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Degree Kirchhoff Index of Unicyclic Graphs[1]

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Abstract

Let G be a connected graph with vertex set $V(G)$. The degree Kirchhoff index of G is defined as $S'(G) = \sum_{\{u,v\}\subseteq V(G)} d(u)d(v)R(u,v)$, where $d(u)$ is the degree of vertex u, and $R(u,v)$ denotes the resistance distance between vertices u and v. In this paper we characterize n-vertex unicyclic graphs having maximum, second–maximum, minimum, and second–minimum degree Kirchhoff index.

1 Introduction

Topological indices (molecular structure descriptors) based on the distances between the vertices of a graph are widely used in theoretical chemistry to establish relations between the structure and the properties of molecules [21, 22]. They provide correlations with physical, chemical, and thermodynamic parameters of chemical compounds.

Let $G = (V(G), E(G))$ be a simple undirected graph with $n = |V(G)|$ vertices and $m = |E(G)|$ edges. In this paper all graphs considered are assumed to be connected. The

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distance $d(v,u) = d(u,v|G)$ between the vertices v and u of the graph G is defined as the length of a shortest path between v and u. The sum of distances between a vertex v of G and all other vertices is denoted by $D(v)$ or, when the underlying graph needs to be specified, by $D(v|G)$, that is

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

The *Wiener index* is defined as the sum of distances between all unordered pairs of vertices

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v) = \frac{1}{2} \sum_{v \in V(G)} D(v) \ .$$

This molecular structure descriptor is one of the most used topological indices, well correlated with many physical and chemical properties of a variety of classes of chemical compounds. For details, see the survey paper [12].

A weighted version of the Wiener index is the *degree distance* defined as [13]

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

where $d(u)$ is the degree (number of first neighbors) of the vertex u. If the underlying graph needs to be specified, then we shall write the vertex degree as $d(u|G)$.

The same quantity $D'(G)$ was examined in the paper [19] under the name *Schultz index*. Namely, somewhat earlier H. P. Schultz [32] proposed a structure descriptor named *molecular topological index*, defined as

$$MTI(G) = \sum_{i=1}^{n} \mathbf{d}(\mathbf{A} + \mathbf{D})_i$$

where $\mathbf{A}$ and $\mathbf{D}$ are the adjacency and distance matrices of the underlying molecular graph G, and $\mathbf{d}$ is the vector of vertex degrees. It can be easily shown that

$$MTI(G) = \sum_{u \in V(G)} d(u)^2 + \sum_{\{u,v\} \subseteq V(G)} [d(u) + d(v)] d(u,v)$$

which means that

$$MTI(G) = M_1(G) + D'(G)$$

with $M_1(G)$ standing for the well-known first Zagreb index (cf. [14, 20]). Klein et al. [27] discovered the simple relation between degree distance and Wiener index:

$$D'(G) = 4W(G) - n(n-1) \tag{1}$$

which holds for trees.

The degree distance of graphs is well studied in the literature. In [4] the authors established the minimum degree distance of graphs with given order and size. Dankelmann et al. [8] presented an asymptotically sharp upper bound on degree distance of graphs with given order and diameter. In [24] the degree distance of partial Hamming graphs was studied. Tomescu [36] presented the graph with minimum degree distance among all connected graphs and disproved a conjecture posed in [13]. Ilić et al. [25] determined the bicyclic graphs with maximum degree distance. Some further properties of the degree distance were reported in [37]. In [35] Tomescu determined the minimum degree distance of unicyclic and bicyclic graphs. Yuan and An [44] determined the maximum degree distance among unicyclic graphs on n vertices.

In [19] a novel proof of the relation (1) was put forward. Then it was noticed that a fully analogous relation can be obtained for the multiplicative variant of the degree distance, namely for

$$S(G) = \sum_{\{u,v\} \subseteq V(G)} d(u)\, d(v)\, d(u,v) \ . \tag{2}$$

This relation reads [19]:

$$S(G) = 4W(G) - (2n-1)(n-1)$$

and also holds for trees. The author of [19] called $S(G)$ the *Schultz index of the second kind* and by no means proposed it for a novel molecular structure descriptor. Unfortunately, not carefully reading the paper [19], the authors of the seminal handbooks [33,34] included $S(G)$ among the topological indices and, even worse, named it *Gutman index*.

The Gutman index of graphs attracted attention only quite recently. In [9] an asymptotic upper bound for $S(G)$ was reported. In [9, 29] relations between the edge–Wiener index and Gutman index were established. The maximal and minimal Gutman indices of bicyclic graphs are determined in [15] and [6], respectively. Some bounds on the Gutman index are established in [1, 46]. Deng [10] calculated the Gutman index of polyhex nanotubes.

In 1993 Klein and Randić [28] introduced a new distance function named resistance distance, based on the theory of electrical networks. They viewed G as an electrical network N by replacing each edge of G with a unit resistor. The resistance distance between the vertices u and v of the graph G, denoted by $R(u,v) = R(u,v|G)$, is then

defined to be the effective resistance between the nodes u and v in N. Similar to the long recognized shortest–path distance, the resistance distance is also intrinsic to the graph, not only with some nice purely mathematical properties, but also with a substantial potential for chemical applications [2, 3, 26, 28, 39–41].

The *Kirchhoff index* (or resistance index) is defined in analogy to the Wiener index as [3]:

$$Kf(G) = \sum_{\{u,v\}\subseteq V(G)} R(u,v) = \frac{1}{2} \sum_{v\in V(G)} R(v)$$

where $R(v)$ stands for the sum of resistance distances between the vertex v and all other vertices of G:

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

The Kirchhoff index is also much studied in the literature. In unicyclic graphs extremal with respect to the Kirchhoff index were determined in [42, 45]. Deng also studied the Kirchhoff index of fully loaded unicyclic graphs [18] and graphs with many cut edges [11]. Zhou [47] characterized the extremal graphs with given matching number, connectivity, and minimal Kirchhoff index. Wang et al. [38] determined the first three minimal Kirchhoff indices among cacti.

Recently, a new index named *degree Kirchhoff index* was put forward in [5], and further studied in [31]. It is defined as

$$S'(G) = \sum_{\{u,v\}\subseteq V(G)} d(u)\, d(v)\, R(u,v) = \frac{1}{2} \sum_{v\in V(G)} d(v)\, S'(v) \tag{3}$$

where

$$S'(v) = S'(v|G) = \sum_{u\in V(G)} d(u)\, R(u,v) \ . \tag{4}$$

Comparing Eqs. (2) and (3) we can see that the degree Kirchhoff index may be viewed as the resistance–distance analogue of the Gutman index. However, there is a much more subtle reason for the introduction of this novel structure descriptor.

Let $\mathbf{L} = \mathbf{D} - \mathbf{A}$ be the Laplacian matrix of the (connected) graph G, and let its eigenvalues be $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} > \mu_n = 0$. For details on Laplacian eigenvalues see [16, 17, 30]. Then a long time known result for the Kirchhoff index is [23]:

$$Kf(G) = n \sum_{i=1}^{n-1} \frac{1}{\mu_i} \ . \tag{5}$$

Let, in addition, $\mathbf{L}^* = \mathbf{D}^{1/2}\mathbf{L}\mathbf{D}^{-1/2}$ be the reduced Laplacian matrix of the graph G, and let its eigenvalues be $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_{n-1} > \rho_n = 0$. For details on the spectral theory of the reduced Laplacian matrix see [7]. A remarkable analogy between the Kirchhoff and degree Kirchhoff indices is the formula [5]:

$$S'(G) = 2m \sum_{i=1}^{n-1} \frac{1}{\rho_i} \ . \tag{6}$$

Comparing Eqs. (5) and (6) we realize that the degree Kirchhoff index provides the reduced–Laplacian analogue of the ordinary Kirchhoff index.

For the following consideration it is important to recall that $R(u,v) = R(v,u)$, $R(u,u) = 0$ and that [28] $d(u,v) \geq R(u,v)$ with equality if and only if there is a unique path linking the vertices u and v. Therefore, for trees, $Kf(G) = W(G)$ and $S'(G) = S(G)$.

In this paper we study the degree Kirchhoff index of unicyclic graphs. The paper is organized as follows. In Section 2 we state some preparatory results, whereas in Section 3 we find the unicyclic graphs with maximum and second–maximum degree Kirchhoff index. In Section 4 we do the same for the minimum and second–minimum case.

2 Preliminary results

Lemma 1. [28] *Let x be a cut vertex of a graph G, and let a and b be vertices occurring in different components which arise upon deletion of x. Then $R(a,b) = R(a,x) + R(x,b)$.*

Lemma 1 has the following important corollary:

Theorem 2. *Let G_1 and G_2 be connected graphs with disjoint vertex sets and with m_1 and m_2 edges, respectively. Let $u_1 \in V(G_1)$, $u_2 \in V(G_2)$. Construct the graph G by identifying the vertices u_1 and u_2, and denote the so obtained vertex by u. Then*

$$S'(G) = S'(G_1) + S'(G_2) + 2m_1\, S'(u_2|G_2) + 2m_2\, S'(u_1|G_1) \ . \tag{7}$$

Proof. Denote the abbreviations

$$V_1 = V(G_1) \setminus \{u_1\} \qquad \text{and} \qquad V_2 = V(G_2) \setminus \{u_2\} \ .$$

In view of the structure of the graph G, from the definition (3) of the degree Kirchhoff index, we have

$$S'(G) = \left[\sum_{\{x,y\} \subseteq V_1} + \sum_{\{x,y\} \subseteq V_2} + \sum_{\substack{x \in V_1 \\ y = u}} + \sum_{\substack{x \in V_2 \\ y = u}} + \sum_{\substack{x \in V_1 \\ y \in V_2}} \right] d(x|G)\, d(y|G)\, R(x,y|G) \ .$$

Now,

$$\begin{aligned}\sum_{\{x,y\}\subseteq V_1} d(x|G)\,d(y|G)\,R(x,y|G) &= S'(G_1) - \sum_{x\in V_1} d(x|G_1)\,d(u_1|G_1)\,R(x,u_1|G_1)\\ &= S'(G_1) - d(u_1|G_1)\sum_{x\in V_1} d(x|G_1)\,R(x,u_1|G_1)\\ &= S'(G_1) - d(u_1)\,S'(u_1|G_1) \qquad (8)\end{aligned}$$

and analogously

$$\sum_{\{x,y\}\subseteq V_2} d(x|G)\,d(y|G)\,R(x,y|G) = S'(G_2) - d(u_2)\,S'(u_2|G_2)\ . \qquad (9)$$

Further,

$$\begin{aligned}\sum_{\substack{x\in V_1\\ y=u}} d(x|G)\,d(y|G)\,R(x,y|G) &= \sum_{x\in V_1} d(x|G_1)\,d(u|G)\,R(x,u_1|G_1)\\ &= d(u|G)\,S'(u_1|G_1) \qquad (10)\end{aligned}$$

and analogously

$$\sum_{\substack{x\in V_2\\ y=u}} d(x|G)\,d(y|G)\,R(x,y|G) = d(u|G)\,S'(u_2|G_2)\ . \qquad (11)$$

Finally,

$$\sum_{\substack{x\in V_1\\ y\in V_2}} d(x|G)\,d(y|G)\,R(x,y|G) = \sum_{\substack{x\in V_1\\ y\in V_2}} d(x|G)\,d(y|G)\,[R(x,u_1|G_1) + R(y,u_2|G_2)]$$

$$= \sum_{\substack{x\in V_1\\ y\in V_2}} d(x|G_1)\,d(y|G_2)\,R(x,u_1|G_1) + \sum_{\substack{x\in V_1\\ y\in V_2}} d(x|G_1)\,d(y|G_2)\,R(y,u_2|G_2)$$

$$= \sum_{x\in V_1} d(x|G_1)\,R(x,u_1|G_1)\sum_{y\in V_2} d(y|G_2) + \sum_{y\in V_2} d(y|G_2)\,R(y,u_2|G_2)\sum_{x\in V_1} d(x|G_1)$$

$$= S'(u_1|G_1)\,[2m_2 - d(u_2|G_2)] + S'(u_2|G_2)\,[2m_1 - d(u_1|G_1)] \qquad (12)$$

because $\sum_{x\in V(G_1)} d(x) = 2m_1$ and $\sum_{x\in V(G_2)} d(x) = 2m_2$.

Adding Eqs. (8)–(12) we obtain Eq. (7). □

Example 3. *Let the graph U_k^n consist of a cycle of size k to which a path with $n-k$ vertices is attached. Then*

$$S'(U_k^n) = \frac{1}{3}\left(3k^3 - 4nk^2 + 2n^3 - n\right)\ . \qquad (13)$$

Proof. The graph U_k^n can be viewed as the graph G in Theorem 2, such that $G_1 \cong C_k$ and $G_2 \cong P_{n-k+1}$, obtained by identifying a vertex u_1 of the cycle C_k of size k with a terminal vertex u_2 of the path P_{n-k+1} on $n-k+1$ vertices. Then Eq. (7) becomes

$$S'(G) = S'(C_k) + S'(P_{n-k+1}) + 2k\, S'(u_2|P_{n-k+1}) + 2(n-k)\, S'(u_1|C_k)\ . \qquad (14)$$

Bearing in mind that C_k is a regular graph of degree two, we have

$$S'(C_k) = 4\, Kf(C_k) = 4\,\frac{k^3-k}{12} = \frac{k^3-k}{3} \quad \text{and} \quad S'(u_1|C_k) = \frac{1}{k}\, S'(C_k) = \frac{k^2-1}{3}\ .$$

Bearing in mind that P_{n-k+1} is a tree, and thus in it the resistance distances and distances coincide, we have [12]

$$\begin{aligned} S'(P_{n-k+1}) &= S(P_{n-k+1}) = 4\, W(P_{n-k+1}) - (2n-2k+1)(n-k) \\ &= 4\binom{n-k+2}{3} - (2n-2k+1)(n-k) \\ &= \frac{2}{3}\,(n-k)^3 + \frac{1}{3}\,(n-k)\ . \end{aligned}$$

and

$$S'(u_2|P_{n-k+1}) = (n-k)^2\ .$$

Substituting the above relations back into (14), we obtain Eq. (13). □

Let v be a vertex of degree $p+1$ in a graph G, which is not a star, such that $vv_1, vv_2, \ldots, vv_p$ are pendent edges incident with v, and u is the neighbor of v distinct from $v_1, v_2, \ldots, v_p$. Form a graph $G' = \sigma(G, v)$ by removing the edges $vv_1, vv_2, \ldots, vv_p$ and adding new edges $uv_1, uv_2, \ldots, uv_p$. We say that G' is a *σ-transform of G* (see Fig. 1).

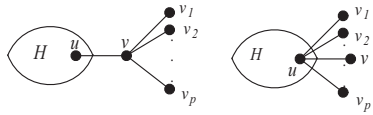

Figure 1: *The σ-transformation at v.*

Theorem 4. *Let $G' = \sigma(G, v)$ be a σ-transform of the graph G. Then $S'(G) \geq S'(G')$. Equality holds if and only if G is a star with v as its center.*

Proof. Let $T = \{v, v_1, v_2, \ldots, v_p\}$ and H denote the subgraph of G induced by the vertex set $V(G) \setminus T$. From the definition of $S'(G)$, we have

$$\begin{aligned} S'(G) &= \left[\sum_{x,y \in V(H-u)} + \sum_{x,y \in T\setminus\{v\}} + \sum_{\substack{x \in V(H-u) \\ y \in T\setminus\{v\}}} \right] d(x)\, d(y)\, R(x,y) \\ &+ d(u) \left[\sum_{x \in V(H-u)} d(x)\, R(x,u) + \sum_{x \in T\setminus\{v\}} d(x)\, R(x,u) \right] \\ &+ d(v) \left[\sum_{x \in V(H-u)} d(x)\, R(x,v) + \sum_{x \in T\setminus\{v\}} d(x)\, R(x,v) \right] + d(u)\, d(v)\, R(u,v) \ . \end{aligned}$$

After the σ-transformation, the degree of the vertex u increases by p, whereas the degree of the vertex v decreases by p. During this transformation, for $x, y \in V(H-u)$ and $x, y \in T \setminus \{v\}$, $\sum_{x,y} d(x)\, d(y)\, R(x,y)$ does not change.

In G,

$$B_1 := \sum_{\substack{x \in V(H-u) \\ y \in T\setminus\{v\}}} d(x)\, d(y)\, R(x,y) = \sum_{\substack{x \in V(H-u) \\ y \in T\setminus\{v\}}} d(x)\, R(x,y)$$

while in G',

$$B_2 := \sum_{\substack{x \in V(H-u) \\ y \in T\setminus\{v\}}} d(x)\, d(y) \Big(R(x,y) - 1 \Big) = \sum_{\substack{x \in V(H-u) \\ y \in T\setminus\{v\}}} d(x) \Big(R(x,y) - 1 \Big) \ .$$

For the vertex u in G,

$$\begin{aligned} B_3 : &= d(u) \left[\sum_{x \in V(H-u)} d(x)\, R(x,u) + \sum_{x \in T\setminus\{v\}} d(x)\, R(x,u) \right] \\ &= d(u) \sum_{x \in V(H-u)} d(x)\, R(x,u) + 2p\, d(u) \end{aligned}$$

whereas for u in G',

$$\begin{aligned} B_4 : &= \sum_{x \in V(H-u)} (d(u)+p) d(x)\, R(x,u) + \sum_{x \in T\setminus\{v\}} (d(u)+p) d(x)\, R(x,u) \\ &= d(u) \sum_{x \in V(H-u)} d(x) R(x,u) + p \sum_{x \in V(H-u)} d(x)\, R(x,u) + p(d(u)+p) \ . \end{aligned}$$

For the vertex v in G,

$$B_5 : = d(v) \left[\sum_{x \in V(H-u)} d(x) R(x,v) + \sum_{x \in T\setminus\{v\}} d(x)\, R(x,v) + d(u)\, R(u,v) \right]$$

$$= \quad (p+1) \sum_{x \in V(H-u)} d(x)\big(R(x,u)+1\big) + p(p+1) + d(u)(p+1)$$

whereas for v in G',

$$B_6 : \ = \sum_{x \in V(H-u)} d(x)\big(R(x,u)+1\big) + 3p + d(u) \ .$$

From the above relations it follows

$$\begin{aligned}
& B_1 - B_2 + B_3 - B_4 + B_5 - B_6 \\
= & \sum_{\substack{x \in V(H-u) \\ y \in T \setminus \{v\}}} d(x)\, R(x,y) - \sum_{\substack{x \in V(H-u) \\ y \in T \setminus \{v\}}} d(x)\Big(R(x,y)-1\Big) \\
+ \ & d(u) \sum_{x \in V(H-u)} d(x)\, R(x,u) + 2p\, d(u) \\
- \ & \left[d(u) \sum_{x \in V(H-u)} d(x)\, R(x,u) + p \sum_{x \in V(H-u)} d(x)\, R(x,u) + p(d(u)+p) \right] \\
+ \ & (p+1) \sum_{x \in V(H-u)} d(x)\big(R(x,u)+1\big) + p(p+1) + d(u)(p+1) \\
- \ & \sum_{x \in V(H-u)} d(x)\big(R(x,u)+1\big) - 3p - d(u) = \sum_{\substack{x \in V(H-u) \\ y \in T \setminus \{v\}}} d(x) \\
- \ & p \sum_{x \in V(H-u)} d(x)\, R(x,u) + p \sum_{x \in V(H-u)} d(x)\big(R(x,u)+1\big) + 2p(d(u)-1) \geq 0 \ .
\end{aligned}$$

The equality holds if and only if H consists of only one vertex u. This completes the proof. □

Theorem 5. *Let G be a unicyclic graph. Let u be one vertex on G such that there are s pendent vertices $u_1, u_2, \ldots, u_s$ attached at u. Let v be a vertex on G, such that there are t pendent vertices $v_1, v_2, \ldots, v_t$ attached at v. Assume that*

$$G_1 = G - \{vv_1, vv_2, \ldots, vv_t\} + \{uv_1, uv_2, \ldots, uv_t\}$$

and

$$G_2 = G - \{uu_1, uu_2, \ldots, uu_s\} + \{vu_1, vu_2, \ldots, vu_s\} \ .$$

Then either $S'(G) > S'(G_1)$ or $S'(G) > S'(G_2)$.

Proof. Let $A = \{u_1, u_2, \ldots, u_s\}$, $B = \{v_1, v_2, \ldots, v_t\}$ and H be the subgraph induced by $V(G) \setminus \{A, B\}$. Further, let $R(u, v) = l$.

In the transformation $G \to G_1$, for any pair of vertices x, y satisfying $x, y \in V(H - u - v)$ or $x, y \in A$ or $x, y \in B$ or $x \in A$, $y \in V(H - u - v)$, the term $\sum\limits_{x,y} d(x)\, d(y)\, R(x, y)$ does not change. Then

$$\begin{aligned}
S'(G) &= \left[\sum_{x,y\in V(H-u-v)} + \sum_{x,y\in A} + \sum_{x,y\in B} + \sum_{\substack{x\in A\\ y\in V(H-u-v)}}\right] d(x)\, d(y)\, R(x, y) \\
&+ \sum_{\substack{x\in A\\ y\in B}} d(x)\, d(y)\, R(x, y) + \sum_{\substack{x\in V(H-u-v)\\ y\in B}} d(x)\, d(y)\, R(x, y) \\
&+ d(u)\left[\sum_{x\in V(H-u-v)} d(x)\, R(x, u) + \sum_{x\in A} d(x)\, R(x, u) + \sum_{x\in B} d(x)\, R(x, u)\right] \\
&+ d(v)\left[\sum_{x\in V(H-u-v)} d(x)\, R(x, v) + \sum_{x\in A} d(x)\, R(x, v) + \sum_{x\in B} d(x)\, R(x, v)\right] \\
&+ d(u)\, d(v)\, R(u, v) \\
&= \left[\sum_{x,y\in V(H-u-v)} + \sum_{x,y\in A} + \sum_{x,y\in B} + \sum_{\substack{x\in A\\ y\in V(H-u-v)}}\right] d(x)\, d(y)\, R(x, y) \\
&+ (l+2)st + t\sum_{x\in V(H-u-v)} \Big(d(x)\, R(x, v) + d(x)\Big) \\
&+ (s+2)\left[\sum_{x\in V(H-u-v)} d(x)\, R(x, u) + s + (l+1)t\right] \\
&+ (t+2)\left[\sum_{x\in V(H-u-v)} d(x)\, R(x, v) + t + (l+1)s\right] + (s+2)(t+2)l
\end{aligned}$$

and analogously,

$$\begin{aligned}
S'(G_1) &= \left[\sum_{x,y\in V(H-u-v)} + \sum_{x,y\in A} + \sum_{x,y\in B} + \sum_{\substack{x\in A\\ y\in V(H-u-v)}}\right] d(x)\, d(y)\, R(x, y) \\
&+ 2st + t\sum_{x\in V(H-u-v)} d(x)\, R(x, u) + t\sum_{x\in V(H-u-v)} d(x)
\end{aligned}$$

$$+ \quad (t+s+2)\left[\sum_{x\in V(H-u-v)} d(x)\,R(x,u)+s+t\right]$$

$$+ \quad 2\left[\sum_{x\in V(H-u-v)} d(x)\,R(x,v)+(l+1)t+(l+1)s\right]+2(s+t+2)l\ .$$

So we get

$$S'(G)-S'(G_1) \;=\; 2t\left[2ls+\sum_{x\in V(H-u-v)} d(x)\big[R(x,v)-R(x,u)\big]\right].$$

By a similar reasoning one arrives at

$$S'(G)-S'(G_2) \;=\; 2s\left[2lt+\sum_{x\in V(H-u-v)} d(x)\big[R(x,u)-R(x,v)\big]\right].$$

Hence, if $S'(G)-S'(G_i)>0$ for $i=1,2$, then the result follows. If at least one difference is negative, say $S'(G)-S'(G_1)<0$, then $\sum_{x\in V(H-u-v)} d(x)\big[R(x,u)-R(x,v)\big] > 2ls$ and therefore $S'(G)-S'(G_2)>2s(2lt+2ls)>0$. This completes the proof. □

3 Unicyclic graphs with maximum and second–maximum degree Kirchhoff index

Let $\mathcal{U}_{n,k}$ be the set of all connected unicyclic graphs of order $n\geq 3$ with girth $k\geq 3$.

Lemma 6. *Among the elements of $\mathcal{U}_{n,k}$, the graph U_k^n defined in Example 3 has maximal degree Kirchhoff index.*

Proof. Let Q_0 be an arbitrary connected graph, possessing m_0 edges. Let u be an arbitrary vertex of Q_0. For brevity, denote $V(Q_0)\setminus\{u\}$ by V.

Construct the graph Q_1 by attaching a new pendent vertex to the vertex u of Q_0. Let this new vertex be denoted by v_1.

Applying Theorem 2 to Q_1, assuming that $G_1\cong Q_0$ and $G_2\cong P_2$, we obtain the following special case of Eq. (7):

$$S'(Q_1)=S'(Q_0)+2\,S'(u|Q_0)+2m_0+1\ . \tag{15}$$

We now compute $S'(v_1|Q_1)$, bearing in mind Eq. (4):

$$S'(v_1|Q_1) = \left[\sum_{x\in V} + \sum_{x=u} + \sum_{x=v_1}\right] d(x|Q_1)\, R(x, v_1|Q_1)\ .$$

Since $R(x, v_1|Q_1) = R(x, u|Q_0) + 1$ and $d(u|Q_1) = d(u|Q_0) + 1$, we have

$$\begin{aligned}\sum_{x\in V} d(x|Q_1)\, R(x, v_1|Q_1) &= \sum_{x\in V} d(x|Q_0)\, [R(x, u|Q_0) + 1] \\ &= \sum_{x\in V(Q_0)} d(x|Q_0)\, R(x, u|Q_0) + 2m_0 - d(u|Q_0) \\ &= S'(u|Q_0) + 2m_0 - d(u|Q_0)\end{aligned}$$

$$\sum_{x=u} d(x|Q_1)\, R(x, v_1|Q_1) = d(u|Q_1)\cdot 1 = d(u|Q_0) + 1$$

and

$$\sum_{x=v_1} d(x|Q_1)\, R(x, v_1|Q_1) = 0$$

which implies

$$S'(v_1|Q_1) = S'(u|Q_0) + 2m_0 + 1\ . \tag{16}$$

Suppose now that $Q_0 \in \mathcal{U}_{n,k}$ and that Q_0 has the maximal degree Kirchhoff index in $\mathcal{U}_{n,k}$. Let u be the vertex of Q_0 with greatest value of $S'(x|Q_0)$. Then by Eq. (15), Q_1 has maximal degree Kirchhoff index in $\mathcal{U}_{n+1,k}$. Further, by Eq. (16), the vertex v_1 in Q_1 has the greatest value of $S'(x|Q_1)$.

Continuing this argument, we conclude that the graph Q_2 obtained by attaching a new pendent vertex v_2 to the vertex v_1 of Q_1 has maximal degree Kirchhoff index in $\mathcal{U}_{n+2,k}$, and that u_2 has the greatest value for $S'(x|Q_2)$, etc.

Start the above described construction at $n = k$, and note that the cycle C_k is the unique element of $\mathcal{U}_{k,k}$. Then the graphs with fixed value of k and $n = k, k+1, k+2, \ldots$ vertices are just the graphs U_k^n. □

Theorem 7. *Among connected unicyclic graphs with n vertices, $n \geq 3$, the graph U_3^n defined in Example 3 has maximal degree Kirchhoff index.*

Proof. In view of Lemma 6, it is sufficient to verify that for any fixed value of $n \geq 3$ and for $k = 3, \ldots, n$, the graph $\mathcal{U}_{n,3}$ has the greatest degree Kirchhoff index.

If $n = 3$, then there exists just one graph $\mathcal{U}_{n,k}$ (namely the cycle C_3) and we are done. Let $n \geq 4$ and consider the right–hand side of Eq. (13) as a function of the variable k.

In the interval $[3, n]$ this function first decreases, reaches a minimum and then increases. Therefore it is sufficient to show that

$$\frac{1}{3}\left(3k^3 - 4nk^2 + 2n^3 - n\right)\Big|_{k=3} > \frac{1}{3}\left(3k^3 - 4nk^2 + 2n^3 - n\right)\Big|_{k=n} ,$$

which is equivalent to

$$n^3 - 36n + 81 > 0 \quad \Leftrightarrow \quad (n-3)^3 + 9(n-3)(n-4) > 0 ,$$

which is evidently satisfied for all $n \geq 4$. □

In order to eliminate trivial cases, in what follows we assume that $n \geq 6$. Denote the unique pendent vertex of U_3^{n-1} by v and its first neighbor by v'. Construct the graph W_3^n by attaching a new pendent vertex to the vertex v' of U_3^{n-1}.

Theorem 8. *Among connected unicyclic graphs with n vertices, $n \geq 6$, the graph W_3^n has second–maximal degree Kirchhoff index.*

Proof. The proof of Theorem 8 is analogous to the proof of Theorem 7, and its details are omitted. It is based on the fact that the vertex v' of U_3^{n-1} has the second–largest value for $S'(x|U_3^{n-1})$. □

4 Unicyclic graphs with minimum and second–minimum degree Kirchhoff index

In this section, for convenience, we represent a unicyclic graph G with the unique cycle $C_k = v_1v_2 \dots v_kv_1$ as $G = U(C_k\,;\, T_1, T_2, \dots, T_k)$, where T_i is the component of $G - E(C_k)$ containing v_i, $1 \leq i \leq k$. Obviously, T_i is a tree rooted at v_i. We say that T_i is trivial if it consists of an isolated vertex. We denote by $H_{n,k}$ the graph obtained from C_k by adding $n - k$ pendent vertices to a vertex of C_k.

Theorem 9. *Let G be a unicyclic graph of order n with girth k. Then $S'(G) \geq S'(H_{n,k})$, with equality if and only if $G \cong H_{n,k}$.*

Proof. Let $G = U(C_k\,;\, T_1, T_2, \dots, T_k)$ be as described above. By Theorem 4, T_i $(1 \leq i \leq k)$ is a star with v_i as its center. From Theorem 5, there exists only one non-trivial star attached at C_k, and this implies the result. □

Let $C_k = v_1v_2 \dots v_kv_1$ be a cycle on k vertices. Then [42], for $1 \le i < j \le k$,

$$R(v_i, v_j) = \frac{(j-i)(k-j+i)}{k} \ge \frac{k-1}{k}$$

and

$$R(v_1|C_k) = \sum_{x \in V(C_k - v_1)} R(x, v_1) = \frac{k^2-1}{6} \qquad , \qquad Kf(C_k) = \frac{k^3-k}{12} \ .$$

For the graph $H_{n,k}$, in view of Theorem 2, let $G_1 = C_k$, $G_2 = H_{n,k} - C_k + u$, where u is the only vertex on C_k with degree larger than 2. It is easy to see that

$$S'(u|G_2) = \sum_{x \in V(G_2)} d(x)R(x,u) = n-k \qquad , \qquad S'(u|G_1) = \frac{k^2-1}{3} \ .$$

Therefore it follows that

$$\begin{aligned} S'(H_{n,k}) &= S'(G_1) + S'(G_2) + 2k\, S'(u|G_2) + 2(n-k)\, S'(u|G_1) \\ &= \frac{k^3-k}{3} + (n-k)(2n-2k-1) + 2k(n-k) + 2(n-k)\frac{k^2-1}{3} \\ &= \frac{1}{3}(4k - k^3 - 5n - 6kn + 2k^2n + 6n^2) \ . \end{aligned}$$

Corollary 10. *Let G be a unicyclic graph of order $n \ge 5$. Then*

$$S'(G) \ge \frac{1}{3}(6n^2 - 5n - 15) \ .$$

The equality holds if and only if $G \cong H_{n,3}$.

Proof. It is easy to see that for $3 \le k \le n-2$,

$$S'(H_{n,k}) - S'(H_{n,3}) = \frac{1}{3}\,(k-3)(2nk - k^2 - 3k - 5) \ge 0 \ .$$

The inequality holds since $f(k) := 2nk - k^2 - 3k - 5$ is increasing for $4 \le k \le n-2$, and hence $f(k) \ge f(4) > 0$.

For $k = n-1, n$, one has

$$\begin{aligned} S'(H_{n,n-1}) - S'(H_{n,3}) &= \frac{1}{3}\,(n-4)(n^2-3n-3) > 0 \\ S'(H_{n,n}) - S'(H_{n,3}) &= \frac{1}{3}\,(n-3)(n^2-3n-5) > 0 \ . \end{aligned}$$

This implies the result. □

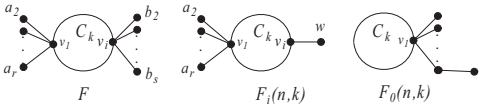

Figure 2: *Graphs mentioned in Lemma 11*

Lemma 11. *Let $F_i(n,k)$ and $F_0(n,k)$ be two graphs as depicted in Fig. 2, $n \geq 12$. Then $S'(F_i(n,k)) \geq S'(F_2(n,k))$, $S'(F_2(n,k)) \geq S'(F_2(n,3))$, $S'(F_0(n,k)) > S'(F_2(n,k))$.*

Proof. For the graph $F_i(n,k)$, let $G_1 = K_{1,r-1}$, $G_2 = H_{k+1,k}$ with common vertex v_1 and $r = n-k$. Assume that the pendent vertex of G_2 is w. It is easy to see that

$$\begin{aligned} S'(K_{1,r-1}) &= S(K_{1,r-1}) = 4W(K_{1,r-1}) - (2r-1)(r-1) = (r-1)(2r-3) \\ S'(H_{k+1,k}) &= \frac{1}{3}(k^3+2k^2+5k+1)\ . \end{aligned}$$

In view of Theorem 2,

$$\begin{aligned} S'(v_1|G_2) &= \sum_{x\in V(G_2)} d(x)R(x,v_1) \\ &= \sum_{x\in V(G_2-w-v_i)} d(x)R(x,v_1) + d(v_i)R(v_i,v_1) + d(w)R(w,v_1) \\ &= 2\sum_{x\in V(G_2-w-v_i)} R(x,v_1) + 3R(v_i,v_1) + R(v_i,v_1) + 1 \\ &= 2\sum_{x\in V(G_2-w)} R(x,v_1) + 2R(v_i,v_1) + 1 \\ &= 2R(v_1|C_k) + 2R(v_i,v_1) + 1 \end{aligned}$$

and

$$S'(v_1|G_1) = \sum_{x\in V(G_1)} d(x)R(x,v_1) = n-k-1\ .$$

Therefore,

$$\begin{aligned} S'(F_i(n,k)) &= (n-k-1)(2n-2k-3) + \frac{1}{3}(k^3+2k^2+5k+1) \\ &+ 2(n-k-1)\Big(2\frac{k^2-1}{6} + 2\frac{(i-1)(k-i+1)}{k} + 1\Big) + 2(k+1)(n-k-1) \\ &\geq (n-k-1)(2n-2k-3) + \frac{1}{3}(k^3+2k^2+5k+1) \\ &+ 2(n-k-1)\Big(2\frac{k^2-1}{6} + 2\frac{k-1}{k} + 1\Big) + 2(k+1)(n-k-1) \end{aligned}$$

$$= S'(F_2(n,k)) = \frac{1}{3k}\Big(12 - 8k^2 - k^4 - 12n + 7kn - 6k^2\,n + 2k^3\,n + 6k\,n^2\Big) .$$

$$S'(F_2(n,3)) = \frac{1}{3}\,(6n^2 + 3n - 47) .$$

From above, we have $S'(F_i(n,k)) \geq S'(F_2(n,k))$, and notice that $F_2(n,k) \cong F_k(n,k)$. Therefore,

$$S'(F_2(n,k)) - S'(F_2(n,3)) = \frac{1}{3k}\,(k-3)(-4 - 17k - 3k^2 - k^3 + 4n + 2k^2\,n) \geq 0 .$$

The inequality holds since $g(k) := -4 - 17k - 3k^2 - k^3 + 4n + 2k^2\,n$ is increasing in the interval $[4,n]$ and hence $g(k) \geq g(4) > 0$.

For $F_0(n,k)$, let $G_1 = F_0(n,k) - C_k + v_1$, $G_2 = C_k$. Assume that the vertex of degree 2 in G_1 is u and its pendent neighbor is w.

In view of Theorem 2, we have

$$S'(v_1|G_2) = \sum_{x \in V(G_2)} d(x)R(x,v_1) = 2R(v_1|C_k) = \frac{k^2-1}{3}$$

and

$$S'(v_1|G_1) = \sum_{x \in V(G_1)} d(x)R(x,v_1) = n - k + 2 .$$

Hence,

$$\begin{aligned} S'(F_0(n,k)) &= \frac{k^3-k}{3} + 2(n-k+1)^2 - (n-k+1) - 9 \\ &+ 2(n-k)\frac{k^2-1}{3} + 2k(n-k+2) \\ &= \frac{1}{3}(-24 + 4k - k^3 + 7n - 6kn + 2k^2n + 6n^2) \end{aligned}$$

which finally yields

$$S'(F_0(n,k)) - S'(F_2(n,k)) = \frac{4}{k}\,(-1 - 2k + k^2 + n) > 0 .$$

This proves the result. □

Theorem 12. *Let $G \neq H_{n,k}$ be a unicyclic graph of order n (≥ 12). Then*

$$S'(G) \geq S'(F_2(n,k)) .$$

The equality holds if and only if $G \cong F_2(n,k)$.

Proof. Suppose that G has the second–smallest degree Kirchhoff index among all connected n-vertex unicyclic graphs. Suppose that the girth of G is k. Then G has the form $U(C_k; T_1, T_2, \ldots, T_k)$ as described above.

First, we claim that at most two of $T_1, T_2, \ldots, T_k$ are not trivial. Otherwise, we may assume that T_1, T_2, T_3 are not trivial. By Theorem 4, they must be stars with centers v_1, v_2, v_3, respectively. Let $V(T_1) = \{v_1, a_2, a_3, \ldots, a_r\}$, $V(T_2) = \{v_2, b_2, b_3, \ldots, b_s\}$, $V(T_3) = \{v_3, c_2, c_3, \ldots, c_t\}$. Then by Theorem 5, $S'(G) > \min\{S'(G - v_2b_2 + v_1b_2), S'(G - v_1a_2 + v_2a_2)\} > S'(H_k)$. This contradicts to the choice of G.

Next, if exactly two of $T_1, T_2, \ldots, T_k$ are not trivial, then without loss of generality, we can assume that T_1 and T_i are not trivial, $1 < i \leq k$. Then by Theorems 4 and 5 they are stars with centers v_1, v_i, respectively. In other words, G is the graph of the form F as shown in Figure 2. Let $V(T_1) = \{v_1, a_2, a_3, \ldots, a_r\}$, $V(T_i) = \{v_i, b_2, b_3, \ldots, b_s\}$, where $r + s + k = n + 2$, $r \geq 2$ and $s \geq 2$. From Lemma 11, we have $r = 2$ or $s = 2$. Without loss of generality, assume that $s = 2$, i. e., $G = F_i(n, k)$ is the graph shown in Figure 2. Then $r + k = n$. From Lemma 11, we have $i = 2$ or $i = k$

If exactly one of $T_1, T_2, \ldots, T_k$ is not trivial, without loss of generality, we assume that it is T_1 . Since $G \neq H_{n,k}$ and T_1 is not a star, from Theorem 4 it follows that G must be the graph $F_0(n, k)$ as shown in Figure 2.

From Lemma 11, $S'(F_0(n, k)) > S'(F_2(n, k))$, so we get the result. □

Corollary 13. *Let $G \neq H_{n,3}$ be a unicyclic graph of order $n \geq 12$. Then*

$$S'(G) \geq \frac{1}{3}\left(6n^2 + 3n - 47\right) .$$

The equality holds if and only if $G \cong F_2(n, 3)$.

Proof. From Theorem 12, we have $S'(G) \geq S'(F_2(n, k))$. By Lemma 11, $S'(F_2(n, k)) \geq S'(F_2(n, 3))$, which implies the result. □

Concluding this paper, we find that the extremal graphs for the degree Kirchhoff index are the same as the extremal graphs for the ordinary Kirchhoff index or the Wiener index [42, 43, 45].

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