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The Minimal Kirchhoff Index of Graphs with a Given Number of Cut Vertices

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Abstract. The resistance distance was introduced by Klein and Randić as a generalization of the classical distance. The Kirchhoff index $Kf(G)$ of a graph G is the sum of resistance distances between all unordered pairs of vertices. In this paper we determine the extremal graphs with minimal Kirchhoff index among all n-vertex graphs with k cut vertices where $1 \leq k < \frac{n}{2}$.

1. Introduction

In 1993, Klein and Randić [11] introduced a distance function named resistance distance on the basis of electrical network theory. They view a connected graph G as an electrical network N by replacing each edge of G with a unit resistor. Let $v_1, v_2, \ldots, v_n$ be labeled vertices of a graph G. The resistance distance between v_i and v_j, denoted by $r_G(v_i, v_j)$, is defined to be the effective resistance between nodes v_i and v_j in G. The conventional distance between v_i and v_j, denoted by $d_G(v_i, v_j)$, is the length of a shortest path between them in a graph G. The famous Wiener index [23] $W(G)$ is the sum of distances between all pairs of vertices, that is $W(G) = \sum\limits_{i<j} d_G(v_i, v_j)$. Analogue to the Wiener index, the Kirchhoff index $Kf(G)$ is defined as:

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

As a useful structure-descriptor, the Kirchhoff index plays an important role in QSAR and QSPR. As the Kirchhoff index and the well-studied Wiener index coincide for trees, it is more interesting to consider the Kirchhoff index of cycle-containing structures. However, the computation of the Kirchhoff index is not an easy task [24] when the size of the graph is very large due to its computational complexity. As it is difficult to get the exact value or analytical formula, it becomes more and more desirable to find bounds

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for the Kirchhoff index of some classes of graphs. For a general graph G, Lukovits et al. [13] showed that $Kf(G) \geq n-1$ with equality holding if and only if G is the complete graph K_n; and it was showed in [16] that the path P_n has maximal Kirchhoff index. For more information on the Kirchhoff index, the readers are referred to recent papers [1, 2, 4, 6–8, 14, 15, 17–22, 25, 26, 28] and the references therein.

All graphs considered in this paper are finite and simple. For two non-adjacent vertices v_i and v_j, we use $G+e$ to denote the graph obtained by inserting a new edge $e = v_iv_j$ in G. Similarly, for $e \in E(G)$ of graph G, let $G-e$ be the subgraph of G obtained by deleting the edge e from $E(G)$. For a subset S of $V(G)$, let $G-S$ be the subgraph of G obtained by deleting the vertices of S and the edges incident with them. A subset S of $V(G)$ is called a *clique* if $G[S]$, the induced subgraph of G by S, is complete. For two graphs G_1 and G_2, we denote by $G_1 \cup G_2$ the graph which consists of two connected components G_1 and G_2. The *join* of two vertex-disjoint graphs G_1 and G_2, denoted by $G_1 \bigvee G_2$, is the graph with vertex set $V(G_1) \cup V(G_2)$ and edge set $E(G_1) \cup E(G_2) \cup \{uv \mid u \in V(G_1), v \in V(G_2)\}$. For a graph G with vertex set $V = \{v_1, v_2, \ldots, v_n\}$, we denote by d_i the degree of the vertex v_i in G for $i = 1, 2, \ldots, n$. Assume that $A(G)$ is the $(0,1)$-adjacency matrix of G and $D(G)$ is the diagonal matrix of vertex degrees. The Laplacian matrix of G is $L(G) = D(G) - A(G)$. The Laplacian polynomial $Q(G,\lambda)$ of G is the characteristic polynomial of its Laplacian matrix, $Q(G,\lambda) = \det(\lambda I_n - L(G)) = \sum_{k=0}^{n} (-1)^k c_k \lambda^{n-k}$. The Laplacian matrix $L(G)$ has nonnegative eigenvalues $n \geq \mu_1 \geq \cdots \geq \mu_n = 0$ [12]. Denote by $S(G) = \{\mu_1, \mu_2, \ldots, \mu_n\}$ the spectrum of $L(G)$, i.e., the Laplacian spectrum of G. If μ_i appears $l_i > 1$ times in $S(G)$, we write $\mu_i^{l_i}$ for short in it.

In 1996, Gutman and Mohar [9] and Zhu et al. [33] independently obtained the following nice result, by which a relation was established between Kirchhoff index and Laplacian spectrum:

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

for any connected graph G of order $n \geq 2$.

In 2010, Deng [5] determined the minimum Kirchhoff index among all connected graphs with n vertices and k cut edges, and characterized the corresponding extremal graphs. Along this line, we consider graphs with minimum Kirchhoff index among all graphs with n vertices and k cut vertices. Assume that k, n are two integers with $1 \leq k < \frac{n}{2}$. Let $\mathcal{G}_{n,k}$ be the class of connected graphs of order n and with k cut vertices. In this paper we have determined the minimum Kirchhoff index of graphs from $\mathcal{G}_{n,k}$ with $1 \leq k < \frac{n}{2}$, and characterized the corresponding extremal graphs.

2. Some Lemmas

In this section we will list or prove some basic but important lemmas as preliminaries.

Lemma 2.1. ([11]) *Let x be a cut vertex of a graph G, and a and b be two vertices in different components of $G-x$. Then*

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

Lemma 2.2. ([13]) *Let G be a non-complete connected graph. If G' is obtained from G by inserting a new edge. Then $Kf(G') < Kf(G)$.*

Lemma 2.3. ([12]) *Suppose that G_i is a graph of order n_i for $i = 1, 2$. Then*

$$S(G_1 \bigvee G_2) = \{n_1+n_2, 0\} \bigcup \{n_1 + \mu_i(G_2) | 1 \leq i \leq n_2 - 1\} \bigcup \{n_2 + \mu_j(G_1) | 1 \leq j \leq n_1 - 1\}.$$

For any connected graph G with vertex $x \in V(G)$, the *resistive eccentricity index* [30] of x, denoted by $Kf_x(G)$, is defined to be the sum of resistance distance between x and all other vertices of G, that is to say,

$Kf_x(G) = \sum_{y\in V(G-x)} r_G(x,y)$. Considering the definition of Kirchhoff index, we have

$$Kf(G) = \frac{1}{2}\sum_{v\in V(G)} Kf_v(G).$$

In the following lemma a formula on calculating the Kirchhoff index is given for a special class of graphs.

Lemma 2.4. ([13]) *Let G_1 and G_2 be two connected graphs with exactly one common vertex x and $G = G_1 \cup G_2$. Then*

$$Kf(G) = Kf(G_1) + Kf(G_2) + (|V(G_1)| - 1)Kf_x(G_2) + (|V(G_2)| - 1)Kf_x(G_1).$$

Lemma 2.5. *Let*

$$f(x) = \frac{n-x-1}{x+1} + \frac{x+1}{n-x-1}$$

be a function on the interval $[1, n-3]$. Then $f(x)$ reaches its maximum $\frac{n-2}{2} + \frac{2}{n-2}$ at $x = 1$ or $n-3$.

Proof. Define a new function

$$h(x) = \frac{n-x-1}{x+1} \quad \text{with} \quad 1 \le x \le n-3 \quad \text{and} \quad g(x) = x + \frac{1}{x}.$$

Then we have $f(x) = g(h(x))$. Taking the second derivative, we arrive at

$$\begin{aligned}
f''(x) &= (g'(h(x))h'(x))' \\
&= g''(h(x))(h'(x))^2 + g'(h(x))h''(x) \\
&= \frac{2}{h^3(x)}\frac{n^2}{(x+1)^4} + (1 - \frac{1}{h^2(x)})\frac{2n}{(x+1)^3} \\
&= \frac{2n}{(x+1)^3}\left[\frac{n}{(x+1)h(x)}\frac{1}{h^2(x)} + 1 - \frac{1}{h^2(x)}\right] \\
&= \frac{2n}{(x+1)^3}\left[\frac{n}{n-x-1}\frac{1}{h^2(x)} + 1 - \frac{1}{h^2(x)}\right] \\
&> 0.
\end{aligned}$$

Therefore, $f(x)$ is a convex function on the interval $[1, n-3]$. Then $f(x)$ attains its maximum at $x = 1$ or $x = n-3$. Noticing that

$$f(1) = f(n-3) = \frac{n-2}{2} + \frac{2}{n-2},$$

we complete the proof of this lemma. □

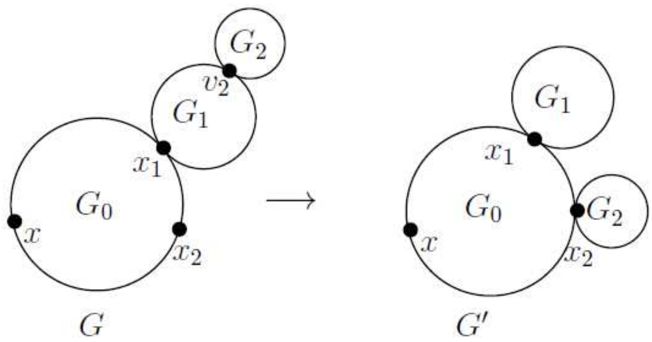

Figure 1: The graphs G and G'

Now we prove the following two properties of the resistive eccentricity index of vertex x in a graph G.

Lemma 2.6. *Let G and G' be the graphs depicted in Figure 1 where G_0 is a connected graph and G_i is a complete graph K_{n_i} for $i = 1, 2$. Assume that x is an arbitrary vertex in G_0 different from x_i with $i = 1, 2$ and $r_{G_0}(x, x_1) = r_{G_0}(x, x_2)$ in G', then we have $Kf_x(G') < Kf_x(G)$.*

Proof. Note that $r_{K_n}(u, v) = \frac{2}{n}$ for any two vertices $u, v \in V(K_n)$. By the definition of the $Kf_x(G)$ and Lemma 2.1, we have

$$\begin{aligned} Kf_x(G) &= Kf_x(G_0) + \sum_{y\in V(G_1-x_1)} r_G(x,y) + \sum_{y\in V(G_2-v_2)} r_G(x,y) \\ &= Kf_x(G_0) + (r_{G_0}(x,x_1) + \frac{2}{n_1})(n_1-1) + (r_{G_0}(x,x_1) + \frac{2}{n_1} + \frac{2}{n_2})(n_2-1), \\ Kf_x(G') &= Kf_x(G_0) + \sum_{y\in V(G_1-x_1)} r_{G'}(x,y) + \sum_{y\in V(G_2-x_2)} r_{G'}(x,y) \\ &= Kf_x(G_0) + (r_{G_0}(x,x_1) + \frac{2}{n_1})(n_1-1) + (r_{G_0}(x,x_2) + \frac{2}{n_2})(n_2-1). \end{aligned}$$

Thus, considering that $r_{G_0}(x, x_1) = r_{G_0}(x, x_2)$ in G', we get

$$Kf_x(G) - Kf_x(G') = \frac{2}{n_1}(n_2 - 1) > 0.$$

Therefore, we have $Kf_x(G') < Kf_x(G)$ as desired. □

Lemma 2.7. *Let G be a connected non-complete graph with $x \in V(G)$ and two non-adjacent vertices $u, v \in V(G)$. Assume that $G' = G + uv$. Then we have $Kf_x(G) > Kf_x(G')$.*

Proof. From Theorem 2.1 of [29], we know that, for any vertex $y \neq x$ in G,

$$r_G(x,y) \quad \geq \quad r_{G'}(x,y),$$

$$\begin{aligned} r_{G'}(x,u) &= r_G(x,u) - \frac{(r_G(x,u) + r_G(u,v) - r_G(x,v))^2}{4(1 + r_G(u,v))}, \\ r_{G'}(x,v) &= r_G(x,v) - \frac{(r_G(x,v) + r_G(u,v) - r_G(x,u))^2}{4(1 + r_G(u,v))}. \end{aligned}$$

Set

$$A = (r_G(x,u) + r_G(x,v)) - (r_{G'}(x,u) + r_{G'}(x,v)).$$

Thus we have

$$\begin{aligned} A &= \frac{(r_G(x,v) + r_G(u,v) - r_G(x,u))^2 + (r_G(x,u) + r_G(u,v) - r_G(x,v))^2}{4(1 + r_G(u,v))} \\ &\geq \frac{[(r_G(x,v) + r_G(u,v) - r_G(x,u)) + (r_G(x,u) + r_G(u,v) - r_G(x,v))]^2}{8(1 + r_G(u,v))} \\ &= \frac{r_G(u,v)^2}{2(1 + r_G(u,v))} \\ &> 0. \end{aligned}$$

From the definition of the resistive eccentricity index of vertex x in a graph G, we conclude that $Kf_x(G) > Kf_x(G')$ as desired. □

Let $n_0 > k$ and $n_i \geq 2$ for $i = 1, \ldots, k$ be positive integers such that $\sum_{i=0}^{k} n_i = n + k$. Denote by $E_n(n_0; n_1, n_2, \cdots, n_k)$ (see Fig. 2) the graph obtained by identifying k distinct vertices of K_{n_0} with one vertex of K_{n_i} with $i = 1, 2, \cdots, k$, respectively. For convenience, we write $E_n(n-k; \overbrace{2, \ldots, 2}^{k})$ as $E_n(n-k; 2^{(k)})$ when $k \geq 2$. Clearly, we have $E_n(n-k; 2^{(k)}) \in \mathcal{G}_{n,k}$.

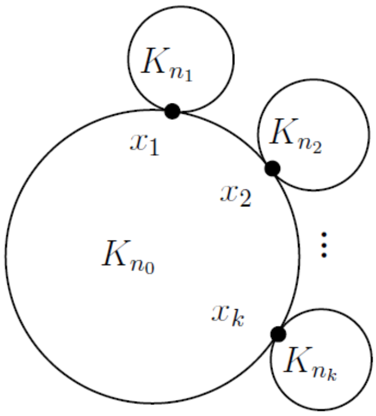

Figure 2: The graph $E_n(n_0; n_1, n_2, \ldots, n_k)$

Lemma 2.8. *Let $G \in \mathcal{G}_{n,k}$ be some $E_n(n_0; n_1, n_2, \ldots, n_k)$ as shown in Fig. 2 where $x_i \in V(G_i) \cap V(G_0)$ with $i = 1, 2, \ldots, k$ and $G_0 = K_{n_0}$, $G_i = K_{n_i}$ for $i \in \{1, 2, \ldots, k\}$. Assume that x is an arbitrary vertex in G_0 different from any vertex in $\{x_i | 1 \leq i \leq k\}$. Then*

$$Kf_x(G) \geq \frac{2}{n-k}(n-k-1) + \Big(1 + \frac{2}{n-k}\Big)k$$

with equality holding if and only if $G \cong E_n(n-k; 2^{(k)})$

Proof. Note that the graph in Fig. 2 is just of the form $E_n(n_0; n_1, n_2, \cdots, n_k)$. By the definition of $Kf_x(G)$ and the structure of G as shown in Fig. 2, considering that $\sum\limits_{i=1}^{k} n_i = n - n_0 + k$, we have

$$\begin{aligned} Kf_x(G) &= \frac{2}{n_0}(n_0-1) + \Big(\frac{2}{n_0} + \frac{2}{n_1}\Big)(n_1-1) + \cdots + \Big(\frac{2}{n_0} + \frac{2}{n_k}\Big)(n_k-1) \\ &= \frac{2}{n_0}(n_0 - 1 + n_1 - 1 + \cdots + n_k - 1) + \sum_{i=1}^{k} \frac{2(n_i-1)}{n_i} \\ &= \frac{2}{n_0}(n-1) + 2k - 2\Big(\frac{1}{n_1} + \frac{1}{n_2} + \cdots + \frac{1}{n_k}\Big). \end{aligned}$$

Now we define a function

$$f(n_0, n_1, n_2, \ldots, n_k) = \frac{2}{n_0}(n-1) + 2k - 2\Big(\frac{1}{n_1} + \frac{1}{n_2} + \cdots + \frac{1}{n_k}\Big)$$

with $n_0 > k$ and $n_i \geq 2$ for $i = 1, 2, \cdots, k$. Set

$$A = f(n_0, n_1, n_2, \ldots, n_k) - f(n_0 + 1, n_1 - 1, n_2, \ldots, n_k).$$

Then we have

$$A = 2(n-1)\Big(\frac{1}{n_0} - \frac{1}{n_0+1}\Big) + 2\Big(\frac{1}{n_1 - 1} - \frac{1}{n_1}\Big) > 0.$$

Thus we have

$$f(n_0, n_1, n_2, \ldots, n_k) > f(n_0 + 1, n_1 - 1, n_2, \ldots, n_k).$$

If $n_i > 2$ for some $1 \leq i \leq k$, then by a similar reasoning as above, we arrive at:

$$\begin{aligned} f(n_0, n_1, n_2, \ldots, n_k) &> f(n_0 + 1, n_1 - 1, n_2, \ldots, n_k) \\ &> \cdots \\ &> f(n-k, 2, 2, \ldots, 2) \\ &= \frac{2}{n-k}(n-k-1) + \Big(1 + \frac{2}{n-k}\Big)k. \end{aligned}$$

Therefore, we claim that any graph G of the form $E_n(n_0; n_1, \ldots, n_k)$ with an arbitrary non-cut vertex x in K_{n_0} can be changed into $E_n(n-k; 2^{(k)})$ with a smaller resistive eccentricity index of x. Then the "only if" part has been proved.

Conversely, if $G \cong E_n(n-k;\, 2^{(k)})$, then we have

$$Kf_x(G) = \frac{2}{n-k}(n-k-1) + \Big(1 + \frac{2}{n-k}\Big)k,$$

finishing the proof of this lemma. □

Recall that a *block* of a connected graph G is a maximal subgraph, which does not contain any cut vertex, in G. We call a block in a graph G an *end-block* if this block contains at most one cut vertex in it as a whole. A graph G is called *block graph* if each block in G is a clique.

Lemma 2.9. *Let $1 \leq k < \frac{n}{2}$ and $G \in \mathcal{G}_{n,k}$ with a non-cut vertex $x \in V(G)$ and $Kf_x(G)$ as small as possible. Then G must be a block graph with k cut vertices each of which connects exactly two cliques in it.*

Proof. From Lemma 2.7, we find that G must be a block graph with k cut vertices. Let x_1 be any cut vertex in G. It suffices to prove that, in G, exactly two cliques, say K_{n_1} and K_{n_2}, share the common vertex x_1.

If not, there exist $s \geq 3$ cliques $K_{n_1}, K_{n_2}, \ldots, K_{n_s}$ share the cut vertex x_1. Choose $v_1 \in V(K_{n_1})$ and $v_s \in V(K_{n_s})$ such that both of them are different from x_1. Now we construct a new graph $G^* = G + v_1v_s$. Obviously, $G^* \in \mathcal{G}_{n,k}$. However, we have $Kf_x(G^*) < Kf_x(G)$ from Lemma 2.7, contradicting to the choice of G. Thus we complete the proof of this lemma. □

From Lemma 2.9, the following remark can be easily deduced.

Remark 2.10. *Let $1 \leq k < \frac{n}{2}$ and $G \in \mathcal{G}_{n,k}$ with a non-cut vertex $x \in V(G)$ and $Kf_x(G)$ as small as possible. Then G can be obtained by identifying an arbitrary vertex in K_{s+1} with a non-cut vertex of $G_1 \in \mathcal{G}_{n-s,k-1}$.*

In the following we present an essential lemma to the structure of extremal graphs from $\mathcal{G}_{n,k}$ with respect to resistive eccentricity index.

Lemma 2.11. *Let n, k be two integers such that $1 \leq k < \frac{n}{2}$ and $G \in \mathcal{G}_{n,k}$ with $x \in V(G)$ being a non-cut vertex and $Kf_x(G)$ as small as possible. Assume that $\{v_1, v_2, \ldots, v_k\}$ is the set of cut vertices in G. Then*

$$G - \{v_1, v_2, \ldots, v_k\} = K_{t_0} \cup K_{t_1} \cup \cdots \cup K_{t_k} \quad \textit{with} \quad \sum_{i=0}^{k} t_i = n - k.$$

Proof. We prove this lemma by induction on k.

For $k = 1$, from Lemma 2.7, our result follows immediately. Assume that this result holds for all positive integers fewer than $k \geq 2$. Now we choose $G \in \mathcal{G}_{n,k}$ with a non-cut vertex x and $Kf_x(G)$ as small as possible. By Lemma 2.9, we conclude that G is a block graph with k cut vertices.

Now we choose an end-block, say K_{s+1}, in G. Then, by Remark 2.10, the graph $G \in \mathcal{G}_{n,k}$ can be viewed as a graph obtained by identifying an arbitrary vertex in K_{s+1} with a non-cut vertex of $G_1 \in \mathcal{G}_{n-s,k-1}$. Denote by $\{v_1, v_2, \ldots, v_{k-1}\}$ the set of all cut vertices in G_1 and by v_k the above vertex intersected in G_1 and K_{s+1}. Then by induction hypothesis, we have $G_1 - \{v_1, v_2, \ldots, v_{k-1}\} = K_{t_0} \cup K_{t_1} \cup \cdots \cup K_{t_{k-1}}$ with $\sum_{i=0}^{k-1} t_i = n - s - k + 1$. Set $s = t_k$, then we have $G - \{v_1, v_2, \ldots, v_k\} = K_{t_0} \cup K_{t_1} \cup \cdots \cup K_{t_k}$ with $\sum_{i=0}^{k} t_i = n - k$, finishing the proof of this lemma. □

Lemma 2.12. *Let k, n be two integers such that $1 \leq k < \frac{n}{2}$. For any graph $G \in \mathcal{G}_{n,k}$ with $x \in V(G)$ being a non-cut vertex, we have*

$$Kf_x(G) \geq \frac{2}{n-k}(n-k-1) + \Big(1 + \frac{2}{n-k}\Big)k$$

with equality holding if and only if $G \cong E_n(n-k; 2^{(k)})$ and x is a non-cut vertex of K_{n-k} in it.

Proof. Assume that $G \in \mathcal{G}_{n,k}$ such that $Kf_x(G)$ is as small as possible with x being a non-cut vertex in G. Let $v_1, v_2, \ldots, v_k$ be all the cut vertices of G. By Lemma 2.11, we have

$$G - \{v_1, v_2, \ldots, v_k\} = K_{t_0} \cup K_{t_1} \cup \cdots \cup K_{t_k} \quad \text{with} \quad \sum_{i=0}^{k} t_i = n - k.$$

Next we will prove the following claim.

Claim 1. $G \cong E_n(n_0; n_1, n_2, \ldots, n_k)$ with $n_i = t_i + h_i$ where $1 \leq h_i \leq k$ for $i = 0, 1, \ldots, k$ and $\sum_{i=0}^{k} h_i = 2k$, and x is a non-cut vertex in K_{n_0} in it.

Proof of Claim 1. We prove this result by induction on k. If $k = 1$, our result holds trivially. Assume that this result holds for all positive integers fewer than k. Now we consider the graphs from $\mathcal{G}_{n,k}$. Thanks to

Remark 2.10, again, any graph $G \in \mathcal{G}_{n,k}$ can be obtained by identifying one non-cut vertex in $G^* \in \mathcal{G}_{n-s,k-1}$ with any vertex of K_{s+1} which is an end-block in G.

By induction hypothesis, we have $G^* \cong E_{n-s}(n_0; n_1, \ldots, n_{k-1})$ with x being a non-cut vertex in K_{n_0} in it. If $G \cong E_n(n_0; n_1, n_2, \ldots, n_k)$, our result follows immediately. Otherwise, by choosing $G_2 = K_{s+1}$ and $G_1 = K_{n_i}$ with $i \in \{1, 2, \ldots, k-1\}$ in $G^* \cong E_{n-s}(n_0; n_1, \ldots, n_{k-1})$ in Lemma 2.6, G can be changed into another graph $G' \cong E_n(n_0; n_1, n_2, \ldots, n_k)$ with $Kf_x(G') < Kf_x(G)$, contradicting to the choice of G. This completes the proof of this claim.

By Claim 1 and Lemma 2.8, our result holds immediately. □

In view of Lemma 2.2, it is straightforward to get the following remark.

Remark 2.13. *Let $1 \le k < \frac{n}{2}$ and $G \in \mathcal{G}_{n,k}$ with Kirchhoff index as small as possible. Then G must be a block graph with k cut vertices.*

By Remark 2.13, we can obtain a parallel remark to Remark 2.10.

Remark 2.14. *Let $1 \le k < \frac{n}{2}$ and $G \in \mathcal{G}_{n,k}$ with $Kf(G)$ as small as possible. Then G can be obtained by identifying an arbitrary vertex in K_{s+1} with a non-cut vertex of $G_1 \in \mathcal{G}_{n-s,k-1}$.*

Based on Remark 2.13, we can easily obtain the following lemma as an analogue of Lemma 2.11.

Lemma 2.15. *Let $G \in \mathcal{G}_{n,k}$ with $Kf(G)$ as small as possible and $v_1, v_2, \ldots, v_k$ all the cut vertices of G. Then we have $G - \{v_1, v_2, \ldots, v_k\} = K_{t_0} \cup K_{t_1} \cup \cdots \cup K_{t_k}$ with $\sum_{i=0}^{k} t_i = n - k$.*

Lemma 2.16. *Let*

$$f(x) = \frac{(k-1)(k-4) + 2x(k-2)}{n-x-k+1}, \quad 1 \le x \le n-2(k-1) \quad \text{and} \quad 3 \le k < \frac{n}{2}.$$

Then $f(x)$ uniquely reaches its minimum $\frac{(k-1)(k-4)+2(k-2)}{n-k}$ at $x = 1$.

Proof. Taking the first derivative, considering the fact that $n \ge 2k$, for any integer $k \ge 3$, we have

$$\begin{aligned} f'(x) &= \frac{2(k-2)n - k(k-1)}{(n-x-k+1)^2} \\ &> \frac{4k(k-2) - k(k-1)}{(n-x-k+1)^2} \\ &> 0. \end{aligned}$$

Thus we conclude that $f(x)$ is monotonically increasing on the interval $[1, n-2(k-1)]$. Therefore

$$f(x) \ge \frac{(k-1)(k-4) + 2(k-2)}{n-k}$$

with equality holding if and only if $x = 1$, which implies our result in this lemma. □

3. Main Results

In this section we will determine the lower bound on Kirchhoff index of graphs from $\mathcal{G}_{n,k}$ with $0 \le k < \frac{n}{2}$ and characterize the corresponding extremal graph at which the lower bound is attained. For $k = 0$, from Lemma 2.2, we deduce that the extremal graph from $\mathcal{G}_{n,k}$ with minimal Kirchhoff index is K_n with $Kf(K_n) = n - 1$. So the in the following we always assume that $k \ge 1$.

Theorem 3.1. *For any graph $G \in \mathcal{G}_{n,1}$, we have*

$$Kf(G) \geq n - 1 + \frac{n^2 - n - 2}{n - 1}$$

with equality holding if and only if $G \cong E_n(n-1; 2)$.

Proof. We choose $G \in \mathcal{G}_{n,1}$ with $Kf(G)$ as small as possible and with x being the cut vertex of G. By Lemma 2.2, we claim that $G - x$ must have two components and both of them are complete graphs. Without loss of generality, we assume that $G - x = K_k \cup K_{n-k-1}$. In view of Lemma 2.2, again, we have $G = K_1 \bigvee (K_{n-k-1} \cup K_k)$ with $1 \leq k \leq \frac{n-1}{2}$. Recall that $S(K_k) = \left\{k^{(k-1)}, 0\right\}$. From Lemma 2.3, we obtain that

$$S(G) = \left\{n, (n-k)^{(n-k-2)}, (k+1)^{(k-1)}, 1, 0\right\}.$$

By Eq. (1), we have

$$Kf(G) = n\Big(\frac{1}{n} + \frac{n-k-2}{n-k} + \frac{k-1}{k+1} + 1\Big) = 1 + 3n - 2n\Big(\frac{1}{n-k} + \frac{1}{k+1}\Big).$$

Now we define a function

$$f(x) = 1 + 3n - 2n\Big(\frac{1}{n-x} + \frac{1}{x+1}\Big) \quad \text{with} \quad 1 \leq x \leq \frac{n-1}{2}.$$

Taking the first derivative of $f(x)$, we get

$$\begin{aligned} f'(x) &= 2n\left[\frac{1}{(x+1)^2} - \frac{1}{(n-x)^2}\right] \\ &> 0 \quad \text{as} \quad 1 \leq x \leq \frac{n-1}{2}. \end{aligned}$$

Thus we have

$$f(x) \geq f(1) = n - 1 + \frac{n^2 - n - 2}{n - 1}$$

with equality holding if and only if $k = 1$ in $G = K_1 \bigvee (K_1 \cup K_{n-2})$, that is, $G \cong E_n(n-1; 2)$, finishing the proof of this theorem. □

Theorem 3.2. *For any graph $G \in \mathcal{G}_{n,2}$, we have*

$$Kf(G) \geq n - 1 + \frac{2n^2 - 4n - 2}{n - 2}$$

with equality holding if and only if $G \cong E_n(n-2, 2^{(2)})$.

Proof. Assume that $G \in \mathcal{G}_{n,2}$ with $Kf(G)$ as small as possible. From Remark 2.14, we find that G can be obtained by identifying one non-cut vertex, say v_1, of $G_1 \in \mathcal{G}_{n-s,1}$ with any one vertex of K_{s+1} where $1 \leq s \leq n-3$. Note that

$$f(x) = \frac{2x}{n-x-1} \quad \text{with} \quad 1 \leq x \leq n-3$$

reaches its minimum at $x = 1$. Therefore, by Lemmas 2.4, 2.5 and 2.12 and Theorem 3.1, we have

$$\begin{aligned}
Kf(G) &= Kf(G_1) + Kf(K_{s+1}) + (n-s-1)Kf_{v_1}(K_{s+1}) + sKf_{v_1}(G_1)\\
&\geq n-s-1+\frac{(n-s)^2-(n-s)-2}{n-s-1}+s+(n-s-1)\frac{2s}{s+1}\\
&\qquad +s\left[\frac{2}{n-s-1}(n-s-2)+\Big(1+\frac{2}{n-s-1}\Big)\right]\\
&= n-1+(n-s-1)\frac{2s}{s+1}+\frac{n^2-2s^2+(s-1)n-2s-2}{n-s-1}\\
&= n-1+(n-s-1)\Big(2-\frac{2}{s+1}\Big)+\Big(1+\frac{2s}{n-s-1}\Big)n-\frac{2(s^2+s+1)}{n-s-1}\\
&= 3n-3-2s-2\Big(\frac{n-s-1}{s+1}+\frac{s+1}{n-s-1}\Big)+n+\frac{2sn}{n-s-1}-\frac{2s^2}{n-s-1}\\
&= 4n-3-2\Big(\frac{n-s-1}{s+1}+\frac{s+1}{n-s-1}\Big)+\frac{2s}{n-s-1}\\
&\geq 4n-3-2\Big(\frac{n-2}{2}+\frac{2}{n-2}\Big)+\frac{2}{n-2}\\
&= n-1+\frac{2n^2-4n-2}{n-2}
\end{aligned}$$

with both equalities holding if and only if $G_1 \cong E_n(n-1;2)$ and $s = 1$. Equivalently, $G \cong E_n(n-2, 2^{(2)})$, finishing the proof of this theorem. □

Theorem 3.3. *Let $G \in \mathcal{G}_{n,k}$ with $2 \leq k < \frac{n}{2}$. Then we have*

$$Kf(G) \geq n-1+\frac{n^2k-nk^2+k^2-3k}{n-k}$$

with equality holding if and only if $G \cong E_n(n-k; 2^{(k)})$.

Proof. We prove this theorem by introduction on k, i.e., the number of cut vertices. When $k = 2$, by Theorem 3.2, our result holds obviously. Therefore, we always assume that $k \geq 3$ in the following proof.

Assume that the result holds for any graph from $\mathcal{G}_{n,k-1}$ for all values of n. Let $G \in \mathcal{G}_{n,k}$ with Kirchhoff index as small as possible. From Lemma 2.15 and the above argument, we find that $G - \{v_1, v_2, \ldots, v_k\} = K_{t_0} \cup K_{t_1} \cup \cdots \cup K_{t_k}$ with $\sum_{p=0}^{k} t_p = n-k$. Now we choose one subgraph K_{t_i} such that any vertex in it has the maximum eccentricity in G. From the definition of eccentricity of vertex in a graph, there exists at least one other subgraph K_{t_j} of G such that any vertex in it has also the maximum eccentricity in G. Moreover, we assume that, in G, v_i is adjacent to every vertices of K_{t_i} and v_j is adjacent to every vertices of K_{t_j}. Suppose that $\min\{t_i, t_j\} = s$. By Remark 2.14, any graph $G \in \mathcal{G}_{n,k}$ can be obtained by identifying one non-cut vertex of $G_1 \in \mathcal{G}_{n-s,k-1}$ with one vertex of K_{s+1}, that is, G_1 and K_{s+1} have only one common vertex, say x. Now we prove the following claim about the property of the set $\mathcal{G}_{n-s,k-1}$.

Claim 1. $k-1 \leq \dfrac{n-s}{2}$ in $\mathcal{G}_{n-s,k-1}$.

Proof of Claim 1. Otherwise, we have $s > n-2(k-1)$. Let

$$G^* = G - \big(V(K_{t_i}) \cup V(K_{t_j})\big).$$

Then $G^* \in \mathcal{G}_{n-t_i-t_j,k-2}$. However, the order of G^* is

$$\begin{aligned} n-t_i-t_j &\le n-2s \\ &< n-2n+4(k-1) \\ &= 4k-4-n \\ &< 2k-4. \end{aligned}$$

Note that the last inequality holds because of the fact that $k < \frac{n}{2}$. Without loss of generality, we assume that $i < j$. From the above argument, we find that $V^* \triangleq \{v_1, v_2, \ldots, v_{i-1}, v_{i+1}, \ldots, v_{j-1}, v_{j+1}, \ldots, v_k\}$ is the set of all cut vertices in G^*, and $G^* - V^* = \bigcup_{1\le p\le k, p\ne i,j} K_{t_p}$. But, the order of $G^* - V^*$ is

$$n^* < 2k-4-(k-2) = k-2.$$

A contradiction occurs to the structure of $G^* - V^*$, which completes the proof of this claim.

Considering the fact that the function

$$h(x) = \frac{2(n-x-1)}{x+1}$$

is monotonically decreasing on the interval $[1, n-2(k-1)]$, by Lemmas 2.12, 2.16 and the induction hypothesis, we have

$$\begin{aligned} Kf(G) &= Kf(G_1) + Kf(K_{s+1}) + (n-s-1)Kf_x(K_{s+1}) + sKf_x(G_1) \\ &\ge n-s-1+\frac{(n-s)^2(k-1)-(n-s)(k-1)^2+(k-1)^2-3(k-1)}{n-s-k+1}+s \\ &\quad + (n-s-1)\frac{2s}{s+1} + s\left[\frac{2(n-s-k)}{n-s-k+1} + \Big(1+\frac{2}{n-s-k+1}\Big)(k-1)\right] \\ &= n-1+(n-s-1)\Big(2-\frac{2}{s+1}\Big) + \frac{(k-1)\left[(n-s)^2-(n-s)(k-1)+k-4\right]}{n-s-k+1} \\ &\quad + s\frac{2(n-s-k)+(n-s-k+3)(k-1)}{n-s-k+1} \\ &= 3n-2s-3-\frac{2(n-s-1)}{s+1}+(n-s)(k-1)+\frac{(k-1)(k-4)}{n-s-k+1} \\ &\quad + \frac{2s(n-s-k)+s(k-1)(n-s-k+3)}{n-s-k+1} \\ &= (n-s)(k+1)+n-3-\frac{2(n-s-1)}{s+1}+\frac{(k-1)(k-4)}{n-s-k+1} \\ &\quad + \frac{s(n-s-k)(k+1)+3(k-1)s}{n-s-k+1} \end{aligned}$$

$$
\begin{aligned}
&= (n-s)(k+1)+n-3-\frac{2(n-s-1)}{s+1}+\frac{(k-1)(k-4+3s)}{n-s-k+1} \\
&\qquad\qquad\qquad\qquad\qquad +\Big(1-\frac{1}{n-s-k+1}\Big)s(k+1) \\
&= n(k+1)+n-3-\frac{2(n-s-1)}{s+1}+\frac{(k-1)(k-4)+2s(k-2)}{n-s-k+1} \\
&\geq n(k+1)+n-3-(n-2)+\frac{(k-1)(k-4)+2(k-2)}{n-k} \\
&= n-1+\frac{n^2k-nk^2+k^2-3k}{n-k}
\end{aligned}
$$

with both equalities holding if and only if $s=1$ and $G_1 \cong E_{n-1}(n-k;2^{(k-1)})$, i.e., $G \cong E_n(n-k;2^{(k)})$. Thus our result follows immediately. □

Combining Theorems 3.1, 3.2 and 3.3, we can obtain the following result:

Theorem 3.4. *For any graph $G \in \mathcal{G}_{n,k}$ with $1 \leq k < \frac{n}{2}$, we have*

$$Kf(G) \geq n-1+\frac{n^2k-nk^2+k^2-3k}{n-k}$$

with equality holding if and only if $G \cong E_n(n-k;2^{(k)})$.

After obtaining Theorem 3.4, naturally we would like to propose the following two problems, by which we end this paper:

(1) Which graphs from $\mathcal{G}_{n,k}$ with $\frac{n}{2} \leq k \leq n-3$ have the minimal Kirchhoff index? Probably Lemma 2.15 also works for this problem, although we can not know the exact extremal graph on this topic.

(2) Which graphs from $\mathcal{G}_{n,k}$ have the maximal Kirchhoff index? Maybe the cycle C_n is a natural candidate we are searching for the case $k=0$. If so, it can be a starting point for this problem.

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