0) - S'(v|G_0) + 2(m_0 + n_0 - 1 - 2l)(s - t + 1) \end{aligned}$$

Hence, if $D_R(G_{s-1,t+1}) - D_R(G_{s,t}) < 0$, then

$$2[r(v|G_0) - r(u|G_0)] + S'(v|G_0) - S'(u|G_0) + 2(m_0 + n_0 - 1 - 2l)(-s + t + 1) < 0,$$

i.e.,

$$2[r(u|G_0) - r(v|G_0)] + S'(u|G_0) - S'(v|G_0) > 2(m_0 + n_0 - 1 - 2l)(-s + t + 1).$$

Therefore,

$$\begin{aligned} & D_R(G_{s+1,t-1}) - D_R(G_{s,t}) \\ &> 2(m_0 + n_0 - 1 - 2l)(-s + t + 1) + 2(m_0 + n_0 - 1 - 2l)(s - t + 1) \\ &= 4(m_0 + n_0 - 1 - 2l) > 0. \end{aligned}$$

This completes the proof.

3 The maximum and second maximum degree resistance distance of $\mathcal{U}(n, l)$

Firstly, we shall investigate unicyclic graph in $\mathcal{U}(n, l)$ with the maximum degree resistance distance.

Theorem 3.1. Let G be a unicyclic graph of order n and girth l . Then $D_R(G) \leq D_R(P_n^l)$, with equality holds if and only if $G \cong P_n^l$.

Proof. Suppose that $G_0 = U(C_l; T_1, T_2, \dots, T_l)$ has maximal degree resistance distance among $\mathcal{U}(n, l)$.

Claim 1. For each i , T_i is a path with v_i as one of its end vertices.

For each i , $D_R(T_i)$ is maximal if and only if T_i is a path by Lemma 2.4, Hence Claim 1 holds.

Claim 2. If $l < n$, all but one of the T_i are trivial.

Suppose that there are two trees T_i and T_j such that they both have more than one vertices. By Claim 1, T_i and T_j are both paths. Suppose that $T_i = v_i u_1 u_2 \cdots u_k$, $T_j = v_j w_1 w_2 \cdots w_m$. Let $G' = G_0 - u_{k-1} u_k + w_m u_k$ or $G' = G_0 - w_{m-1} w_m + u_k w_m$, then $D_R(G') > D_R(G_0)$, this contradicts to the choice of G_0 , which implies Claim 2.

Claim 1 and Claim 2 yield to Theorem.

From Theorem 3.1, the degree resistance distance of P_n^l is computed as follows:

$$\begin{aligned} & D_R(P_n^l) \\ &= D_R(C_l) + 2(n-l)r(v|C_l) + (n-l)S'(v|C_l) + l(n-l)(n-l+1) + (l-1)(n-l)^2 \\ & \quad + \frac{2}{3}(n-l)^3 + (n-l)^2 + \frac{1}{3}(n-l) \\ &= l^3 - \frac{1}{3}(4n+3)l^2 + nl + \frac{2}{3}n^3 - \frac{1}{3}n \end{aligned}$$

Combining above results and Theorem 3.1, one arrives at,

Theorem 3.2. Let $G \in \mathcal{U}(n, l)$, then

$$D_R(G) \leq l^3 - \frac{1}{3}(4n+3)l^2 + nl + \frac{2}{3}n^3 - \frac{1}{3}n, \quad (7)$$

the equality holds if and only if $G \cong P_n^l$.

Secondly, we shall investigate unicyclic graph in $\mathcal{U}(n, l)$ with the second maximum degree resistance distance.

Theorem 3.3. Let $G \in \mathcal{U}(n, l)$, $3 \leq l \leq n-3$ and $G \not\cong P_n^l$, then

$$D_R(G) \leq l^3 - \frac{1}{3}(4n+3)l^2 + nl + \frac{2}{3}n^3 - \frac{13}{3}n + 10, \quad (8)$$

the equality holds if and only if $G \cong U(C_l; T(n-l+1, n-l-1, 1))$.

Proof. Suppose that $G = U(C_l; T_1, T_2, \dots, T_l)$ has the second maximum degree resistance distance among $\mathcal{U}(n, l)$.

Firstly, at most two of T_1, T_2, \dots, T_l are not trivial.

Otherwise, without loss of generality, we assume that T_1, T_2, T_3 are not trivial. They must be paths by Lemmas 2.4.

Let $T_1 = v_1 a_1 a_2 \cdots a_r$, $T_2 = v_2 b_1 b_2 \cdots b_s$, $T_3 = v_3 c_1 c_2 \cdots c_t$. Then

$D_R(G) < D_R(G - a_{r-1} a_r + b_s a_r)$ or $D_R(G) < D_R(G - a_{r-1} a_r + c_t a_r)$ by Lemma 2.5.

This contradicts to the choice of G .

Nextly, if exactly two of T_1, T_2, \dots, T_l are not trivial, then they are paths from Lemmas 2.4. Without loss of generality, we assume that $T_1 = v_1 a_2 \cdots a_r$ and $T_i = v_i b_2 \cdots b_s$

($1 < i \leq l$), where $r + s + l = n + 2$, $r \geq 2$ and $s \geq 2$, are not trivial. By Lemma 2.5, one has

$$D_R(G) < D_R(G - a_{r-1}a_r + b_s a_r), \text{ or } D_R(G) < D_R(G - b_{s-1}b_s + a_r b_s).$$

Repeating above steps, one arrives at $r = 2$ or $s = 2$ at last.

Without loss of generality, we assume that $s = 2$, i.e., $G = H_i(2 \leq i \leq l)$ is the graph shown in Figure 1(1).

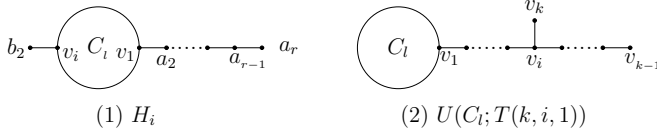


Figure 1.

It is easy to calculate out the degree resistance distance by Lemma 2.3 as follows:

$$\begin{aligned} & D_R(H_i) \\ &= \frac{1}{3}(2k^3 + l^3 + 6k^2l + 2kl^2 - 9kl + 5k + 11l - 6) + \frac{4}{l}(k-1)[-i^2 + (2+l)i - l - 1] \\ &= l^3 - \frac{1}{3}(4n-9)l^2 - (3n-2)l + \frac{4}{l}(n-l-1)[-i^2 + (2+l)i - l - 1] \\ &+ \frac{1}{3}(2n^3 + 5n - 6) \end{aligned}$$

and

$$D_R(H_i) \leq \begin{cases} l^3 - \frac{1}{3}(4n-6)l^2 - (2n-1)l + \frac{1}{3}(2n^3 + 5n - 6), & \text{if } l \text{ is even;} \\ l^3 - \frac{1}{3}(4n-6)l^2 - (2n-1)l + \frac{1}{3}(2n^3 + 5n - 3) - \frac{n-1}{l}, & \text{if } l \text{ is odd.} \end{cases}$$

with the equality if and only if $i = \frac{l}{2} + 1$ for l is even, or $i = \frac{l+1}{2} + 1$ for l is odd.

If exactly one of T_1, T_2, \dots, T_l is not trivial, without loss of generality, we assume that T_1 is not trivial. Since $G \not\cong P_n^l$, then $T_1 \neq P_{n-l+1}$. From Lemma 2.4, we know that G is the graph shown in Figure 1(2).

Let $G = U(C_l; T(k, i, 1))$ ($l \geq 3, 2 \leq i \leq k-2, k+l = n+1$) be the graph depicted in Figure 1(2). $G_1 = C_l, G_2 = T(k, i, 1)$, then G_1 and G_2 sharing the common vertex v_1 . It is noted that $V(G_1) = E(G_1) = l, V(G_2) = k, E(G_2) = k-1$;

$$r(v_1|G_1) = \frac{l^2 - 1}{6}, \quad r(v_1|G_2) = \frac{1}{2}(k-2)(k-1) + i;$$

$$S'(v_1|G_1) = \frac{l^2 - 1}{3}, \quad S'(v_1|G_2) = 2 \sum_{i=1}^{k-3} (k-2) + 2i - 1 = k^2 - 4k + 3 + 2i.$$

$$D_R(G_1) = \frac{1}{3}(l^3 - l), \quad D_R(G_2) = \frac{2}{3}k^3 - k^2 + \frac{13}{3}k + 4i^2 - 4ki - 4.$$

Thus,

$$\begin{aligned} D_R(G) &= D_R(G_1) + D_R(G_2) + 2(k-1)r(v_1|G_1) + 2lr(v_1|G_2) \\ &\quad + (k-1)S'(v_1|G_1) + (l-1)S'(v_1|G_2) \\ &= \frac{1}{3}(l^3 - l) + \frac{2}{3}k^3 - k^2 + \frac{13}{3}k + 4i^2 - 4ki - 4 + 2(k-1) \cdot \frac{l^2 - 1}{6} \\ &\quad + 2l \cdot \left[\frac{1}{2}(k-2)(k-1) + i \right] + (k-1) \cdot \frac{l^2 - 1}{3} + (l-1) \cdot (k^2 - 4k + 3 + 2i) \end{aligned}$$

Bearing in the mind that $k = n + 1 - l$, then

$$D_R(G) = 4i^2 - 2(2n + 3 - 4l)i + \frac{1}{3}(3l^3 - 4nl^2 + 9l^2 - 9nl - 18l + 2n^3 + 17n).$$

In the following, we shall investigate graphs in $U(C_l; T(k, i, 1))$ with the maximum degree resistance distance.

Let $f(x) = 4x^2 - 2(2n + 3 - 4k)x + \frac{1}{3}(3l^3 - 4nl^2 + 9l^2 - 9nl - 18l + 2n^3 + 17n)$, $2 \leq x \leq n - l - 1$. Then

(1) when $\frac{n}{2} - l + \frac{3}{4} \leq 2$, i.e., $l \leq n \leq 2l + 3$.

$f(x)$ is increasing in $[2, n - l - 1]$, thus,

$$f(x) \leq l^3 - \frac{4n+3}{3}l^2 + nl + \frac{2}{3}n^3 - \frac{13}{3}n + 10,$$

the equality holds if and only if $G \cong U(C_l; T(n - l + 1, n - l - 1, 1))$.

(2) when $n \geq 2l + 3$.

$f(x)$ is decreasing in $[2, \frac{n}{2} - l + \frac{3}{4}]$ and increasing in $[\frac{n}{2} - l + \frac{3}{4}, n - l - 1]$. Then

$$D_R(G) \leq l^3 - \frac{4n+3}{3}l^2 + nl + \frac{2}{3}n^3 - \frac{13}{3}n + 10,$$

the equality holds if and only if $G \cong U(C_l; T(n - l + 1, n - l - 1, 1))$.

Finally, we need to compare degree resistance distance between $H_{\frac{l}{2}+1}(H_{\frac{l}{2}+1})$ and $U(C_l; T(n - l + 1, n - l - 1, 1))$.

(1) If $l \geq 4$ is even, then

$$\begin{aligned} &D_R(U(C_l; T(n - l + 1, n - l - 1, 1))) - D_R(H_{\frac{l}{2}+1}) \\ &= -3l^2 + (3n - 1)l - 6n + 12 \\ &= n(3l - 6) - 3l^2 - l + 12 \\ &\geq (l + 3)(3l - 6) - 3l^2 - l + 12 \quad (\text{since } n \geq l + 3) \\ &= 2l - 6 > 0 \end{aligned}$$

(2) If $l \geq 3$ is odd, then

$$\begin{aligned} & D_R(U(C_l; T(n-l+1, n-l-1, 1))) - D_R(H_{\frac{l+1}{2}+1}) \\ &= -3l^2 + (3n-1)l - 6n + 11 + \frac{n-1}{l} \\ &= n(3l + \frac{1}{l} - 6) - 3l^2 - l - \frac{1}{l} + 11 \\ &\geq (l+3)(3l + \frac{1}{l} - 6) - 3l^2 - l - \frac{1}{l} + 11 \quad (\text{since } n \geq l+3) \\ &= 2l + \frac{2}{l} - 6 > 0 \end{aligned}$$

This completes the proof.

4 The maximum and second maximum degree resistance distance of $\mathcal{U}(n)$

Theorem 4.1. $\max_{3 \leq l \leq n} \{D_R(P_n^l)\} = D_R(P_n^3)$.

Proof. Let $f(l) := D_R(P_n^l) = l^3 - \frac{1}{3}(4n+3)l^2 + nl + \frac{2}{3}n^3 - \frac{1}{3}n$.

In what follows, we will find the maximum value of $f(l)$ on $I := [3, 4, \dots, n]$.

The first derivative of $f(l)$ is

$$\frac{\partial f(l)}{\partial l} = 3l^2 - \frac{2}{3}(4n+3)l + n.$$

The roots of $\frac{\partial f(l)}{\partial l} = 0$ are $l_{1,2} = \frac{(4n+3) \mp \sqrt{16n^2 - 3n + 9}}{9}$.

It is easy to see that for $n \geq 3$,

$$l_1 < \frac{4n+3 - (4n-24)}{9} = 3, \quad l_2 > \frac{4n+3 + (24-4n)}{9} = 3.$$

In the following, we will show that $f(3)$ is the maximum value of $f(l)$ on I .

For $n \geq 3$, it's easy to verify that $l_2 \leq n$. Then, one has

(i) when $l \in [3, l_2)$, $\frac{\partial f(l)}{\partial l} < 0$, which indicates that $f(l)$ is decreasing on $[3, l_2)$;

(ii) when $l \in [l_2, n]$, $\frac{\partial f(l)}{\partial l} > 0$, which indicates that $f(l)$ is increasing on $[l_2, n]$.

So, the maximum value of $D_R(P_n^l)$ must occurred between $f(3)$ and $f(n)$.

It's suffice to see that $f(3) - f(n) = \frac{1}{3}(n^3 - 27n + 54)$.

Let $g(x) = \frac{1}{3}(x^3 - 27x + 54)$ ($x \geq 3$), then $\frac{\partial g(x)}{\partial x} = x^2 - 9 \geq 0$, $g(x)$ is increasing when $x \geq 3$.

Since $g(3) = 0$, then $g(x) \geq 0$ for $n \geq 3$, i.e., $f(3) \geq f(n)$ for $n \geq 3$.

This completes the proof.

Theorem 4.2. Let $G \in \mathcal{U}(n)$ be an arbitrary unicyclic graph, then

$$D_R(G) \leq \frac{2n^3}{3} - \frac{28n}{3} + 18,$$

with the equality holds if and only if $G \cong P_n^3$.

Analogously, one arrives at

Theorem 4.3. $\max_{3 \leq l \leq n-3} \{D_R(U(C_l; T(n-l+1, n-l-1, 1)))\} = D_R(U(C_3; T(n-2, n-4, 1)))$.

Corollary 4.4. Let $G \in U(C_l; T(n-l+1, n-l-1, 1))$, $3 \leq l \leq n-3$. Then

$$D_R(G) \leq \frac{2n^3}{3} - \frac{40n}{3} + 28,$$

with the equality holds if and only if $G \cong U(C_3; T(n-2, n-4, 1))$.

Theorem 4.5. Let $G \in \mathcal{U}(n)$ ($n \geq 6$), be an arbitrary unicyclic graph, $G \not\cong P_n^3$. Then

$$D_R(G) \leq \frac{2n^3}{3} - \frac{40n}{3} + 28,$$

with the equality holds if and only if $G \cong U(C_3; T(n-2, n-4, 1))$.

Proof. Firstly, we shall find graphs in $P_n^l \setminus P_n^3$ with the maximum degree resistance distance.

Similar to the proof of Theorem 4.1, $\max_{4 \leq l \leq n} \{D_R(P_n^l)\} = \{D_R(P_n^4), D_R(P_n^n)\}$.

By Theorem 3.2, we have

$$D_R(P_n^4) = \frac{2}{3}n^3 - \frac{53}{3}n + 48, \quad D_R(P_n^n) = \frac{1}{3}n^3 - \frac{1}{3}n.$$

It is easy to verify that $D_R(P_n^4) > D_R(P_n^n)$.

Secondly, we compare $D_R(P_n^4)$ with $D_R(U(C_3; T(n-2, n-4, 1)))$.

$$\begin{aligned} & D_R(U(C_3; T(n-2, n-4, 1))) - D_R(P_n^4) \\ &= \frac{2n^3}{3} - \frac{40n}{3} + 28 - \left(\frac{2}{3}n^3 - \frac{53}{3}n + 48\right) \\ &= \frac{13}{3}n - 20 > 0. \end{aligned}$$

The proof is completed.

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References

- [1] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20.
- [2] D. J. Klein, M. Randić, Resistance distance, *J. Math. Chem.* **12** (1993) 81–95.
- [3] D. Bonchev, A. T. Balaban, X. Liu, D. J. Klein, Molecular cyclicity and centrality of polycyclic graphs. Cyclicity based on resistance distances or reciprocal distances, *Int. J. Quantum Chem.* **50** (1994) 1–20.
- [4] J. L. Palacios, Foster's formulas via probability and the Kirchhoff index, *Meth. Comput. Appl. Prob.* **6** (2004) 381–387.
- [5] I. Lukovits, S. Nikolić, N. Trinajstić, Resistance distance in regular graphs, *Int. J. Quantum Chem.* **71** (1999) 217–225.
- [6] J. L. Palacios, Resistance distance in graphs and random walks, *Int. J. Quantum Chem.* **81** (2001) 29–33.
- [7] H. P. Zhang, Y. J. Yang, Resistance distance and Kirchhoff index in circulant graphs, *Int. J. Quantum Chem.* **107** (2007) 330–339.
- [8] W. Zhang, H. Deng, The second maximal and minimal Kirchhoff indices of unicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **61** (2009) 683–695.
- [9] H. P. Zhang, X. Jiang, Y. J. Yang, Bicyclic graphs with extremal Kirchhoff index, *MATCH Commun. Math. Comput. Chem.* **61** (2009) 697–712.
- [10] Q. Guo, H. Deng, D. Chen, The extremal Kirchhoff index of a class of unicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **61** (2009) 713–722.
- [11] H. Deng, On the minimum Kirchhoff index of graphs with a given number of cut-edges, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 171–180.
- [12] R. Li, Lower bounds for the Kirchhoff index, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 163–174.
- [13] A. A. Dobrynin, A. A. Kochetova, Degree distance of a graph: A degree analogue of the Wiener index, *J. Chem. Inf. Comput. Sci.* **34** (1994) 1082–1086.
- [14] I. Gutman, L. Feng, G. Yu, Degree resistance distance of unicyclic graphs, *Trans. Comb.* **1** (2012) 27–40.
- [15] J. L. Palacios, Upper and lower bounds for the additive degree Kirchhoff index, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 651–655.
- [16] A. A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: Theory and applications, *Acta Appl. Math.* **66** (2001) 211–249.