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Extremal Properties of Kirchhoff Index and Degree Resistance Distance of Unicyclic Graphs

Xuli Qi[a,b], Zhibin Du[c,d,*], Xutao Zhang[e]

[a] *School of Mathematics and Statistics, Central China Normal University, Wuhan 430079, P. R. China*
[b] *Department of Mathematics and Statistics, Georgia State University, Atlanta, GA 30303, USA*
qixuli-1212@163.com

[c] *School of Software, South China Normal University, Foshan, Guangdong 528225, P. R. China*
[d] *School of Mathematics and Statistics, Zhaoqing University, Zhaoqing, Guangdong 526061, P. R. China*
zhibindu@126.com

[e] *Hebei University of Science and Technology, Shijiazhuang, Hebei 050018, P. R. China*
xutao_zhang@yeah.net

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Abstract

Let G be a connected graph with vertex set $V(G)$. The Kirchhoff index of G is defined as $Kf(G) = \sum_{\{u,v\}\subseteq V(G)} R(u,v|G)$, and the degree resistance distance of G is defined as $D_R(G) = \sum_{\{u,v\}\subseteq V(G)}[d(u|G)+d(v|G)]R(u,v|G)$, where $R(u,v|G)$ denotes the resistance distance between vertices u and v in G, and $d(u|G)$ denotes the degree of the vertex u in G. In this paper, we mainly determine maximum Kirchhoff index and maximum degree resistance distance of n-vertex unicyclic graphs with given maximum degree, and characterize their extremal graphs. In addition, maximum Kirchhoff index and maximum degree resistance distance of n-vertex unicyclic graphs can be determined as corollaries, which are results in [3, 24, 26].

*Corresponding author.

1 Introduction

All graphs considered in this paper are finite, simple and connected. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. For $u, v \in V(G)$, the (ordinary) distance between u and v in G, denoted by $d(u, v|G)$, is the length of a shortest path connecting them in G.

Graph invariants, based on the distances between the vertices of a graph [2], are widely used in theoretical chemistry to establish relations between the structure and the properties of molecules [10, 11]. Topological indices are numerical graph invariants, in which the Wiener index is one of the oldest and the most thoroughly studied indices [23, 25]. The Wiener index of G is defined as [6, 13]

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

A number of modifications of the Wiener index were proposed, and the degree distance is such a graph invariant, which is defined as [7]

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

where $d(u|G)$ is the degree of the vertex u in G. If G is a tree on n-vertex, then the Wiener index and the degree distance are related as [7]

$$D(G) = 4W(G) - n(n-1).$$

In 1993 Klein and Randić [15] introduced a new distance function named resistance distance. For $u, v \in V(G)$, the resistance distance between u and v in G, denoted by $R(u, v|G)$, is defined as the effective resistance between nodes u and v of the electrical network for which nodes correspond to vertices of G and each edge of G is replaced by a resistor of unit resistance.

The Kirchhoff index of G is defined in analogy to the Wiener index as [15]

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

The Kirchhoff index is also an important topological index and much studied in the literature [4, 12, 17–20, 22, 26, 28, 29]. It found a lot of applications in chemistry, electrical network, Markov chains, averaging networks and experiment design, see [1, 8, 14].

The degree resistance distance was put forward in [9], which is defined as

$$D_R(G) = \sum_{\{u,v\}\subseteq V(G)} [d(u|G) + d(v|G)]R(u, v|G).$$

This quantity is sometimes referred to as the additive degree-Kirchhoff index, and more results can be referred to [3, 5, 20, 24, 27].

It is well-known [15] that

$$R(u,v|G) \leq d(u,v|G)$$

with equality if and only if there is a unique path connecting vertices u and v in G. As an immediate consequence, if G is a tree, then $Kf(G) = W(G)$ and $D_R(G) = D(G)$. Thus in the research on the Kirchhoff index and the degree resistance distance of graphs, it is primarily of interest in the case of cycle-containing graphs. Note that $|E(G)| = |V(G)| - 1$ for trees, and $|E(G)| = |V(G)|$ for unicyclic graphs. In this paper, we mainly characterize the unique unicyclic graph with maximum Kirchhoff index, which is the Theorem 1.1, and the unique unicyclic graphs with maximum degree resistance distance, which is the Theorem 1.2, when order n and maximum degree Δ are given and $2 \leq \Delta \leq n-1$.

First, we introduce some notations and special graphs. Let $\mathbb{U}(n,\Delta)$ be the set of n-vertex unicyclic graphs with maximum degree Δ, where $2 \leq \Delta \leq n-1$. Let P_n and C_n be the path and the cycle on n vertices, respectively. For $3 \leq \Delta \leq n-1$, let $U_{n,\Delta}$ be the n-vertex unicyclic graph obtained by attaching $\Delta - 3$ pendent vertices and a path $P_{n-\Delta}$ to one vertex of C_3 (see Figure 1). For $3 \leq \Delta \leq n-3$, let $U'_{n,\Delta}$ be the n-vertex unicyclic graph obtained by joining one vertex of C_3 and the center of the star on Δ vertices with a path of length $n - \Delta - 2$ (see Figure 1). In particular, $\mathbb{U}(n,2) = \{C_n\}$ for $\Delta = 2$ and $\mathbb{U}(n, n-1) = \{U_{n,n-1}\}$ for $\Delta = n-1$.

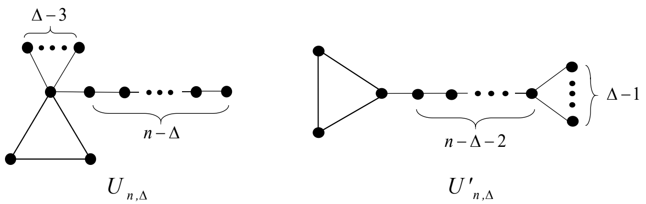

Figure 1. The graphs $U_{n,\Delta}$ and $U'_{n,\Delta}$.

Now we give the main results in this paper.

Theorem 1.1 *Among the graphs in $\mathbb{U}(n,\Delta)$ with $3 \leq \Delta \leq n-1$, $U_{n,\Delta}$ is the unique graph with maximum Kirchhoff index, which is equal to*

$$\frac{1}{6}[2\Delta^3 - (3n+3)\Delta^2 + (9n-5)\Delta + n^3 - 11n + 6].$$

Let $f(x) = \frac{1}{6}[2x^3 - (3n+3)x^2 + (9n-5)x + n^3 - 11n + 6]$, where $3 \le x \le n-1$. Denote by x_1 and x_2 the two roots of $f'(x) = 0$, where $x_1 < x_2$. It is easy to check that $x_1 < 3$ and $x_2 > n-1$. Then $f(x)$ is decreasing in the interval $[3, n-1]$ and $f(x) \le f(3) = \frac{1}{6}(n^3 - 11n + 18)$. Note that $Kf(C_n) < Kf(U_{n,3})$ for $n \ge 4$. Thus we obtain that $U_{n,3}$ is the unique graph with maximum Kirchhoff index among all n-vertex unicyclic graphs, which is one of the main results in [26].

Corollary 1 *[26] For n-vertex unicyclic graph G with $n \ge 4$,*

$$Kf(G) \le \frac{1}{6}(n^3 - 11n + 18)$$

with equality if and only if $G = U_{n,3}$.

Theorem 1.2 *Among the graphs in $\mathbb{U}(n, \Delta)$ with $3 \le \Delta \le n-1$,*

(i) if $\Delta = 3, 4, 5, n-2, n-1$, or $\Delta \ge 6$ and $n < \Delta + 4 + \frac{9}{\Delta - 5}$, then $U_{n,\Delta}$ is the unique graph with maximum degree resistance distance, which is equal to

$$\frac{1}{3}[4\Delta^3 - (6n+3)\Delta^2 + (12n-7)\Delta + 2n^3 - 10n - 6];$$

(ii) if $\Delta \ge 6$ and $n > \Delta + 4 + \frac{9}{\Delta - 5}$, then $U'_{n,\Delta}$ is the unique graph with maximum degree resistance distance, which is equal to

$$\frac{1}{3}[4\Delta^3 - (6n+9)\Delta^2 + (18n-1)\Delta + 2n^3 - 40n + 60];$$

(iii) if $\Delta \ge 6$ and $n = \Delta + 4 + \frac{9}{\Delta - 5}$ (i.e., $\Delta = 6, n = 19; \Delta = 8, n = 15; \Delta = 14, n = 19$), then $U_{n,\Delta}$ and $U'_{n,\Delta}$ are the unique graphs with maximum degree resistance distance, which is equal to $3833\frac{1}{3}$ for $\Delta = 6$ and $n = 19$, 1358 for $\Delta = 8$ and $n = 15$, and $1553\frac{1}{3}$ for $\Delta = 14$ and $n = 19$.

Let $f_1(x) = \frac{1}{3}[4x^3 - (6n+3)x^2 + (12n-7)x + 2n^3 - 10n - 6]$, where $3 \le x \le n-1$. Let $f_2(x) = \frac{1}{3}[4x^3 - (6n+9)x^2 + (18n-1)x + 2n^3 - 40n + 60]$, where $3 \le x \le n-3$. By similar arguments about $f(x)$ as above, we have $f_1(x)$ and $f_2(x)$ are respectively decreasing in the interval $[3, n-1]$ and $[3, n-3]$, and so $f_1(x) \le f_1(3) = \frac{2}{3}(n^3 - 14n + 27)$ and $f_2(x) \le f_2(3) = \frac{2}{3}(n^3 - 20n + 42)$. Note that $f_2(3) < f_1(3)$ and $D_R(C_n) < D_R(U_{n,3})$ for $n \ge 4$. Thus we obtain that $U_{n,3}$ is the unique graph with maximum degree resistance distance among all n-vertex unicyclic graphs, which is one of the main results in [3, 24].

Corollary 2 *[3, 24] For n-vertex unicyclic graph G with $n \ge 4$,*

$$D_R(G) \le \frac{2}{3}(n^3 - 14n + 27)$$

with equality if and only if $G = U_{n,3}$.

2 Preliminaries

Note that $R(v,v|G)=d(v,v|G)=0$ for $v\in V(G)$. Let

$$Kf(v|G)=\sum_{u\in V(G)}R(u,v|G)=\sum_{u\in V(G)\setminus\{v\}}R(u,v|G),$$

$$D_R(v|G)=\sum_{u\in V(G)}d(u|G)R(u,v|G)=\sum_{u\in V(G)\setminus\{v\}}d(u|G)R(u,v|G).$$

Then $Kf(G)=\frac{1}{2}\sum_{v\in V(G)}Kf(v|G)$ and $D_R(G)=\sum_{v\in V(G)}d(v|G)\sum_{u\in V(G)}R(u,v|G)$.

Let $P_n(u,v)$ be the n-vertex path from the vertex u to the vertex v. Then

$$Kf(u|P_n(u,v))=Kf(v|P_n(u,v))=\frac{1}{2}n(n-1),$$

$$Kf(P_n)=W(P_n)=\frac{1}{6}n(n-1)(n+1),$$

$$D_R(u|P_n(u,v))=D_R(v|P_n(u,v))=(n-1)^2,$$

$$D_R(P_n)=D(P_n)=4W(P_n)-n(n-1)=\frac{1}{3}(2n^3-3n^2+n).$$

Let $C_n=v_1v_2\cdots v_nv_1$ be the n-vertex cycle with vertices labeled consecutively by $v_1,v_2,\dots,v_n$. Then it is known that [26]

$$R(v_i,v_j|C_n)=\frac{(j-i)\cdot[n-(j-i)]}{n},$$

where $1\le i<j\le n$ and $R(v_i,v_j|C_n)$ is increasing for $1\le j-i\le\lfloor\frac{n}{2}\rfloor$. And from [9]

$$Kf(C_n)=\frac{n^3-n}{12},\ D_R(C_n)=4Kf(C_n)=\frac{n^3-n}{3},$$

$$Kf(v_i|C_n)=\frac{n^2-1}{6},\ D_R(v_i|C_n)=2Kf(v_i|C_n)=\frac{n^2-1}{3}\ \text{for } 1\le i\le n.$$

Let $C_l(T_1,T_2,\dots,T_l)$ be the unicyclic graph with cycle $C_l=v_1v_2\cdots v_lv_1$ such that the deletion of all edges on C_l results in l vertex-disjoint trees $T_1,T_2,\dots,T_l$ with $v_i\in V(T_i)$, and we say T_i is a branch at v_i for $i=1,2,\dots,l$. Then any n-vertex unicyclic graph G with a cycle on l vertices is of the form $C_l(T_1,T_2,\dots,T_l)$, where $\sum_{i=1}^{l}|V(T_i)|=n$. In particular, if $T_i=P_{|V(T_i)|}$ and v_i is one end vertex of $P_{|V(T_i)|}$, then we denote T_i as $P_{|V(T_i)|}$ for $1\le i\le l$. Obviously, if T_i is trivial, then $T_i=P_1$ for $1\le i\le l$.

For a subset S of $V(G)$ ($E(G)$, respectively), $G-S$ denotes the graph obtained from G by deleting the vertices in S and their incident edges (the edges in S, respectively). For a subset S^* of the edge set of the complement of G, $G+S^*$ denotes the graph obtained from G by adding the edges in S^*.

For a graph G with $x \in V(G)$ and a graph W that is vertex-disjoint with G, a graph obtained by attaching W at its vertex y to the vertex x is such a graph obtained from G and W by adding an edge xy. In particular, if we attach a path at its one end vertex to the vertex x of G, then we simply say attaching the path to the vertex x.

For a graph G with a vertex x of degree at least three, a pendant path at the vertex x is a path in G connecting the vertex x and a pendant vertex such that all internal vertices (if exist) in this path have degree two.

The following Lemmas 2.1-2.3 are some basic properties about resistance distance, Kirchhoff index and degree resistance distance.

Lemma 2.1 *[15] Let x be a cut vertex of a graph G, and let u and v be vertices occurring in different components which arise upon deletion of x. Then*

$$R(u,v|G) = R(u,x|G) + R(x,v|G).$$

Lemma 2.1 has the following important application.

Lemma 2.2 *[9, 28] 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 $x_1 \in V(G_1)$ and $x_2 \in V(G_2)$. Construct the graph G by identifying the vertices x_1 and x_2, and denote the obtained vertex by x. Then*

(i)

$$Kf(G) = Kf(G_1) + Kf(G_2) + (n_2-1)\,Kf(x|G_1) + (n_1-1)\,Kf(x|G_2),$$

$$\begin{aligned} D_R(G) &= D_R(G_1) + D_R(G_2) + (n_2-1)\,D_R(x|G_1) + (n_1-1)\,D_R(x|G_2) \\ &\quad +2m_2Kf(x|G_1) + 2m_1Kf(x|G_2); \end{aligned}$$

(ii) in particular, for $G_2 = P_2$,

$$Kf(G) = Kf(G_1) + Kf(x|G_1) + n_1,$$

$$D_R(G) = D_R(G_1) + D_R(x|G_1) + 2Kf(x|G_1) + 2m_1 + n_1 + 1.$$

Lemma 2.3 *For an n-vertex unicyclic graph G with a pendant path P at a vertex y and a pendant vertex x of the path P, let $R(x,y|G) = a$. Then*

$$Kf(x|G) - Kf(y|G) = a(n-a-1)$$

and

$$D_R(x|G) - D_R(y|G) = 2a(n-a).$$

Proof. It is easy to see that

$$\begin{aligned} Kf(x|G) - Kf(y|G) &= Kf(x|P_{a+1}(x,y)) + Kf(x|G - V(P_{a+1}(x,y))) \\ &\quad - Kf(y|P_{a+1}(x,y)) - Kf(y|G - V(P_{a+1}(x,y))) \\ &= Kf(x|G - V(P_{a+1}(x,y))) - Kf(y|G - V(P_{a+1}(x,y))) \\ &= a(n-a-1). \end{aligned}$$

Let y' be the neighbor of y on the pendant path $P_{a+1}(x,y)$ in G. In particular, if $a = 1$, then $y' = x$. So

$$\begin{aligned} D_R(x|G) - D_R(y|G) &= D_R(x|P_{a+1}(x,y)) + D_R(x|G - V(P_{a+1}(x,y))) \\ &\quad - D_R(y|P_{a+1}(x,y)) - D_R(y|G - V(P_{a+1}(x,y))) \\ &= a \cdot d(y|G) - a \cdot d(x|G) + a \cdot \sum_{v \in V(G) \setminus V(P_{a+1}(x,y))} d(v|G) \\ &= a \cdot 2|E(G - V(P_a(x,y')))| = 2a(n-a) \ . \end{aligned}$$

The result follows easily. ■

The following Lemmas 2.4-2.8 are some useful transformations of graphs and numerical comparisons of their Kirchhoff index and degree resistance distance, which will used in the proof of Theorems 1.1 and 1.2.

Lemma 2.4 *Let W_1 and W_2 be vertex-disjoint connected graphs with $n_1 \geq 2$ and $n_2 \geq 2$ vertices, and with $m_1 \geq 1$ and $m_2 \geq 1$ edges, respectively. Let $x_1 \in V(W_1)$ and $x_2 \in V(W_2)$. Construct the graph G_1 by joining x_1 and x_2 with a path of length $r \geq 1$. And construct the graph G_2 by identifying x_1 and x_2, which is denoted by x, and attaching a path P_r to x. Then $Kf(G_1) > Kf(G_2)$ and $D_R(G_1) > D_R(G_2)$.*

Proof. In G_1, x_2 is a cut vertex, and let $G_{11} = G_1 - (V(W_2) \setminus \{x_2\})$ and $G_{12} = W_2$. In G_2, x is a cut vertex, and let $G_{21} = G_2 - (V(W_2) \setminus \{x\})$ and $G_{22} = W_2$. Obviously, $G_{11} = G_{21}$, $G_{12} = G_{22}$, $Kf(x_2|G_{12}) = Kf(x|G_{22})$, $Kf(x_1|W_1) = Kf(x|W_1)$, $D_R(x_2|G_{12}) = D_R(x|G_{22})$ and $D_R(x_1|W_1) = D_R(x|W_1)$. Let x_1' be the neighbor of x_1 on the path $P_{r+1}(x_1,x_2)$ in G_1. In particular, if $r = 1$, then $x_1' = x_2$. Let y be the pendant vertex of the pendant path P_{r+1} at x in G_2. Note that $R(x_1,x_2|G_1) = R(x,y|G_2) = r$. Then by Lemma 2.2 (i) and Lemma 2.3, we have

$$Kf(G_1) - Kf(G_2) = (n_2 - 1)[Kf(x_2|G_{11}) - Kf(x|G_{21})] = r(n_1-1)(n_2-1) > 0,$$

and

$$
\begin{aligned}
& D_R(G_1) - D_R(G_2) \\
= \ & (n_2-1)[D_R(x_2|G_{11}) - D_R(x|G_{21})] + 2m_2[Kf(x_2|G_{11}) - Kf(x|G_{21})] \\
= \ & 2r[m_1(n_2-1) + m_2(n_1-1)] > 0,
\end{aligned}
$$

implying that $Kf(G_1) > Kf(G_2)$ and $D_R(G_1) > D_R(G_2)$. The result follows. ■

Lemma 2.5 *For fixed integers i, j and l with $1 \le i < j \le l$, let $G_{a_i,a_j} = C_l(T_1, \dots, T_i, \dots, T_j, \dots, T_l)$ be an n-vertex unicyclic graph, where $T_i = P_{a_i+1}$ and $T_j = P_{a_j+1}$ with a_i, $a_j \ge 1$, and all branches not at v_i and v_j are fixed. For a_i, $a_j \ge 1$, let x $(y, respectively)$ be the pendant vertex of T_i $(T_j, respectively)$, and v_i' $(v_j', respectively)$ the neighbor of v_i $(v_j, respectively)$ in T_i $(T_j, respectively)$. In particular, if $a_i = 1$ $(a_j = 1, respectively)$, then $x = v_i'$ $(y = v_j', respectively)$. Then*

$$Kf(G_{a_i,a_j}) < \max\{Kf(G_{a_i+a_j,0}), Kf(G_{0,a_i+a_j})\}$$

and

$$D_R(G_{a_i,a_j}) < \max\{D_R(G_{a_i+a_j,0}), D_R(G_{0,a_i+a_j})\}.$$

Proof. Note that $G_{a_i+a_j,0} = G_{a_i,a_j} - \{v_jv_j'\} + \{xv_j'\}$ and $G_{0,a_i+a_j} = G_{a_i,a_j} - \{v_iv_i'\} + \{yv_i'\}$. For G_{a_i,a_j}, v_i and v_j are cut vertices, and let $G_{11} = G_{a_i,a_j} - (V(P_{a_j+1}) \setminus \{v_j\})$, $G_{12} = P_{a_j+1}$, $G_{21} = G_{a_i,a_j} - (V(P_{a_i+1}) \setminus \{v_i\})$ and $G_{22} = P_{a_i+1}$. Note that $|V(G_{12})| = a_j + 1$, $|E(G_{12})| = a_j$, $|V(G_{22})| = a_i + 1$ and $|E(G_{22})| = a_i$. Then by Lemma 2.3, we have

$$Kf(x|G_{11}) - Kf(v_i|G_{11}) = a_i(n - a_i - a_j - 1),$$

$$Kf(y|G_{21}) - Kf(v_j|G_{21}) = a_j(n - a_i - a_j - 1),$$

$$D_R(x|G_{11}) - D_R(v_i|G_{11}) = 2a_i(n - a_i - a_j),$$

and

$$D_R(y|G_{21}) - D_R(v_j|G_{21}) = 2a_j(n - a_i - a_j).$$

Note that

$$Kf(v_i|G_{21}) = Kf(v_i|G_{11}) - \sum_{v \in V(P_{a_i}(v_i',x))} R(v, v_i|G_{11}) + \sum_{v \in V(P_{a_j}(v_j',y))} R(v, v_i|G_{21}),$$

$$Kf(v_j|G_{21}) = Kf(v_j|G_{11}) - \sum_{v \in V(P_{a_i}(v_i',x))} R(v, v_j|G_{11}) + \sum_{v \in V(P_{a_j}(v_j',y))} R(v, v_j|G_{21}),$$

$$
\begin{aligned}
D_R(v_i|G_{21}) &= D_R(v_i|G_{11}) - d(v_j|G_{11})R(v_j, v_i|G_{11}) - \sum_{v\in V(P_{a_i}(v_i', x))} d(v|G_{11})R(v, v_i|G_{11}) \\
&+ d(v_j|G_{21})R(v_j, v_i|G_{21}) + \sum_{v\in V(P_{a_j}(v_j', y))} d(v|G_{21})R(v, v_i|G_{21}),
\end{aligned}
$$

and

$$
\begin{aligned}
D_R(v_j|G_{21}) &= D_R(v_j|G_{11}) - d(v_i|G_{11})R(v_i, v_j|G_{11}) - \sum_{v\in V(P_{a_i}(v_i', x))} d(v|G_{11})R(v, v_j|G_{11}) \\
&+ d(v_i|G_{21})R(v_i, v_j|G_{21}) + \sum_{v\in V(P_{a_j}(v_j', y))} d(v|G_{21})R(v, v_j|G_{21}).
\end{aligned}
$$

Then by Lemma 2.2 (i), we have

$$
\begin{aligned}
& Kf(G_{a_i+a_j,0}) - Kf(G_{a_i,a_j}) \\
=\ & (|V(G_{12})| - 1)[Kf(x|G_{11}) - Kf(v_j|G_{11})] \\
=\ & (|V(G_{12})| - 1)[Kf(x|G_{11}) - Kf(v_i|G_{11}) + Kf(v_i|G_{11}) - Kf(v_j|G_{11})] \\
=\ & a_j[a_i(n - a_i - a_j - 1) + Kf(v_i|G_{11}) - Kf(v_j|G_{11})].
\end{aligned}
$$

Let $A = a_i(n - a_i - a_j - 1)$ and $B = Kf(v_j|G_{11}) - Kf(v_i|G_{11})$. If $A > B$, then $Kf(G_{a_i+a_j,0}) > Kf(G_{a_i,a_j})$. Otherwise, if $B \geq A$, then we have

$$
\begin{aligned}
Kf(G_{0,a_i+a_j}) - Kf(G_{a_i,a_j}) &= (|V(G_{22})| - 1)[Kf(y|G_{21}) - Kf(v_i|G_{21})] \\
&= a_i[Kf(y|G_{21}) - Kf(v_j|G_{21}) + Kf(v_j|G_{21}) - Kf(v_i|G_{21})] \\
&= a_i[a_j(n - a_i - a_j - 1) + Kf(v_j|G_{21}) - Kf(v_i|G_{21})] \\
&\geq a_i(a_i + a_j)[n - a_i - a_j - 1 - R(v_i, v_j|C_l)] \\
&\geq a_i(a_i + a_j)[n - a_i - a_j - 1 - d(v_i, v_j|C_l)] > 0,
\end{aligned}
$$

implying that $Kf(G_{0,a_i+a_j}) > Kf(G_{a_i,a_j})$.

Similarly, by Lemma 2.2 (i), we have

$$
\begin{aligned}
& D_R(G_{a_i+a_j,0}) - D_R(G_{a_i,a_j}) \\
=\ & (|V(G_{12})| - 1)[D_R(x|G_{11}) - D_R(v_j|G_{11})] + 2|E(G_{12})|[Kf(x|G_{11}) - Kf(v_j|G_{11})] \\
=\ & a_j[D_R(x|G_{11}) - D_R(v_i|G_{11}) + D_R(v_i|G_{11}) - D_R(v_j|G_{11})] \\
& +2a_j[Kf(x|G_{11}) - Kf(v_i|G_{11}) + Kf(v_i|G_{11}) - Kf(v_j|G_{11})] \\
=\ & a_j[2a_i(2n - 2a_i - 2a_j - 1) + D_R(v_i|G_{11}) + 2Kf(v_i|G_{11}) - D_R(v_j|G_{11}) - 2Kf(v_j|G_{11})].
\end{aligned}
$$

+ Let $C = 2a_i(2n - 2a_i - 2a_j - 1)$ and $D = D_R(v_j|G_{11}) + 2Kf(v_j|G_{11}) - D_R(v_i|G_{11}) - 2Kf(v_i|G_{11})$. If $C > D$, then $D_R(G_{a_i+a_j,0}) > D_R(G_{a_i,a_j})$. Otherwise, if $D \geq C$, then we have

$$
\begin{aligned}
& D_R(G_{0,a_i+a_j}) - D_R(G_{a_i,a_j}) \\
=\ & (|V(G_{22})| - 1)[D_R(y|G_{21}) - D_R(v_i|G_{21})] + 2|E(G_{22})|[Kf(y|G_{21}) - Kf(v_i|G_{21})] \\
=\ & a_i[D_R(y|G_{21}) - D_R(v_j|G_{21}) + D_R(v_j|G_{21}) - D_R(v_i|G_{21})] \\
& +2a_i[Kf(y|G_{21}) - Kf(v_j|G_{21}) + Kf(v_j|G_{21}) - Kf(v_i|G_{21})] \\
=\ & a_i[2a_j(2n - 2a_i - 2a_j - 1) + D_R(v_j|G_{21}) + 2Kf(v_j|G_{21}) - D_R(v_i|G_{21}) - 2Kf(v_i|G_{21})]
\end{aligned}
$$

$$\geq 2a_i(a_i + a_j)[2(n - a_i - a_j - R(v_i, v_j|C_l)) - 1]$$
$$\geq 2a_i(a_i + a_j)[2(n - a_i - a_j - d(v_i, v_j|C_l)) - 1] > 0,$$

implying that $D_R(G_{0,a_i+a_j}) > D_R(G_{a_i,a_j})$.

Now the result follows. ■

Lemma 2.6 *For any unicyclic graph W with $w \in V(W)$, let $W(a_1, a_2, \ldots, a_t)$ be the graph obtained from W by attaching $t \geq 2$ paths $P_{a_1}, P_{a_2}, \ldots, P_{a_t}$ to w, where $0 \leq a_1 \leq a_2 \leq \cdots \leq a_t$. For fixed $k = a_1 + a_2 + \cdots + a_t$, if $1 \leq a_1 \leq a_2 \leq \cdots \leq a_t$, then*

$$Kf(W(a_1, a_2, \ldots, a_t)) \leq Kf(W(1, \ldots, 1, k - t + 1))$$

and

$$D_R(W(a_1, a_2, \ldots, a_t)) \leq D_R(W(1, \ldots, 1, k - t + 1))$$

with either equality if and only if $a_t = k - t + 1$ and $a_i = 1$ for $i = 1, 2, \ldots, t - 1$.

Proof. Let $G_1 = W(a_1, a_2, \ldots, a_t)$ with $1 \leq a_1 \leq a_2 \leq \cdots \leq a_t$. First assume that there is some i such that $a_i \geq 2$ with $1 \leq i \leq t - 1$. Let $G_2 = W(b_1, b_2, \ldots, b_t)$ with $b_i = a_i - 1$, $b_t = a_t + 1$ and $b_j = a_j$ for $j \neq i, t$. Let x, y be respectively the pendant vertices of the path P_{a_t} and P_{a_i}, and z the neighbor of y in G_1. Then $G_2 = G_1 - \{zy\} + \{xy\}$. Let $G_3 = G_1 - \{zy\} + \{wy\}$ and $G_0 = G_1 - \{y\} = G_2 - \{y\} = G_3 - \{y\}$. By Lemma 2.3, we have

$$\begin{aligned}
Kf(x|G_0) - Kf(w|G_0) &= a_t(|V(G_0)| - a_t - 1), \\
Kf(w|G_0) - Kf(z|G_0) &= -(a_i - 1)(|V(G_0)| - a_i), \\
D_R(x|G_0) - D_R(w|G_0) &= 2a_t(|V(G_0)| - a_t), \\
D_R(w|G_0) - D_R(z|G_0) &= -2(a_i - 1)(|V(G_0)| - a_i + 1).
\end{aligned}$$

Together with Lemma 2.2 (ii), we have

$$\begin{aligned}
Kf(G_2) - Kf(G_1) &= Kf(G_2) - Kf(G_3) + Kf(G_3) - Kf(G_1) \\
&= Kf(x|G_0) - Kf(w|G_0) + Kf(w|G_0) - Kf(z|G_0) \\
&= (a_t - a_i + 1)(|V(G_0)| - a_t - a_i) > 0
\end{aligned}$$

and

$$D_R(G_2) - D_R(G_1) = D_R(G_2) - D_R(G_3) + D_R(G_3) - D_R(G_1)$$

$$
\begin{aligned}
&= D_R(x|G_0) - D_R(w|G_0) + 2[Kf(x|G_0) - Kf(w|G_0)] \\
&\quad + D_R(w|G_0) - D_R(z|G_0) + 2[Kf(w|G_0) - Kf(z|G_0)] \\
&= 2(a_t - a_i + 1)(2|V(G_0)| - 2a_t - 2a_i + 1) > 0,
\end{aligned}
$$

implying that $Kf(G_2) > Kf(G_1)$ and $D_R(G_2) > D_R(G_1)$. Repeating the above transformation from G_1 to G_2, we can finally have $Kf(W(a_1, a_2, \ldots, a_t)) \leq Kf(W(1, \ldots, 1, k - t + 1))$ and $D_R(W(a_1, a_2, \ldots, a_t)) \leq D_R(W(1, \ldots, 1, k-t+1))$ with either equality if and only if $a_t = k - t + 1$ and $a_i = 1$ for $i = 1, 2, \ldots, t-1$. Then the result follows. ■

For $3 \leq l \leq n$, let $U_n^l = C_l(P_{n-l+1}, P_1, \ldots, P_1)$. In particular, $U_n^3 = U_{n,3}$ and $U_n^n = C_n$. It was shown in [3, 26] that

$$Kf(U_n^l) = \frac{1}{12}[3l^3 - (4n+6)l^2 + (6n+3)l + 2n^3 - 4n]$$

and

$$D_R(U_n^l) = \frac{1}{3}[3l^3 - (4n+3)l^2 + 3nl + 2n^3 - n].$$

And we have

$$Kf(v_{\lfloor \frac{l}{2} \rfloor + 1}|U_n^l) = \begin{cases} \frac{1}{2}(n-l)(n-l+1) + \frac{l^2-1}{6} + \frac{l(n-l)}{4} & \text{if } l \text{ is even} \\ \frac{1}{2}(n-l)(n-l+1) + \frac{l^2-1}{6} + \frac{(l^2-1)(n-l)}{4l} & \text{if } l \text{ is odd,} \end{cases}$$

$$D_R(v_{\lfloor \frac{l}{2} \rfloor + 1}|U_n^l) = \begin{cases} (n-l)^2 + \frac{l^2-1}{3} + \frac{l(n-l)}{2} & \text{if } l \text{ is even} \\ (n-l)^2 + \frac{l^2-1}{3} + \frac{(l^2-1)(n-l)}{2l} & \text{if } l \text{ is odd.} \end{cases}$$

Lemma 2.7 *For fixed integers a, l and i with $a \geq 0$, $l \geq 3$ and $2 \leq i \leq \lfloor \frac{l}{2} \rfloor + 1$, let $G_i(a, l) = C_l(T_1, T_2, \ldots, T_l)$ be the n-vertex unicyclic graph, where T_1 is fixed, T_i is P_{a+1} with end vertex v_i, and all branches not at v_1 and v_i are P_1. Let $G(a, l) = G_{\lfloor \frac{l}{2} \rfloor + 1}(a, l)$ and $k = a + l$. Then for fixed $k \geq 4$,*

$$Kf(G_i(a, l)) < \max\{Kf(G(k-3, 3)), Kf(G(k-4, 4))\}$$

and

$$D_R(G_i(a, l)) < \max\{D_R(G(k-3, 3)), D_R(G(k-4, 4))\}$$

with $l = 4$ and $i = 2$, or $l \geq 5$.

Proof. First, we claim that $Kf(G_i(a, l)) \leq Kf(G(a, l))$ and $D_R(G_i(a, l)) \leq D_R(G(a, l))$ with equalities if and only if $G_i(a, l) = G(a, l)$. If $|T_1| = 1$ or $a = 0$, then $G_i(a, l) = G(a, l)$. Assume that $|T_1| \geq 2$, $a \geq 1$, and $G_i(a, l) \neq G(a, l)$, i.e., $2 \leq i \leq \lfloor \frac{l}{2} \rfloor$. In $G(a, l)$, $v_{\lfloor \frac{l}{2} \rfloor + 1}$

is a cut vertex, and let $G_{11} = G(a,l) - (V(T_{\lfloor \frac{l}{2} \rfloor+1}) \setminus \{v_{\lfloor \frac{l}{2} \rfloor+1}\})$ and $G_{12} = T_{\lfloor \frac{l}{2} \rfloor+1}$. In $G_i(a,l)$, v_i is a cut vertex, and let $G_{21} = G_i(a,l) - (V(T_i) \setminus \{v_i\})$ and $G_{22} = T_i$. Obviously, $G_{11} = G_{21}$, $G_{12} = G_{22}$, $Kf(v_{\lfloor \frac{l}{2} \rfloor+1}|G_{12}) = Kf(v_i|G_{22})$ and $D_R(v_{\lfloor \frac{l}{2} \rfloor+1}|G_{12}) = D_R(v_i|G_{22})$. By Lemma 2.2 (i), we have

$$\begin{aligned} Kf(G(a,l)) - Kf(G_i(a,l)) &= a[Kf(v_{\lfloor \frac{l}{2} \rfloor+1}|G_{11}) - Kf(v_i|G_{21})] \\ &= a(|V(T_1)| - 1)[R(v_1, v_{\lfloor \frac{l}{2} \rfloor+1}|C_l) - R(v_1, v_i|C_l)] > 0 \end{aligned}$$

and

$$\begin{aligned} D_R(G(a,l)) - D_R(G_i(a,l)) &= a[D_R(v_{\lfloor \frac{l}{2} \rfloor+1}|G_{11}) - D_R(v_i|G_{21})] \\ &\quad +2a[Kf(v_{\lfloor \frac{l}{2} \rfloor+1}|G_{11}) - Kf(v_i|G_{21})] \\ &= 4a|E(T_1)|[R(v_1, v_{\lfloor \frac{l}{2} \rfloor+1}|C_l) - R(v_1, v_i|C_l)] > 0, \end{aligned}$$

implying that $Kf(G(a,r)) > Kf(G_i(a,r))$ and $D_R(G(a,r)) > D_R(G_i(a,r))$. This proves the claim.

If $l = 4$ and $i = 2$, then $k = a + 4$, $G_2(a,4) \neq G_3(a,4) = G(k-4,4)$, and thus by the above claim,

$$Kf(G_2(a,4)) < Kf(G(k-4,4)) \leq \max\{Kf(G(k-3,3)), Kf(G(k-4,4))\}$$

and

$$D_R(G_2(a,4)) < D_R(G(k-4,4)) \leq \max\{D_R(G(k-3,3)), D_R(G(k-4,4))\}.$$

Assume that $l \geq 5$. By the above claim, we only need to show that

$$Kf(G(a,l)) < \max\{Kf(G(k-3,3)), Kf(G(k-4,4))\}$$

and

$$D_R(G(a,l)) < \max\{D_R(G(k-3,3)), D_R(G(k-4,4))\}.$$

Note that the vertex v_1 in $G(a,l)(G(a+2,l-2)$, respectively) is just the vertex $v_{\lfloor \frac{l}{2} \rfloor+1}$ ($v_{\lfloor \frac{l}{2} \rfloor}$, respectively) in $U^l_{l+a}(U^{l-2}_{l+a}$, respectively). By Lemma 2.2 (i) and the expressions of $Kf(U^l_n)$, $Kf(v_{\lfloor \frac{l}{2} \rfloor+1}|U^l_n)$, $D_R(U^l_n)$ and $D_R(v_{\lfloor \frac{l}{2} \rfloor+1}|U^l_n)$, we have

$$\begin{aligned} &Kf(G(a+2,l-2)) - Kf(G(a,l)) \\ = \ &Kf(U^{l-2}_{l+a}) - Kf(U^l_{l+a}) + (|V(T_1)| - 1)[Kf(v_{\lfloor \frac{l}{2} \rfloor}|U^{l-2}_{l+a}) - Kf(v_{\lfloor \frac{l}{2} \rfloor+1}|U^l_{l+a})] \end{aligned}$$

$$= \begin{cases} \frac{1}{6}(-nl+9na+16n-9a^2-30a-27) & \text{if } l \text{ is even} \\ \frac{1}{6}(-l^2+16l+8al-14a-27) & \\ +(n-a-l)\left(\frac{6a-2l+11}{3}+\frac{l^3-(a+4)l^2+(2a+3)l-a}{2l(l-2)}\right) & \text{if } l \text{ is odd,} \end{cases}$$

and

$$\begin{aligned} & D_R(G(a+2,l-2)) - D_R(G(a,l)) \\ = \; & D_R(U_{l+a}^{l-2}) - D_R(U_{l+a}^{l}) + (|V(T_1)|-1)[D_R(v_{\lfloor\frac{l}{2}\rfloor}|U_{l+a}^{l-2}) - D_R(v_{\lfloor\frac{l}{2}\rfloor+1}|U_{l+a}^{l})] \\ & +2|E(T_1)|[Kf(v_{\lfloor\frac{l}{2}\rfloor}|U_{l+a}^{l-2}) - Kf(v_{\lfloor\frac{l}{2}\rfloor+1}|U_{l+a}^{l})] \\ = \; & \begin{cases} \frac{2}{3}(-nl+9na+13n-9a^2-24a-18) & \text{if } l \text{ is even} \\ \frac{2}{3}(-l^2+13l+8al-11a-18) & \\ +2(n-a-l)\left(\frac{12a-4l+19}{3}+\frac{l^3-(a+4)l^2+(2a+3)l-a}{l(l-2)}\right) & \text{if } l \text{ is odd.} \end{cases} \end{aligned}$$

For even $l \geq 6$, let $g_1(l) = -nl+9na+16n-9a^2-30a-27$ and $g_2(l) = -nl+9na+13n-9a^2-24a-18$ be two functions of the variable l. Then

$$\begin{aligned} g_1(6) &= (9a+10)n-9a^2-30a-27 \geq (9a+10)(a+6)-9a^2-30a-27 \\ &= 34a+33>0 \end{aligned}$$

and

$$\begin{aligned} g_2(6) &= (9a+7)n-9a^2-24a-18 \geq (9a+7)(a+6)-9a^2-24a-18 \\ &= 37a+24>0\;. \end{aligned}$$

Let l_0^1 and l_0^2 be respectively the roots of $g_1(l)$ and $g_2(l)$. Thus $g_1(l) \geq 0$ when $6 \leq l \leq l_0^1$, and $g_1(l)<0$ when $l>l_0^1$. And $g_2(l) \geq 0$ when $6 \leq l \leq l_0^2$, and $g_2(l)<0$ when $l>l_0^2$. If k is even, then $l \leq k$. Thus $Kf(G(a,l))$ is maximum only if $(a,l)=(k-4,4)$ for $k \leq l_0^1$, and $(a,l)=(k-4,4)$ or $(0,k)$ for $k>l_0^1$. And $D_R(G(a,l))$ is maximum only if $(a,l)=(k-4,4)$ for $k \leq l_0^2$, and $(a,l)=(k-4,4)$ or $(0,k)$ for $k>l_0^2$. Note that v_1 is a cut vertex in $G(k-4,4)$ and $G(0,k)$. By Lemma 2.2 (i), we have

$$\begin{aligned} Kf(G(k-4,4)) - Kf(G(0,k)) &= \frac{1}{12}(k^3-43k+108)+\frac{1}{6}(n-k)(2k^2-15k+28) \\ &\geq \frac{1}{12}(k^3-43k+108)>0 \end{aligned}$$

and

$$D_R(G(k-4,4)) - D_R(G(0,k)) = \frac{1}{3}(k^3-52k+144)+\frac{1}{3}(n-k)(4k^2-33k+68)$$

$$\geq \frac{1}{3}(k^3 - 52k + 144) > 0,$$

implying that $Kf(G(k-4,4)) > Kf(G(0,k))$ and $D_R(G(k-4,4)) > D_R(G(0,k))$. Similarly, if k is odd, then $l \leq k-1$, $Kf(G(a,l))$ and $D_R(G(a,l))$ are maximum only if $(a,l) = (k-4,4)$ or $(1,k-1)$, and we have by direct calculations that $Kf(G(k-4,4)) > Kf(G(1,k-1))$ and $D_R(G(k-4,4)) > D_R(G(1,k-1))$. Thus $Kf(G(a,l)) < Kf(G(k-4,4))$ and $D_R(G(a,l)) < D_R(G(k-4,4))$.

For odd $l \geq 5$, by similar arguments as above, we have $Kf(G(a,l)) < Kf(G(k-3,3))$ and $D_R(G(a,l)) < D_R(G(k-3,3))$. Then the result follows. ■

For integers $a \geq 1$, $b \geq 0$ and $l = 3,4$, let $U_n^l(a,b)$ be the n-vertex unicyclic graph obtained by attaching $n-a-b-l$ pendant vertices and a path P_a to $v_1 \in V(W)$, where W is $C_3(P_1,P_1,P_{b+1})$ for $l=3$ and $C_4(P_1,P_1,P_{b+1},P_1)$ for $l=4$. Let $k = n-a-b-l$. Note that v_1 is a cut vertex in $U_n^l(a,b)$. Let $G_1 = U_n^l(a,b) - (V(T_1) \setminus \{v_1\})$ and $G_2 = T_1$ in $U_n^l(a,b)$. By Lemma 2.2 (i), we have

$$Kf(U_n^l(a,b)) = \frac{1}{6}(a+1)(a+2)(a+3k) + k(k-1)$$
$$+\begin{cases} \frac{1}{6}[(b+4)^3 - 22b - 34] + \frac{1}{2}(b+3)(a^2+a+2k) + \frac{1}{2}(a+k)(b^2+3b+5) & \text{if } l=4 \\ \frac{1}{6}[(b+3)^3 - 11b - 15] + \frac{1}{2}(b+2)(a^2+a+2k) + \frac{1}{2}(a+k)(b^2+\frac{7}{3}b+\frac{8}{3}) & \text{if } l=3 \end{cases}$$

and

$$D_R(U_n^l(a,b)) = \frac{2}{3}a(a+1)(a+2) + 2k(a+1)(a+2) + 4k(k-1) - (a+k)(a+k+1)$$
$$+\begin{cases} \frac{1}{3}[2(b+4)^3 - 53b - 68] + (a+k)(2b^2+5b+10) & \\ +b(2a^2+a+3k) + 7a^2 + 4a + 11k & \text{if } l=4 \\ \frac{1}{3}[2(b+3)^3 - 28b - 30] + (a+k)(2b^2+\frac{11}{3}b+\frac{16}{3}) & \\ +b(2a^2+a+3k) + 5a^2 + 3a + 8k & \text{if } l=3. \end{cases}$$

Lemma 2.8 *For integers $a \geq 1$, $b \geq 0$ and $l = 3,4$, let $s = a+b \geq 2$ and $k = n-s-l$. Then*

$$Kf(U_n^l(a,b)) \leq Kf(U_n^l(s,0))$$

and

$$D_R(U_n^l(a,b)) \leq D_R(U_n^l(s,0))$$

with either equality if and only if $U_n^l(a,b) = U_n^l(s,0)$.

Proof. For $U_n^l(a,b)$, let x be the pendant vertex of the path attached to v_1, y the pendant vertex of P_{b+1} if $b \geq 1$, and z a pendant neighbor of v_1 if $k \geq 1$. Let $G_1 = U_n^l(a,b)$. Let

w be the neighbor of x in G_1. For $a \geq 2$, let $G_2 = G_1 - \{wx\} + \{yx\} = U_n^l(a-1, b+1)$, $G_3 = G_1 - \{wx\} + \{v_3x\}$, $G_4 = G_1 - \{wx\} + \{v_1x\}$ and $G_0 = G_1 - \{x\} = G_2 - \{x\} = G_3 - \{x\} = G_4 - \{x\}$. Then by Lemma 2.2 (ii) and Lemma 2.3, we have

$$\begin{aligned}
& Kf(U_n^l(a-1,b+1)) - Kf(U_n^l(a,b)) \\
= \;& Kf(G_2) - Kf(G_1) \\
= \;& Kf(G_2) - Kf(G_3) + Kf(G_3) - Kf(G_4) + Kf(G_4) - Kf(G_1) \\
= \;& Kf(y|G_0) - Kf(v_3|G_0) + Kf(v_3|G_0) - Kf(v_1|G_0) + Kf(v_1|G_0) - Kf(w|G_0) \\
= \;& b(n-b-2) + \frac{2(l-2)}{l}(a-b+k-1) - (a-1)(n-a-1) \\
= \;& \begin{cases} (1-a+b)(k+2)+k & \text{if } l=4 \\ (1-a+b)(k+\frac{4}{3}) + \frac{2k}{3} & \text{if } l=3 \end{cases}
\end{aligned}$$

and

$$\begin{aligned}
& D_R(U_n^l(a-1,b+1)) - D_R(U_n^l(a,b)) \\
= \;& D_R(G_2) - D_R(G_1) \\
= \;& D_R(G_2) - D_R(G_3) + D_R(G_3) - D_R(G_4) + D_R(G_4) - D_R(G_1) \\
= \;& D_R(y|G_0) - D_R(v_3|G_0) + D_R(v_3|G_0) - D_R(v_1|G_0) + D_R(v_1|G_0) - D_R(w|G_0) \\
& +2[Kf(y|G_0) - Kf(v_3|G_0) + Kf(v_3|G_0) - Kf(v_1|G_0) + Kf(v_1|G_0) - Kf(w|G_0)] \\
= \;& 2b(n-b-1) + \frac{4(l-2)}{l}(a-b+k-1) - 2(a-1)(n-a) \\
& +2b(n-b-2) + \frac{4(l-2)}{l}(a-b+k-1) - 2(a-1)(n-a-1) \\
= \;& \begin{cases} 2(1-a+b)(2k+5)+4k & \text{if } l=4 \\ 2(1-a+b)(2k+\frac{11}{3}) + \frac{8k}{3} & \text{if } l=3. \end{cases}
\end{aligned}$$

If $l=3$, then $Kf(U_n^3(a-1,b+1)) \geq Kf(U_n^3(a,b))$ if and only if $a-b \leq 1 + \frac{2k}{3k+4} < 2$ and $D_R(U_n^3(a-1,b+1)) \geq D_R(U_n^3(a,b))$ if and only if $a-b \leq 1+\frac{4k}{6k+11} < 2$, implying that $Kf(U_n^3(a,b))$ and $D_R(U_n^3(a,b))$ are maximum only if $(a,b) = (1, s-1)$ or $(s,0)$. Similarly, if $l=4$, then $Kf(U_n^4(a,b))$ and $D_R(U_n^4(a,b))$ are maximum only if $(a,b) = (1, s-1)$ or $(s,0)$. By the expressions of $Kf(U_n^l(a,b))$ and $D_R(U_n^l(a,b))$, we have

$$Kf(U_n^l(s,0)) - Kf(U_n^l(1,s-1)) = \begin{cases} 2(s-1) > 0 & \text{if } l=4 \\ \frac{1}{3}(k+4)(s-1) > 0 & \text{if } l=3, \end{cases}$$

$$D_R(U_n^l(s,0)) - D_R(U_n^l(1,s-1)) = \begin{cases} 10(s-1) > 0 & \text{if } l=4 \\ \frac{1}{3}(4k+22)(s-1) > 0 & \text{if } l=3. \end{cases}$$

Then the result follows. ■

3 Proof of Theorems 1.1 and 1.2

At this stage, we are ready to present the proofs of Theorems 1.1 and 1.2.

Proof. The case $\Delta = n-1$ is trivial. Assume that $3 \le \Delta \le n-2$. Let $G_1 = C_l(T_1, T_2, \dots, T_l)$ ($G_2 = C_l(T_1, T_2, \dots, T_l)$, respectively) be a graph with maximum Kirchhoff index (degree resistance distance, respectively) in $\mathbb{U}(n, \Delta)$. Obviously, $3 \le l \le n-1$.

Claim 1. If there exists one vertex of maximum degree Δ on the cycle C_l in G_1 (G_2, respectively), then $G_1 = U_{n,\Delta}$ ($G_2 = U_{n,\Delta}$, respectively).

Suppose without loss of generality that v_1 is one vertex of maximum degree Δ on C_l. By Lemma 2.4, the vertices outside C_l are of degree one or two, and the vertices on C_l different from v_1 are of degree two or three. By Lemma 2.5, there is at most one vertex on C_l different from v_1 of degree three. Thus G_1 (G_2, respectively) is a graph obtainable from the cycle C_l by attaching $\Delta - 2$ paths to v_1 and at most one path to another vertex on C_l different from v_1. By Lemmas 2.6 and 2.7, we have $G_1 = U_n^l(a, b)$ ($G_2 = U_n^l(a, b)$, respectively) with $\Delta = n - a - b - l + 3$, where $l = 3, 4$. Then by Lemma 2.8, if $l = 3$, then $G_1 = U_n^3(n - \Delta, 0) = U_{n,\Delta}$ ($G_2 = U_n^3(n - \Delta, 0) = U_{n,\Delta}$, respectively); if $l = 4$, then $G_2 = U_n^4(n - \Delta - 1, 0)$ ($G_2 = U_n^4(n - \Delta - 1, 0)$, respectively). By the expressions of $Kf(U_n^l(a, b))$ and $D_R(U_n^l(a, b))$, we have

$$Kf(U_{n,\Delta}) = \frac{1}{6}[2\Delta^3 - (3n+3)\Delta^2 + (9n-5)\Delta + n^3 - 11n + 6],$$

$$Kf(U_n^4(n-\Delta-1, 0)) = \frac{1}{6}[2\Delta^3 - (3n-3)\Delta^2 + (3n-5)\Delta + n^3 - 4n - 12],$$

$$D_R(U_{n,\Delta}) = \frac{1}{3}[4\Delta^3 - (6n+3)\Delta^2 + (12n-7)\Delta + 2n^3 - 10n - 6],$$

$$D_R(U_n^4(n-\Delta-1, 0)) = \frac{1}{3}[4\Delta^3 - (6n-9)\Delta^2 - \Delta + 2n^3 + n - 42].$$

Note that $n \ge \Delta + 2$. Then it is easily checked that $Kf(U_{n,\Delta}) > Kf(U_n^4(n - \Delta - 1, 0))$ and $D_R(U_{n,\Delta}) > D_R(U_n^4(n - \Delta - 1, 0))$. And thus $G_1 = U_{n,\Delta}$ and $G_2 = U_{n,\Delta}$, proving Claim 1.

Claim 2. If there is no vertex of maximum degree Δ on the cycle C_l in G_1 (G_2, respectively), then $G_1 = U'_{n,\Delta}$ ($G_2 = U'_{n,\Delta}$, respectively).

Assume that there is one vertex w of maximum degree Δ outside C_l , where $4 \le \Delta \le n-3$. Suppose without loss of generality that v_1 is the vertex on C_l that is nearest to w. By Lemma 2.4, the vertices outside C_l different from w are of degree one or two, and the vertices on C_l are of degree two or three. By Lemma 2.5, there is at most one vertex on C_l different from v_1 of degree three. By Lemma 2.6, there is at most one pendant path at w with length at least two. Assume that there is such a pendant path P at w with length at least two. Then let x be the neighbor of the pendant vertex of the path P, and $t = d(w, x|G) \geq 1$. Let $x_1, x_2, \ldots, x_{\Delta-2}$ be the pendant neighbors of w. Let $G_{10} = G_1 - \{x_1, x_2, \ldots, x_{\Delta-2}\}$ and $G_1' = G_1 - \{wx_1, wx_2, \ldots, wx_{\Delta-2}\} + \{xx_1, xx_2, \ldots, xx_{\Delta-2}\} \in \mathbb{U}(n, \Delta)$ ($G_{20} = G_2 - \{x_1, x_2, \ldots, x_{\Delta-2}\}$ and $G_2' = G_2 - \{wx_1, wx_2, \ldots, wx_{\Delta-2}\} + \{xx_1, xx_2, \ldots, xx_{\Delta-2}\} \in \mathbb{U}(n, \Delta)$, respectively). Note that $n - \Delta - t \geq 3$. By Lemma 2.2 (i), we have

$$\begin{aligned} Kf(G_1') - Kf(G_1) &= (\Delta - 2)[Kf(x|G_{10}) - Kf(w|G_{10})] \\ &= t(\Delta - 2)(n - \Delta - t - 1) > 0 \end{aligned}$$

and

$$\begin{aligned} D_R(G_2') - D_R(G_2) &= (\Delta - 2)[D_R(x|G_{20}) - D_R(w|G_{20})] \\ &\quad +2(\Delta - 2)[Kf(x|G_{20}) - Kf(w|G_{20})] \\ &= 2t(\Delta - 2)(2n - 2\Delta - 2t - 1) > 0, \end{aligned}$$

implying that $Kf(G_1') > Kf(G_1)$ and $D_R(G_2') > D_R(G_2)$, contradictions. Thus there is no pendant path at w with length at least two, i.e., w has $\Delta - 1$ pendant neighbors in G_1 and G_2.

Let H_1 (H_2, respectively) be the graph obtained from G_1 (G_2, respectively) by deleting the vertices of the branch T_1 except v_1. By Lemma 2.7, we have $G_1 = G(k - 3, 3)$ or $G(k - 4, 4)$ ($G_2 = G(k - 3, 3)$ or $G(k - 4, 4)$, respectively), where $k = |W_1|$ and $W_1 = C_3(P_1, P_{k-2}, P_1)$ or $C_4(P_1, P_1, P_{k-3}, P_1)$ ($k = |W_2|$ and $W_2 = C_3(P_1, P_{k-2}, P_1)$ or $C_4(P_1, P_1, P_{k-3}, P_1)$, respectively). Assume that $W_1 \neq C_3, C_4$ ($W_2 \neq C_3, C_4$, respectively). Let y be the neighbor of v_1 in T_1 and z the pendant vertex in W_1 (W_2, respectively). Let $G_1'' = G_1 - \{v_1y\} + \{zy\} \in \mathbb{U}(n, \Delta)$ ($G_2'' = G_2 - \{v_1y\} + \{zy\} \in \mathbb{U}(n, \Delta)$, respectively). Note that $k \geq 4$ for $l = 3$ and $k \geq 5$ for $l = 4$. By Lemma 2.2 (i), we have

$$\begin{aligned} Kf(G_1'') - Kf(G_1) &= |E(T_1)|[Kf(z|H_1) - Kf(v_1|H_1)] \\ &= \begin{cases} 2(k-4)|E(T_1)| > 0 & \text{if } l = 4 \\ \frac{4}{3}(k-3)|E(T_1)| > 0 & \text{if } l = 3 \end{cases} \end{aligned}$$

and

$$\begin{aligned} D_R(G_2'') - D_R(G_2) &= |E(T_1)|[D_R(z|H_1) - D_R(v_1|H_1)] \\ &\quad +2|E(T_1)|[Kf(z|H_1) - Kf(v_1|H_1)] \\ &= \begin{cases} 10(k-4)|E(T_1)| > 0 & \text{if } l = 4 \\ \frac{22}{3}(k-3)|E(T_1)| > 0 & \text{if } l = 3, \end{cases} \end{aligned}$$

implying that $Kf(G_1'') > Kf(G_1)$ and $D_R(G_2'') > D_R(G_2)$, contradictions. Thus $W_1 = C_3$ or C_4, and $W_2 = C_3$ or C_4. For $3 \le \Delta \le n-4$, let $U''_{n,\Delta}$ be the n-vertex unicyclic graph obtained by joining a vertex of C_4 and the center of the star on Δ vertices with a path of length $n-\Delta-3$. Note that v_1 is a cut vertex in $U'_{n,\Delta}$ and $U''_{n,\Delta}$. By Lemma 2.2 (i), we have

$$\begin{aligned} Kf(U'_{n,\Delta}) &= \frac{1}{6}[2\Delta^3 - (3n+3)\Delta^2 + (9n-5)\Delta + n^3 - 17n + 24], \\ Kf(U''_{n,\Delta}) &= \frac{1}{6}[2\Delta^3 - (3n+3)\Delta^2 + (9n-5)\Delta + n^3 - 28n + 60], \\ D_R(U'_{n,\Delta}) &= \frac{1}{3}[4\Delta^3 - (6n+9)\Delta^2 + (18n-1)\Delta + 2n^3 - 40n + 60], \\ D_R(U''_{n,\Delta}) &= \frac{1}{3}[4\Delta^3 - (6n+9)\Delta^2 + (18n-1)\Delta + 2n^3 - 65n + 150]. \end{aligned}$$

Then it is easily checked that $Kf(U'_{n,\Delta}) > Kf(U''_{n,\Delta})$ and $D_R(U'_{n,\Delta}) > D_R(U''_{n,\Delta})$. And thus $G_1 = U'_{n,\Delta}$ and $G_2 = U'_{n,\Delta}$, proving Claim 2.

Combining Claims 1 and 2, we have $G_1 = U_{n,\Delta}$ for $3 \le \Delta \le n-1$ or $G_1 = U'_{n,\Delta}$ for $4 \le \Delta \le n-3$. If $4 \le \Delta \le n-3$, then it is easily checked that $Kf(U_{n,\Delta}) > Kf(U'_{n,\Delta})$. Then the result of Theorem 1.1 follows.

Similarly, we have $G_2 = U_{n,\Delta}$ for $3 \le \Delta \le n-1$ or $G_2 = U'_{n,\Delta}$ for $4 \le \Delta \le n-3$. If $4 \le \Delta \le n-3$, then it is easily checked that

$$\begin{aligned} D_R(U_{n,\Delta}) - D_R(U'_{n,\Delta}) &= 2[(\Delta-5)(\Delta-n+4)+9] \\ & \begin{cases} > 0 & \text{if } \Delta = 4,5 \\ > 0 & \text{if } \Delta \ge 6 \text{ and } n < \Delta + 4 + \frac{9}{\Delta-5} \\ = 0 & \text{if } \Delta \ge 6 \text{ and } n = \Delta + 4 + \frac{9}{\Delta-5} \\ < 0 & \text{if } \Delta \ge 6 \text{ and } n > \Delta + 4 + \frac{9}{\Delta-5}. \end{cases} \end{aligned}$$

Note that if $\Delta \ge 6$ and $n = \Delta + 4 + \frac{9}{\Delta-5}$, then $\Delta = 6, n = 19; \Delta = 8, n = 15; \Delta = 14, n = 19$. Then the result of Theorem 1.2 follows. ■

4 Concluding Remarks

It is worth mentioning that when we try to determine the maximum degree resistance distance (also called additive degree-Kirchhoff index in some papers) among n-vertex unicyclic graphs with given maximum degree, we find that the maximum Kirchhoff index of n-vertex unicyclic graphs with given maximum degree can be determined, by using a similar method. So compared with the method in [16], our proof would be more rational and universal.

More precisely, our methods are valid for the determinations of maximum values for three types of Kirchhoff indices (Kirchhoff index, additive degree-Kirchhoff index, multiplicative degree-Kirchhoff index) among n-vertex unicyclic graphs with given maximum degree. The extremal graphs of additive degree-Kirchhoff and multiplicative degree-Kirchhoff indices are the same ($U_{n,\Delta}$ or $U'_{n,\Delta}$) [21]. However, the case for Kirchhoff index is somewhat different, which can only be $U_{n,\Delta}$.

In our further research, we will try to get more properties of these three types of Kirchhoff indices, especially the additive degree-Kirchhoff index.

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