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# Unicyclic graphs with extremal Kirchhoff index*

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**Abstract**

Resistance distance was introduced by Klein and Randić (J. Math. Chem. 12 (1993) 81–95). The Kirchhoff index $Kf(G)$ of a graph $G$ is the sum of resistance distances between all pairs of vertices. Let $S_n^l$ denote the graph obtained from cycle $C_l$ by adding $n-l$ pendant edges to a vertex of $C_l$. Let $P_n^l$ denote the graph obtained by identifying one endvertex of path $P_{n-l+1}$ with any vertex of $C_l$. In this paper, we show that among $n$-vertex unicyclic graphs, (i) if $n < 8$, $C_n$ has minimal Kirchhoff index; if $8 \leq n < 12$, $S_n^4$ has minimal Kirchhoff index; if $n = 12$, both $S_n^3$ and $S_n^4$ have minimal Kirchhoff index; otherwise, $S_n^3$ has minimal Kirchhoff index; (ii)$P_n^3$ has maximal Kirchhoff index. Sharp bounds for Kirchhoff index of unicyclic graphs are also obtained.

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# 1 Introduction

Let $G$ be a connected graph with vertices labeled as $v_1, v_2, \cdots, v_n$. The distance between vertices $v_i$ and $v_j$, denoted by $d(v_i, v_j)$, is the length of a shortest path between them. The famous Wiener index $W(G)$ [1] is the sum of distances between all pairs of vertices, that is,

$$W(G) = \sum_{i<j} d(v_i, v_j).$$

In 1993, Klein and Randić [2] introduced a new distance function named resistance distance basing on electrical network theory. They view $G$ as an electrical network $N$ such that each edge of $G$ is assumed to be a unit resistor. The resistance distance between vertices $v_i$ and $v_j$, denoted by $r(v_i, v_j)$ (if more than one graphs are considered, we use $r_G(v_i, v_j)$ to avoid confusion), is defined to be the effective resistance between nodes $v_i$ and $v_j$ in $N$. Analogue to Wiener index, the Kirchhoff index $Kf(G)$ [3] is defined as:

$$Kf(G) = \sum_{i<j} r(v_i, v_j).$$

As an intrinsic graph metric and a relevant tool to characterize wave- or fluid-like communication between two vertices [4], resistance distance is well studied both in mathematical and chemical literatures [5, 6, 7, 8, 9, 10, 11, 12]. It is computed in various ways: in algebra using generalized inverse of Laplacian matrix [2], Laplacian eigenvalues and eigenvectors [13] and normalized Laplacian eigenvalues and eigenvectors [16]; in combinatorics using spanning trees and spanning bi-trees [14]; in probability using random walks [15]. As a new useful structure-descriptor [17], Kirchhoff index attracts more and more attention. Much work has been done to compute Kirchhoff index of some classes of graphs [20, 21, 22, 23, 24, 25, 26].

Though it is usually difficult to compute Kirchhoff index of graphs, we can give some bounds for Kirchhoff index of graphs and characterize extremal graphs as well. Let $P_n$ (resp. $C_n$) denote the path (resp. cycle) on $n$ vertices. For a general graph $G$, Lukovits et al. [18] 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 [19] proved 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. [25] showed that

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

The first equality holds if and only if $G$ is $K_n$ and the second does if and only if $G$ is $C_n$.

In this paper, we concentrate on unicyclic graphs. A graph $G$ is called a unicyclic graph if it contains exactly one cycle. We may use the following notation to represent a unicyclic graph:

$$G = U(C_l; T_1, T_2, \cdots, T_l),$$

where $C_l$ is the unique cycle in $G$ with $V(C_l) = \{v_1, v_2, \cdots, v_l\}$ such that $v_i$ is adjacent to $v_{i+1}$ (subscript module $l$) for $1 \leq i \leq l$. For each $i$, let $T_i$ be the component of $G-(V(C_l)-v_i)$ containing $v_i$. Obviously $T_i$ is a tree. We say $T_i$ trivial if it is an isolated vertex. For example, see Fig. 1.

For convenience, we employ the following notation. Let $\mathcal{G}(n, l)$ be the set of all unicyclic graphs on $n$ vertices containing cycle $C_l$. Let $S_n^l$ denote the graph obtained from cycle $C_l$ by adding $n - l$ pendant edges to a vertex of $C_l$. Let $P_n^l$ denote the graph obtained by identifying one endvertex of $P_{n-l+1}$ with any vertex of $C_l$. $S_n^l$ and $P_n^l$ are depicted in Fig. 2. It is obvious that $S_n^n = P_n^n = C_n$.

Let $W_{v_i}(G)$ denote the sum of all distances between vertex $v_i$ and the other vertices of $G$, that is

$$W_{v_i}(G) = \sum_{j \neq i} d(v_i, v_j).$$

Similarly, we define $Kf_{v_i}(G)$ as follows:

$$Kf_{v_i}(G) = \sum_{j \neq i} r(v_i, v_j).$$

In this paper, first of all, simple explicit formula for Kirchhoff index of unicyclic graphs is derived in terms of their structure. In the following, we prove that among $\mathcal{G}(n, l)$, $S_n^l$ and $P_n^l$

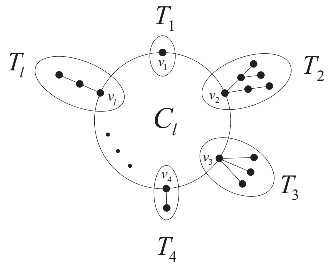


Fig. 1. $U(C_l; T_1, T_2, \cdots, T_l)$.

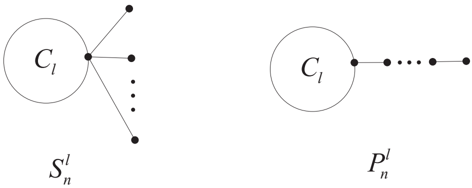


Fig. 2. $S_n^l$ and $P_n^l$.

have minimal and maximal Kirchhoff index, respectively. It enables us to search for $n$-vertex unicyclic graphs with minimal and maximal Kirchhoff index only among $S_n^3, S_n^4, \cdots, S_n^n$ and $P_n^3, P_n^4, \cdots, P_n^n$, respectively. In addition, bounds for Kirchhoff index of $\mathcal{G}(n, l)$ are obtained accordingly. In order to characterize unicyclic graphs with extremal Kirchhoff index, $\min\limits_{3 \le l \le n}\{Kf(S_n^l)\}$ (Lemma 4.1) and $\max\limits_{3 \le l \le n}\{Kf(P_n^l)\}$ (Lemma 4.2) are determined by analytical method. According to the above two Lemmas, we obtain that among $n$-vertex unicyclic graphs, (i) if $n < 8$, $C_n$ has minimal Kirchhoff index; if $8 \le n < 12$, $S_n^4$ has minimal Kirchhoff index; if $n = 12$, both $S_n^3$ and $S_n^4$ have minimal Kirchhoff index; otherwise, $S_n^3$ has minimal Kirchhoff index; (ii) $P_n^3$ has maximal Kirchhoff index. Sharp bounds for Kirchhoff index of unicyclic graphs are derived as well.

## 2 Kirchhoff index of unicyclic graphs

**Lemma 2.1.** *[2] Let $x$ be a cutvertex of a graph, and let $a$ and $b$ be vertices occurring in different components which arise upon deletion of $x$. Then*

$$r(a,b) = r(a,x) + r(x,b).$$

**Theorem 2.2.** *Let $G = U(C_l; T_1, T_2, \cdots, T_l)$. Then*

$$Kf(G) = \sum_{i=1}^{l} W(T_i) + \sum_{i<j} \big(|V(T_j)|W_{v_i}(T_i) + |V(T_i)||V(T_j)|\frac{(j-i)(l-j+i)}{l} + |V(T_i)|W_{v_j}(T_j)\big). \tag{1}$$

*Proof.* The Kirchhoff index of $G$ is the sum of two types of resistance distances, namely between pairs of vertices from $T_i$ ($1 \le i \le l$), and between a vertex $a$ from $T_i$ and another vertex $b$ from $T_j$ ($1 \le i < j \le l$). By Lemma 2.1,

$$r(a,b) = r(a,v_i) + r(v_i,v_j) + r(v_j,b) = d(a,v_i) + r(v_i,v_j) + d(v_j,b).$$

Noticing that $r(v_i,v_j) = \frac{(j-i)(l-j+i)}{l}$ [27], we have

$$r(a,b) = d(a,v_i) + \frac{(j-i)(l-j+i)}{l} + d(v_j,b).$$

Hence

$$\begin{aligned} Kf(G) &= \sum_{i=1}^{l} W(T_i) + \sum_{i<j} \sum_{a\in V(T_i)} \sum_{b\in V(T_j)} \big(d(a,v_i) + \frac{(j-i)(l-j+i)}{l} + d(v_j,b)\big) \\ &= \sum_{i=1}^{l} W(T_i) + \sum_{i<j} \sum_{a\in V(T_i)} \big(|V(T_j)|d(a,v_i) + |V(T_j)|\frac{(j-i)(l-j+i)}{l} + W_{v_j}(T_j)\big) \\ &= \sum_{i=1}^{l} W(T_i) + \sum_{i<j} \big(|V(T_j)|W_{v_i}(T_i) + |V(T_i)||V(T_j)|\frac{(j-i)(l-j+i)}{l} \\ &\quad + |V(T_i)|W_{v_j}(T_j)\big). \end{aligned}$$

□

**Remark.** Eq. (1) can also be written as:

$$\begin{aligned} Kf(G) &= \frac{l^3-l}{12} + \sum_{i=1}^{l} W(T_i) \\ &\quad + \sum_{i<j} \Big( |V(T_j)| W_{v_i}(T_i) + (|V(T_i)||V(T_j)| - 1) \frac{(j-i)(l-j+i)}{l} + |V(T_i)| W_{v_j}(T_j) \Big). \end{aligned} \tag{2}$$

We first compute the resistance distances between vertices of $C_l$ and bearing in mind that $Kf(C_l) = \frac{l^3-l}{12}$ [18], then Eq. (2) is derived from Eq. (1).

## 3 Bounds for Kirchhoff index of $\mathcal{G}(n,l)$

**Lemma 3.1.** *[28] Let $T$ be a n-vertex tree different from $P_n$ and $S_n$. Then*

$$W(S_n) < W(T) < W(P_n).$$

It is also obtained in [28] that

$$W(S_n) = (n-1)^2, \tag{3}$$

$$W(P_n) = \binom{n+1}{3} = \frac{n^3-n}{6}. \tag{4}$$

The following two Lemmas show that among $\mathcal{G}(n,l)$, $S_n^l$ and $P_n^l$ has minimal and maximal Kirchhoff index, respectively.

**Lemma 3.2.** *Let $G \in \mathcal{G}(n,l)$ and $G \neq S_n^l$. Then $Kf(G) > Kf(S_n^l)$.*

*Proof.* Suppose that $G_0 = U(C_l; T_1, T_2, \cdots, T_l)$ has minimal Kirchhoff index among $\mathcal{G}(n,l)$.

**Claim 1**. For each $i$, $T_i$ is a star with $v_i$ as its central vertex.

For each $i$, $W(T_i)$ is minimal if and only if $T_i$ is a star by Lemma 3.1 and it is obvious that $W_{v_i}(T_i)$ is minimal if and only if $T_i$ is a star with $v_i$ as its central vertex. Hence Claim 1 holds by Eq. (1).

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

Suppose to the contrary 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 stars. We choose $a \in V(T_i)$ and $b \in V(T_j)$ such that $a \neq v_i$ and $b \neq v_j$. Without loss of generality, assume that $Kf_a(G_0) \leq Kf_b(G_0)$. Let $G_0' = G_0 - v_j b + v_i b$. We will show that $Kf(G_0') < Kf(G_0)$.

For any two vertices $x$, $y$ different from $b$, $r_{G_0}(x,y) = r_{G_0'}(x,y)$, hence

$$Kf(G_0) - Kf_b(G_0) = Kf(G_0') - Kf_b(G_0').$$

On the other hand,

$$Kf_b(G_0') = Kf_a(G_0') = Kf_a(G_0) - r_{G_0}(a,b) + 2 < Kf_a(G_0) \leq Kf_b(G_0).$$

Hence

$$Kf(G_0') = Kf(G_0) - Kf_b(G_0) + Kf_b(G_0') < Kf(G_0).$$

This contradicts the choice of $G_0$, which implies Claim 2.

Claims 1 and 2 yield Lemma 3.2. □

**Lemma 3.3.** *Let $G \in \mathcal{G}(n,l)$ and $G \neq P_n^l$. Then $Kf(G) < Kf(P_n^l)$.*

*Proof.* Suppose that $G_0 = U(C_l; T_1, T_2, \cdots, T_l)$ has maximal Kirchhoff index among $\mathcal{G}(n,l)$.

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

For each $i$, $W(T_i)$ is maximal if and only if $T_i$ is a path by Lemma 3.1 and it is easy to observe that $W_{v_i}(T_i)$ is maximal if and only if $T_i$ is a path with $v_i$ as one of its end-vertices. Hence Claim 1 holds by Eq. (1).

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

Suppose to the contrary that there exists at least two trees such that they all have more than one vertices. Let $T_i$ and $T_j$ be two such trees. By Claim 1, $T_i$ and $T_j$ are both paths. Let $a \neq v_i$ and $b \neq v_j$ be endvertices of $T_i$ and $T_j$, respectively. Without losing generality, assume that $Kf_a(G_0) \geq Kf_b(G_0)$. Let $c$ be the neighbor of $b$ and $G_0' = G_0 - cb + ab$. Now we show that $Kf(G_0') > Kf(G_0)$.

For any two vertices $x$, $y$ different from $b$, $r_{G_0}(x,y) = r_{G_0'}(x,y)$, hence

$$Kf(G_0) - Kf_b(G_0) = Kf(G_0') - Kf_b(G_0').$$

On the other hand,

$$Kf_b(G_0') = Kf_a(G_0') + n - 2 = Kf_a(G_0) + 1 - r_{G_0}(a,b) + n - 2.$$

Since $r_{G_0}(a,b) < d_{G_0}(a,b) < n-1$, it follows that $Kf_b(G_0') > Kf_a(G_0) \geq Kf_b(G_0)$. Hence

$$Kf(G_0') = Kf(G_0) - Kf_b(G_0) + Kf_b(G_0') > Kf(G_0).$$

This contradicts the choice of $G_0$, which implies Claim 2.

Claims 1 and 2 yield Lemma 3.3. □

By Eqs. (2), (3) and (4), Kirchhoff index of $S_n^l$ and $P_n^l$ are computed as follows:

$$\begin{aligned} Kf(S_n^l) &= \frac{l^3 - l}{12} + (n-l)^2 + \frac{(n-l)(l^2-1)}{6} + (n-l)(l-1) \\ &= -\frac{l^3}{12} + \frac{nl^2}{6} + (\frac{13}{12} - n)l + n^2 - \frac{7n}{6}, \end{aligned} \tag{5}$$

$$\begin{aligned} Kf(P_n^l) &= \frac{l^3 - l}{12} + \frac{(n-l+1)^3 - (n-l+1)}{6} + \frac{(n-l)(l^2-1)}{6} + \frac{(n-l)(n-l+1)(l-1)}{2} \\ &= \frac{l^3}{4} - \frac{(3+2n)l^2}{6} + \frac{(3+6n)l}{12} + \frac{n^3 - 2n}{6}. \end{aligned} \tag{6}$$

Together with Lemmas 1 and 2, the following Theorem is immediate.

**Theorem 3.4.** *For $G \in \mathcal{G}(n,l)$, we have*

$$-\frac{l^3}{12} + \frac{nl^2}{6} + (\frac{13}{12} - n)l + n^2 - \frac{7n}{6} \leq Kf(G) \leq \frac{l^3}{4} - \frac{(3+2n)l^2}{6} + \frac{(3+6n)l}{12} + \frac{n^3 - 2n}{6}.$$

*The first equality holds if and only if $G = S_n^l$ and the second does if and only if $G = P_n^l$.*

# 4 Unicyclic graphs with extremal Kirchhoff index

In this section, we characterize unicyclic graphs with extremal Kirchhoff index and determine bounds for Kirchhoff index of unicyclic graphs.

By Lemmas 3.2 and 3.3, $n$-vertex unicyclic graphs with minimal and maximal Kirchhoff index belong to sets $\{S_n^3, S_n^4, \cdots, S_n^n\}$ and $\{P_n^3, P_n^4, \cdots, P_n^n\}$, respectively. In what follows, we apply ourselves to finding $\min\limits_{3\leq l\leq n}\{Kf(S_n^l)\}$ and $\max\limits_{3\leq l\leq n}\{Kf(P_n^l)\}$ by analytical method.

**Lemma 4.1.**

$$\min_{3\leq l\leq n}\{Kf(S_n^l)\} = \begin{cases} Kf(C_n) & \text{if } n<8, \\ Kf(S_n^4) & \text{if } 8\leq n<12, \\ Kf(S_n^3)=Kf(S_n^4) & \text{if } n=12, \\ Kf(S_n^3) & \text{otherwise.} \end{cases}$$

*Proof.* Let

$$f(l) := Kf(S_n^l) = -\frac{l^3}{12} + \frac{nl^2}{6} + (\frac{13}{12} - n)l + n^2 - \frac{7n}{6}$$

and $I := \{3, 4, \cdots, n\}$.

Our aim is to find the minimum value of $f(l)$ on $I$. To this end, we first find the first derivative of $f(l)$:

$$f^{'}(l) = -\frac{l^2}{4} + \frac{nl}{3} - n + \frac{13}{12}.$$

Solving $f^{'}(l) = 0$ for $l$ we obtain $l_{1,2} = \frac{2n\mp\sqrt{(2n-9)^2-42}}{3}$. By setting $\Delta := (2n-9)^2 - 42 = 0$, we have $n_{1,2} = \frac{9\mp\sqrt{42}}{2}$. It is easy to verify that $1 < n_1 < 2$ and $7 < n_2 < 8$. For convenience, we distinguish the following two cases:

**Case 1.** $3 \leq n \leq 7$. In this case, $\Delta < 0$. Hence $f^{'}(l) < 0$ and $f(l)$ is decreasing on $[3, n]$. So $f(n)$ is the minimum value of $f(l)$ on $I$.

**Case 2.** $n \geq 8$. In this case, $\Delta > 0$.

**Subcase 2.1** $n = 8, 9, 10$. It is easy to verify that $f(4)$ is the minimum value of $f(l)$ on $I$.

**Subcase 2.2** $n \geq 11$. In this case, it is easy to obtain that $l_2 > n$. On the other hand, since $(2n-12)^2 < (2n-9)^2 - 42 < (2n-9)^2$, it follows that $3 < l_1 < 4$. Hence $f^{'}(l) < 0$ on $[3, l_1)$ and $f^{'}(l) > 0$ on $(l_1, n]$, which implies that $f(l)$ is decreasing on $[3, l_1)$ and increasing on $(l_1, n]$. So $\min\{f(3), f(4)\}$ is the minimum value of $f(l)$ on $I$. Since

$$f(3) - f(4) = 2 - \frac{n}{6},$$

$$\min\{f(3), f(4)\} = \begin{cases} f(4) & \text{if } n < 12, \\ f(3) = f(4) & \text{if } n = 12, \\ f(3) & \text{otherwise.} \end{cases}$$

Hence Lemma 4.1 follows. □

**Lemma 4.2.** $\max\limits_{3 \leq l \leq n}\{Kf(P_n^l)\} = Kf(P_n^3)$.

*Proof.* Let

$$g(l) := Kf(P_n^l) = \frac{l^3}{4} - \frac{(3+2n)l^2}{6} + \frac{(3+6n)l}{12} + \frac{n^3 - 2n}{6}.$$

In what follows, we will find the maximum value of $g(l)$ on $I$.

The first derivative of $g(l)$ is

$$g^{'}(l) = \frac{1}{12}(9l^2 - (12+8n)l + 3 + 6n).$$

The roots of $g^{'}(l) = 0$ are $l_{1,2} = \frac{6+4n \mp \sqrt{16n^2 - 6n + 9}}{9}$. For $n \geq 3$, , $l_1 < \frac{6+4n-\sqrt{(4n-21)^2}}{9} = 3$ since $16n^2 - 6n + 9 > (4n-21)^2$ and it is easy to verify that $l_2 > 3$. In the following, we will show that $g(3)$ is the maximum value of $g(x)$ on $I$ no matter $l_2$ is more than or less than $n$.

(i) If $l_2 \geq n$, then $g^{'}(l) < 0$ and $g(l)$ is decreasing on $[3, n]$. So $g(3)$ is the maximum value of $g(l)$ on $I$.

(ii) If $3 < l_2 < n$, then $g^{'}(l) < 0$ on $[3, l_2)$ and $g^{'}(l) > 0$ on $(l_2, n]$, which indicates that $g(l)$ is decreasing on $[3, l_2)$ and increasing on $(l_2, n]$. So $\max\{g(3), g(n)\}$ is the maximum value of $g(l)$ on $I$. It is easy to obtain that

$$g(3) - g(n) = \frac{1}{12}(n^3 - 21n + 36).$$

Let $F(x) := \frac{1}{12}(x^3 - 21x + 36)$. Then $F^{'}(x) = 3x^2 - 21$. It is easy to verify that $F^{'}(x) > 0$ for $x \geq 3$. Hence $F(x)$ is increasing on $[3, n]$. Since $F(3) = 0$, it follows that $F(n) > 0$ for $n > 3$. So, as in (i), $g(3)$ is also the maximum value of $g(l)$ on $I$. □

Now we arrive at our main result:

**Theorem 4.3.** *Among n-vertex unicyclic graphs,*

(i)*if* $n < 8$, $C_n$ *has minimal Kirchhoff index; if* $8 \leq n < 12$, $S_n^4$ *has minimal Kirchhoff index; if* $n = 12$, *both* $S_n^3$ *and* $S_n^4$ *have minimal Kirchhoff index; otherwise,* $S_n^3$ *has minimal Kirchhoff index.*

(ii)$P_n^3$ *has maximal Kirchhoff index.*

By Eqs. (5) and (6), it is easy to obtain the following formulae:

(i) $Kf(C_n) = \frac{n^3-n}{12}$;

(ii) $Kf(S_n^3) = n^2 - \frac{8}{3}n + 1$;

(iii) $Kf(S_n^4) = n^2 - \frac{5}{2}n - 1$;

(iv) $Kf(P_n^3) = \frac{n^3-11n+18}{6}$.

Combining these formulae with Theorem 4.3, sharp bounds for Kirchhoff index of unicyclic graphs are determined:

**Theorem 4.4.** *For n-vertex unicyclic graph G,*

(i) *if* $n < 8$, $\frac{n^3-n}{12} \leq Kf(G) \leq \frac{n^3-11n+18}{6}$,

(ii) *if* $8 \leq n \leq 12$, $n^2 - \frac{5}{2}n - 1 \leq Kf(G) \leq \frac{n^3-11n+18}{6}$,

(iii) *if* $n > 12$, $n^2 - \frac{8}{3}n + 1 \leq Kf(G) \leq \frac{n^3-11n+18}{6}$.

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