Cacti with minimum, second-minimum, and third-minimum Kirchhoff indices

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Abstract. Resistance distance was introduced by Klein and Randić. The Kirchhoff index $Kf(G)$ of a graph $G$ is the sum of resistance distances between all pairs of vertices. A graph $G$ is called a cactus if each block of $G$ is either an edge or a cycle. Denote by $\text{Cat}(n;t)$ the set of connected cacti possessing $n$ vertices and $t$ cycles. In this paper, we give the first three smallest Kirchhoff indices among graphs in $\text{Cat}(n;t)$, and characterize the corresponding extremal graphs as well.

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1. Introduction

Let $G = (V(G), E(G))$ be a graph whose sets of vertices and edges are $V(G) = \{v_1, v_2, \ldots, v_n\}$ and $E(G)$, respectively.

In 1993, Klein and Randić [1] posed a new distance function named resistance distance on the basis of electrical network theory. The term resistance distance was used for the physical interpretation: one imagines unit resistors on each edge of a connected graph $G$ with vertices $v_1, v_2, \ldots, v_n$ and takes the resistance distance between vertices $v_i$ and $v_j$ of $G$ to be the effective resistance between vertices $v_i$ and $v_j$, denoted by $r_G(v_i, v_j)$. Recall that the conventional distance between vertices $v_i$ and $v_j$, denoted by $d_G(v_i, v_j)$, is the length of a shortest path between them and the famous Wiener index [2] is the sum of distances between all pairs of vertices; that is,

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

Analogous to the Wiener index, the Kirchhoff index [3] is defined as

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

Similarly to the conventional distance, the resistance distance is also intrinsic to the graph, not only with some nice purely mathematical and physical interpretations.
[4,5], but with a substantial potential for chemical applications. In fact, for those two distance functions, the shortest-path might be imagined to be more relevant when there is corpuscular communication (along edges) between two vertices, whereas the resistance distance might be imagined to be more relevant when the communication is wave- or fluid-like. Then, that chemical communication in molecules is rather wavelike suggests the utility of this concept in chemistry. So in recent years, the resistance distance has become much studied in the chemical literature [6-17]. It is found that the resistance distance is closely related with many well-known graph invariants, such as the connectivity index, the Balaban index, etc. This further suggests the resistance distance is worthy of being investigated. The resistance distance is also well studied in the mathematical literature. Much work has been done to compute the Kirchhoff index of some classes of graphs, or give bounds for the Kirchhoff index of graphs and characterize extremal graphs [10,15,18]. For instance, unicyclic graphs with the extremal Kirchhoff index are characterized and sharp bounds for the Kirchhoff index of such graphs are obtained [19]. In [20], the authors further investigated the Kirchhoff index in unicyclic graphs, and determined graphs with second- and third-minimal Kirchhoff indices as well as those graphs with second- and third-maximal Kirchhoff indices.

A graph $G$ is called a cactus if each block of $G$ is either an edge or a cycle. Denote by $\text{Cat}(n,t)$ the set of connected cacti possessing $n$ vertices and $t$ cycles. In this paper, we give the first three smallest Kirchhoff indices among graphs in $\text{Cat}(n,t)$ and characterize the corresponding extremal graphs as well.

2. Lemmas and main results

Before we state and prove our main results, we introduce some lemmas.

**Lemma 1** (see [7]). Let $x$ be a cut vertex of a connected graph $G$ and $a$ and $b$ 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.** Let $G_1$ and $G_2$ be connected graphs. If we identify any vertex, say $x_1$, of $G_1$ with any other vertex, say $x_2$, of $G_2$ as a new common vertex $x$, and we obtain a new graph $G$, then

$$Kf(G) = Kf(G_1) + Kf(G_2) + n_1Kf_{x_2}(G_2) + n_2Kf_{x_1}(G_1),$$

where $Kf_{x_1}(G_i) = \sum_{y_i \in G_i} r_{G_i}(x_i,y_i)$ and $n_i = |V(G_i)| - 1$ for $i = 1,2$.

![Figure 1.](image)
Let $G_3$, $G_4$ and $G_5$ be connected graphs as depicted in Fig. 1. By **Operation I** we mean the graph transformation from $G_3$ to $G_4$, or from $G_3$ to $G_5$.

The following lemma is our main lemma, which shall play an important role in proving our main results.

**Lemma 3.** Let $G_3$, $G_4$ and $G_5$ be connected graphs as depicted in Fig. 1. Then the following holds:

(a) If $K_{f_v}(X) \geq K_{f_u}(X)$, then $K_f(G_3) > K_f(G_4)$;

(b) If $K_{f_u}(X) \geq K_{f_v}(X)$, then $K_f(G_3) > K_f(G_5)$.

**Proof.** By Lemmas 1 and 2, one obtains

$$K_f(G_4) = K_f(X) + K_f(Y \cup Z) + (|X| - 1)K_{f_u}(Y \cup Z) + (|Y| + |Z| - 2)K_{f_u}(X)$$

and

$$K_f(G_3) = K_f(Y) + K_f(X \cup Z) + (|Y| - 1)K_{f_u}(X \cup Z) + (n - |Y|)K_{f_u}(Y)$$

Therefore,

$$K_f(G_4) - K_f(G_3) = (|Y| - 1)K_{f_v}(Z) + (|Z| - 1)K_{f_u}(Y) + (|X| - 1)K_{f_u}(Y)$$

$$+ (|X| - 1)K_{f_v}(Z) + (|Y| + |Z| - 2)K_{f_u}(X)$$

$$- (|X| - 1)K_{f_v}(Z) - (|Z| - 1)K_{f_u}(X) - (|Y| - 1)K_{f_u}(X)$$

$$- (|Y| - 1)K_{f_v}(Z) - (|Y| - 1)(|Z| - 1)r_X(u,v)$$

$$- (n - |Y|)K_{f_u}(Y)$$

$$= (|Z| - 1)(K_{f_u}(X) - K_{f_v}(X)) - (|Y| - 1)(|Z| - 1)r_X(u,v).$$

If $K_{f_v}(X) \geq K_{f_u}(X)$, it then follows from the above equation that

$$K_f(G_4) - K_f(G_3) \leq -(|Y| - 1)(|Z| - 1)r_X(u,v) < 0,$$

which proves (a).

The same reasoning can be used to prove (b). $\square$
Figure 2.

Now, we are in a position to state and prove our main results of this paper.

**Theorem 1.** Among all graphs in \( \text{Cat}(n, t) \) with \( n \geq 13 \) and \( t \geq 1 \), \( G^0(n, t) \) is the unique graph having the minimum Kirchhoff index.

**Proof.** Let \( G_{\text{min}} \) be the graph in \( \text{Cat}(n, t) \) with the minimal Kirchhoff index. Our goal is to prove that \( G_{\text{min}} \cong G^0(n, t) \).

By contradiction. Suppose to the contrary that \( G_{\text{min}} \not\cong G^0(n, t) \).

We first assume that \( G_{\text{min}} \) has no cut-edges. From Lemma 3, all cycles in \( G_{\text{min}} \) must share exactly one common vertex, say \( v \).

Figure 3.

By **Operation II** we mean the graph transformation from \( G^* \) to \( G^{**} \).

We first prove the following assertion.

**Assertion 1.** Let \( G^* \) and \( G^{**} \) be two graphs as depicted in Fig. 3., then \( Kf(G^*) > Kf(G^{**}) \).

**Proof.** From Lemma 2 we obtain

\[
Kf(G^*) = Kf(C_l) + Kf(H) + (l - 1)Kf_v(H) + (|H| - 1)Kf_v(C_l),
\]

\[
Kf(G^{**}) = Kf(S^{l-1}_l) + Kf(H) + (l - 1)Kf_v(H) + (|H| - 1)Kf_v(S^{l-1}_l),
\]

(\( t \) times

(\( n - 2t - 1 \) times

\( G^0(n, t) \))
For any graph $G$ with $n = 13$ and $t = 1$, $Kf(G) \geq 3$.

**Corollary 1.** For any graph $G$ in $\text{Cat}(n, t)$ with $n \geq 13$ and $t \geq 1$, $Kf(G) \geq n^2 - 2t^2 - 3n + t + 2 + \frac{n}{t}$ with equality if and only if $G \cong G^0(n, t)$.
Proof. According to Lemma 2, we obtain
\[
K_f(G^0(n, t)) = K_f(\underbrace{C_3vC_3 \cdots vC_3}_{t \text{ times}}) + K_f(S_{n-2t}) + 2tK_f(S_{n-2t})
\]
\[
+ (n - 2t - 1)K_f(\underbrace{C_3vC_3 \cdots vC_3}_{t \text{ times}})
\]
\[
= K_f(\underbrace{C_3vC_3 \cdots vC_3}_{t \text{ times}}) + (n - 2t - 1) + 2t(n - 2t - 1)
\]
\[
+ \frac{4t}{3}(n - 2t - 1) + 2\left(\frac{n - 2t - 1}{2}\right),
\]
\[
K_f(\underbrace{C_3vC_3 \cdots vC_3}_{t \text{ times}}) = K_f(C_3) + K_f(\underbrace{C_3vC_3 \cdots vC_3}_{(t-1) \text{ times}})
\]
\[
+ 2K_f(\underbrace{C_3vC_3 \cdots vC_3}_{(t-1) \text{ times}}) + 2K_f(C_3)
\]
\[
= K_f(\underbrace{C_3vC_3 \cdots vC_3}_{(t-1) \text{ times}}) + \frac{16t - 10}{3}.
\]

Note that $K_f(C_3) = 2$. Hence, we obtain $K_f(\underbrace{C_3vC_3 \cdots vC_3}_{t \text{ times}}) = \frac{8n^2 - 2t}{3}$ by an elementary calculation, and then $K_f(G^0(n, t)) = n^2 - 2t^2 - 3n + t + 2 + \frac{n}{3}$. Combining this fact and Theorem 1, we get the desired result. \qed

In the following we shall consider the cacti with the second and the third smallest Kirchhoff indices.

Suppose first that $G$ has the second smallest Kirchhoff index among all elements of $Cat(n, t)$. Evidently, $G$ can be changed into $G^0(n, t)$ by using exactly one step of Operation I or II, for otherwise, one can employ one step of Operation I or II on $G$, and obtain a new graph $G'$, which is still in $Cat(n, t)$ but not isomorphic to $G^0(n, t)$, which gives
\[
K_f(G) > K_f(G') > K_f(G^0(n, t)),
\]
contradicting our choice of $G$.

By the above arguments, one can conclude that $G$ must be one of the graphs $G_6$, $G_7$, and $G_8$ as shown in Fig. 4.
Theorem 2. Among all graphs in $\text{Cat}(n, t)$ with $n \geq 13$ and $t \geq 1$, the cactus with the second-minimum Kirchhoff index is $G_8$ (see Fig. 4).

Proof. (i): Let $H_1$ denote the common subgraph of $G_6$ and $G^0(n, t)$. Thus, we can view graphs $G_6$ and $G^0(n, t)$ as the graphs depicted in Fig. 5.

![Figure 5](image)

Using Lemma 2, we have

$$Kf(G^0(n, t)) = Kf(S_3) + Kf(H_1) + 2Kf_{v_1}(H_1) + (n - 3)Kf_{v_1}(S_3)$$

$$= 4 + Kf(H_1) + 2Kf_{v_1}(H_1) + 2(n - 3),$$

$$Kf(G_6) = Kf(P_3) + Kf(H_1) + 2Kf_{v_1}(H_1) + (n - 3)Kf_{v_1}(P_3)$$

$$= 4 + Kf(H_1) + 2Kf_{v_1}(H_1) + 3(n - 3).$$

Therefore,

$$Kf(G_6) = Kf(G^0(n, t)) + (n - 3).$$

(ii): Let $H_2$ be the common subgraph of $G_7$ and $G^0(n, t)$ (see Fig. 6). Here we also let $v_1$ denote the unique maximum-degree vertex in $G^0(n, t)$.

![Figure 6](image)

In view of Lemma 2,

$$Kf(G^0(n, t)) = Kf(P_2) + Kf(H_2) + Kf_{v_1}(H_2) + (n - 2)Kf_{v_1}(P_2)$$

$$= Kf(H_2) + Kf_{v_1}(H_2) + (n - 1),$$

$$Kf(G_7) = Kf(H_2) + Kf_{v_2}(H_2) + (n - 1)$$

$$= Kf(H_2) + Kf_{v_1}(H_2) + \frac{2}{3}(n - 4) + (n - 1).$$
Therefore,

\[ Kf(G_7) = Kf(G^0(n, t)) + \frac{2}{3}(n - 4). \]  

\[ \text{(1)} \]

(iii): Let \( H_3 \) be the common subgraph of \( G_8 \) and \( G^0(n, t) \)(see Fig. 7).

\[ G_8 \]

\[ G^0(n, t) \]

\[ H_3 \]

\[ C_4 \]

\[ v_1 \]

\[ H_3 \]

\[ C_3 \]

\[ v_1 \]

\[ S_3^4 \]

\[ C_3 \]

\[ S_3^4 \]

\[ v_1 \]

\[ C_4 \]

\[ H_3 \]

Denote by \( S_3^4 \) the graph obtained by attaching one pendant edge to any vertex of \( C_3 \). So,

\[ Kf(G_8) = kf(C_4) + Kf(H_3) + 3Kf_v_1(H_3) + (n - 4)Kf_v_1(C_4), \]

\[ Kf(G^0(n, t)) = Kf(S_3^4) + Kf(H_3) + 3Kf_v_1(H_3) + (n - 4)Kf_v_1(S_3^4). \]

Recall that \( Kf_v_1(C_4) = \frac{17}{6} \), and that \( Kf(C_4) = \frac{4^2 - 4}{12} = 5 \), we thus have

\[ Kf(G_8) - Kf(G^0(n, t)) = \frac{4^2 - 11 \times 4 + 12}{12} + (n - 4)(\frac{2 \times 4 - 7}{6}) \]

\[ = \frac{32}{12} + \frac{n - 4}{6} \]

\[ = \frac{n}{6} - 2. \]

Therefore, \( Kf(G_8) = Kf(G^0(n, t)) + \frac{n}{6} - 2 \).

By the above expressions obtained for the Kirchhoff indices of \( G_6 \), \( G_7 \) and \( G_8 \), we immediately have the desired result.

From Theorem 2 we immediately have the following result.

**Corollary 2.** For a graph \( G \), not isomorphic to \( G^0(n, t) \), in \( \text{Cat}(n, t) \) with \( n \geq 13 \) and \( t \geq 1 \), it holds that \( Kf(G) \geq n^2 - 2t^2 - \frac{17n}{6} + t + \frac{n}{3} \), with equality if and only if \( G \cong G_8 \) (see Fig.4).
By the same reasonings as those used in Theorem 2, we conclude that the possible candidates having the third smallest Kirchhoff index must come from one graph of $G_7, G_9 - G_{13}$ (see Figs. 4 and 9).

**Theorem 3.** Among all graphs in $Cat(n, t)$ with $n \geq 13$ and $t \geq 1$, the cactus with the third-minimum Kirchhoff index is $G_{11}$ (see Fig. 9).

**Proof.** By above discussions, we need only to determine the minimum cardinality among $Kf(G_7), Kf(G_9), Kf(G_{10}), Kf(G_{11}), Kf(G_{12})$ and $Kf(G_{13})$.

Let $H_4$ be the common subgraph of $G_7, G_9$ and $G_{10}$ (see Figs. 4, 8 and 9). Also, we let $G_0$ be a subgraph of $G_7$ (see Fig. 8). It is now reduced to

\[
Kf(G_9) = Kf(S_1^2) + Kf(H_4) + 4Kf_{v_3}(H_4) + (n - 5)Kf_{v_3}(S_1^2)
\]

\[
= \frac{23}{2} + Kf(H_4) + 4Kf_{v_3}(H_4) + \frac{17}{4}(n - 5),
\]

\[
Kf(G_7) = Kf(G_0) + Kf(H_4) + 4Kf_{v_3}(H_4) + (n - 5)Kf_{v_3}(G_0)
\]

\[
= \frac{40}{3} + Kf(H_4) + 4Kf_{v_3}(H_4) + 4(n - 5),
\]

where $S_1^2$ denotes the graph obtained by attaching one pendant edge to any vertex of $C_4$.

Therefore,

\[
Kf(G_9) - Kf(G_7) = \frac{3n - 37}{12} > 0,
\]

since $n \geq 13$.

Furthermore,

\[
Kf(G_{10}) = Kf((S_1^2)) + Kf(H_4) + 4Kf_{v_3}(H_4) + (n - 5)Kf_{v_3}((S_1^2))
\]

\[
= \frac{23}{2} + Kf(H_4) + 4Kf_{v_3}(H_4) + \frac{9}{2}(n - 5).
\]
Therefore
\[ Kf(G_{10}) - Kf(G_9) = \frac{n-5}{4} > 0 \quad (n \geq 13). \]

Then
\[ Kf(G_{10}) > Kf(G_9) > Kf(G_7) \quad (n \geq 13). \]

In the following, we need only to compare \( G_7, G_{11}, G_{12} \) and \( G_{13} \).
Evidently, \( G_{11} \) can be changed into \( G_8 \) by using exactly one step of Operation II. Hence, by the Assertion in Theorem 1, we have
\[ Kf(G_{11}) = Kf(G_8) + \frac{l^2 - 11l + 12}{12} + (|H| - 1)(\frac{2l - 7}{6}). \]

Here, \( l = 4 \) and \( |H| - 1 = n - 4 \). Therefore,
\[
Kf(G_{11}) = Kf(G_8) + \frac{4^2 - 11 \times 4 + 12}{12} + (n - 4)(\frac{2 \times 4 - 7}{6}) \\
= Kf(G_8) + \frac{n}{6} - 2 \\
= Kf(G^0(n,t)) + \frac{n}{3} - 4. \tag{2}
\]

From Eqs.(1) and (2) it follows that
\[ Kf(G_{11}) - Kf(G_7) = -\frac{1}{3}n - \frac{4}{3} < 0. \]

Evidently, \( G_{12} \) can be changed into \( G_7 \) by using exactly one step of Operation II. So we have
\[ Kf(G_{12}) = Kf(G_7) + \frac{n}{6} - 2 = Kf(G^0(n,t)) + \frac{5n - 28}{6}. \]

Thus
\[ Kf(G_{12}) > Kf(G_7) > Kf(G_{11}) \quad (n \geq 13). \]

It is obvious that \( G_{13} \) can be changed into \( G_8 \) by using exactly one step of Operation II, thus by the same reasoning as above, we get
\[ Kf(G_{13}) = Kf(G_8) + \frac{5^2 - 11 \times 5 + 12}{12} + (n - 5)(\frac{2 \times 5 - 7}{6}). \]

Here, \( l = 5 \) and \( |H| - 1 = n - 5 \). Therefore,
\[
Kf(G_{13}) = Kf(G_8) + \frac{5^2 - 11 \times 5 + 12}{12} + (n - 5)(\frac{2 \times 5 - 7}{6}) \\
= Kf(G_8) + \frac{n}{2} - 4.
\]

Combining this fact and the expression that \( Kf(G_8) = Kf(G^0(n,t)) + \frac{n}{6} - 2 \), we arrive at
\[ Kf(G_{13}) - Kf(G_{11}) = \frac{1}{3}n - 2 = \frac{n - 6}{3}. \]

So \( Kf(G_{11}) < Kf(G_{13}) \) for \( n \geq 13 \).
The proof of Theorem 3 is thus completed.
Corollary 3. For a graph $G$ in $Cat(n,t)$ with $n \geq 13$ and $t \geq 1$, not isomorphic to \{${G^0}(n,t), G_8$\},

$$Kf(G) \geq n^2 - 2t^2 - \frac{8n}{3} + t - 2 + \frac{nt}{3}$$

with equality if and only if $G \cong G_{11}$ (see Fig. 9).

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