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The Maximal Kirchhoff Index of Theta Shape Graph

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Abstract. The resistance distance between any two vertices of a connected graph G is defined as the effective resistance between them in the electrical network constructed from G by replacing each edge of G with unit resistor. The Kirchhoff index of a graph is a structure-descriptor based on resistance distance. The investigation on the Kirchhoff index of graph is an important topic in the theory of graph. It is difficult to implement some algorithms to compute resistance distance and Kirchhoff index in a graph from their computational complexity. Hence, it makes sense to find closed-form formulae or solve extreme problems for the Kirchhoff index. For the connected graphs whose cyclomatic number less than two, their resistance distances and the Kirchhoff indices have been described well. In this paper, we discuss the graphs with cyclomatic number two, by graph transformations the maximal Kirchhoff index and the corresponding graph in the theta shape graphs (a specified class of bicycle graphs) are obtained.

Keywords: electrical network, resistance distance, Kirchhoff index, theta shape graph.

1. Introduction

The graph G considered here is simple undirected, with the vertex set V(G) and edge set E(G). We denote the number of the vertices of G by |V(G)|, and the number of the edges of G by |E(G)|. The distance between vertices u and v of graph G, denoted by d(u,v), is the length of the shortest path between them. If e is an edge of a connected graph G, we denoted by G-e the graph obtained from G by deleting the edge e, and G\e the graph obtained by removing the edge e and identifying its two end-vertices.

On the basis of electrical network theory, Klein and Randic introduced the novel concept of resistance distance[1]. Let G be a connected graph with vertices set $v_1, v_2, \cdots, v_n$, they viewed a graph 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 $r(v_i, v_j)$ or r_{ij} , is defined to be the effective resistance between nodes v_i and v_j as computed with Ohm's law in N. The Kirchhoff index of G, defined as [1], $Kf(G) = \sum_{i<j} r_{ij}$, is the sum of resistance distances between all pairs of vertices in G. The famous Wiener index was denoted as W(G)[2], $W(G) = \sum_{i<j} d_{ij}$, which counts the sum of distances between pairs of vertices of G. Klein and Randic proved that $r_{ij} \le d_{ij}$ and $Kf(G) \le W(G)$ with equality if and only if G is a tree[1]. Kirchhoff index is a structure-descriptor based on resistance distance. The investigation on the Kirchhoff index of graph is an important topic in the theory of graph. It is difficult to implement some algorithms to compute resistance distance and Kirchhoff index in a graph from their computational complexity. Hence, it makes sense to find closed-form formulae for the Kirchhoff index [1,3]. In present, to compute resistance distance, various methods have been developed, and relevant for resistance distance have been given for some classes of graphs, and some relevant indices to Kirchhoff index are discussed[3-16]. For the connected graphs whose cyclomatic number less than two, their resistance distances and the Kirchhoff indices have been described well. In this paper, we discuss the bicycle graphs, whose cyclomatic number is two.

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The bicycle graphs are connected graphs whose number of vertices is one more than the number of edges. The first and second classes of these graphs have been discussed, and their ordering relations and extreme graphs are obtained [11]. In this paper, we will pay attention to the third class of graphs, i.e. the theta shape graphs (as shown in Fig.1 (1)). We denote the theta shape graph with n vertices by Θ_n . Θ_n^t denotes the theta shape graph with n vertices, and the number of the vertices on the essential circles is t. In [16], We have investigated the ordering relations of the Kirchhoff index of the theta shape graphs and the minimal Kirchhoff index and the corresponding graph in this class of graphs are also discussed. In this paper, by the graph transformation, we find some ordering relations of Kirchhoff indices and discuss the maximal Kirchhoff index for this class of graphs.

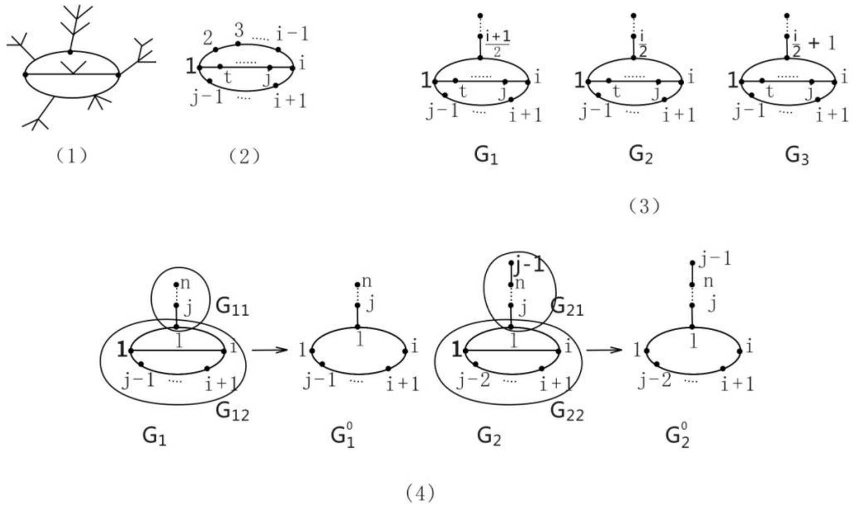

Fig. 1: Θ_n , Θ_n^t and their extreme graphs

The sum of the resistance distance from v_i to other vertices of G is denoted by $\mathrm{Kf}_{v_i}(G)$. The following lemmas will be used in sequel:

Lemma 1.1([8]) For a general graph G, $Kf(G) \geq n-1$, the equality holds if and only if G is a complete graph.

Lemma 1.2([9]) For a graph G, $Kf(G) \leq (n^3-n)/6$ with equality if and only if G is a path.

Lemma 1.3([10]) For a circulate graph G, $n-1 \leq Kf(G) \leq (n^3-n)/12$, the first equality holds if and only if G is K_n and the second does if and only if G is C_n .

Lemma 1.4([11]) Let C_n be the cycle on $n \geq 3$ vertices, for any two vertices $v_i, v_j \in V(C_n)$ with $i<j$, by ohm's law, we have $r_{C_n}(v_i,v_j)=(j-i)(n+i-j)/n$.

Lemma 1.5([12]) Let x be a cut vertex of a connected graph G such that G-x has exactly two branches G_1 and G_2. Let G_i' be the subgraph induced by $G_i \cup \{x\} (i=1,2)$. Then

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

Where $Kf_x(G_i')=\sum_{v\in V(G_i')} r(x,v), i=1,2.$

Lemma 1.6([13]) Let G' be a connected graph with $e=ij$ being an edge, $G=G'-e$, then for any $p,q \in V(G)(=V(G'))$

$$r'(p,q)=r(p,q)-\frac{[r(p,i)+r(q,j)-r(p,j)-r(q,i)]^2}{4[1+r(i,j)]}$$

Lemma 1.7([13]) Let G' be a connected graph with $e=ij$ being an edge, $G=G'-e$, then

$$Kf(G')=Kf(G)-\frac{n\sum_{k=1}^{n}[r(i,k)-r(j,k)]^2-[\sum_{k=1}^{n}r(i,k)-\sum_{k=1}^{n}r(j,k)]^2}{4[1+r(i,j)]}.$$

Lemma 1.8([13]) Let G be a connected graph with $e=ij$ being an edge. Let $G'=G-e$ and $G^*=G\setminus e$. Then for any $p,q\in V(G)$, $r(p,q)=[1-r(i,j)]r'(p,q)+r(i,j)r^*(p,q)$.

2. Main Results

2.1. Two graph transformations and some ordering relations

Transformation 1: The graph G is a connected graph with vertex set $\{v_1, v_2, \cdots, v_p\}$, and each vertex $v_i (1 \le i \le p)$ with hanging tree T_i, without loss of generality, we suppose the tree T_i with the maximal diameter q. We choose one path of length equal to the diameter of T_i, with the corresponding vertices $v_i, v_{i1}, v_{i2}, \cdots, v_{ij}, \cdots, v_{iq}$. If each vertex v_{ij} with hanging tree T_i, we denote such graph as G_1. If the tree T_{ij} is adhered to v_{iq}, we have the graph G_2 (see Fig. 2(1)). We denote the set of vertices of $T_{ij} \setminus v_{ij}$ as V_1, the set $\{v_{i,j+1}, \cdots, v_{iq}\}$ as V_2.

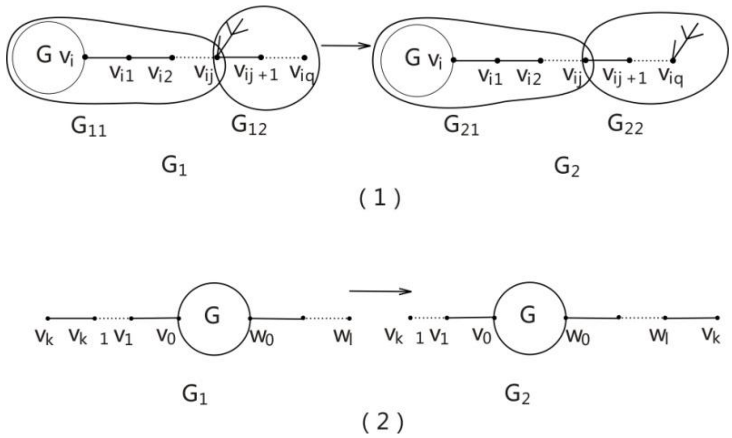

Fig. 2: Two graph transformations

Theorem 2.1 The graph G_1 and G_2 are such graphs given in Fig.2 (1), then $Kf(G_2) > Kf(G_1)$.

Proof. By Lemma 1.5, we have $Kf(G_1) = Kf(G_{11}) + Kf(G_{12}) + (|V(G_{11})|-1)Kf_{v_{ij}}(G_{12}) + (|V(G_{12})|-1)Kf_{v_{ij}}(G_{11})$ and

$$Kf(G_2) = Kf(G_{21}) + Kf(G_{22}) + (|V(G_{21})|-1)Kf_{v_{ij}}(G_{22}) + (|V(G_{22})|-1)Kf_{v_{ij}}(G_{21}).$$

As $G_{11} \cong G_{21}$, $G_{12} \cong G_{22}$, $Kf(G_{11}) = Kf(G_{21})$, $Kf(G_{12}) = Kf(G_{22})$. And $Kf_{v_{ij}}(G_{11}) = Kf_{v_{ij}}(G_{21})$, $|V(G_{11})| = |V(G_{21})|$, $|V(G_{12})| = |V(G_{22})|$. So we are sufficient to compare $Kf_{v_{ij}}(G_{12})$ with $Kf_{v_{ij}}(G_{22})$,

$$Kf_{v_{ij}(G_{12})} = \sum\nolimits_{v\in V_1} r_{G_{12}}(v_{ij}, v) + \sum\nolimits_{v\in V_2} r_{G_{12}}(v_{ij}, v),$$

$$Kf_{v_{ij}}(G_{22}) = \sum\nolimits_{v\in V_1} r_{G_{22}}(v_{ij}, v) + \sum\nolimits_{v\in V_2} r_{G_{22}}(v_{ij}, v) = \sum\nolimits_{v\in V_1} [d(v_{ij}, v_{iq}) + r_{G_{12}}(v_{ij}, v)] + \sum\nolimits_{v\in V_2} r_{G_{22}}(v_{ij}, v)$$

As $d(v_{ij}, v_{iq}) > 0$, then $Kf_{v_{ij}}(G_{12}) < Kf_{v_{ij}}(G_{22})$. The result is obtained.

Transformation 2: The graph G with $|V(G)| \ge 3$ and we choose two vertices of G, for example v_0 and w_0 with $d(v_0, w_0) \ge 2$, there is an automorphism Φ of G such that $\Phi(w_0) = \Phi(v_0)$, then for any $u \in V(G)$, $r(v_0, u) = r(w_0, u)$. P_k and P_l are two paths with length k and l respectively, and $k \le l$. The graph G_1 is obtained from G if v_0 and w_0 with hanging path P_k and P_l respectively, and G_2 is obtained from G if v_0 and w_0 with hanging path P_{k-1} and P_{l+1} respectively.(see Fig.2(2))

Theorem 2.2 The graph G_1 and G_2 are such graphs given in Fig.2 (2), then $Kf(G_1) < Kf(G_2)$.

Proof. By Lemma 1.5,

$$Kf_{v_k}(G_1) = \sum\nolimits_{u\in V_{P_k}} r(v_k, u) + \sum\nolimits_{u\in V(G)} r(v_k, u) + \sum\nolimits_{u\in V_{P_l}} r(v_k, u) = \frac{k(k-1)}{2} + \sum\nolimits_{u\in V(G)} [k + r(v_0, u)] + \sum\nolimits_{i=1}^{l} [k + r(v_0, w_0) + i]$$

$$= \frac{k(k-1)}{2} + k|V(G)| + Kf_{v_0}(G) + kl + \frac{l(l+1)}{2} + lr(v_0, w_0)$$

$$Kf_{w_l}(G_1) = \sum\nolimits_{u\in V_{P_k}} r(w_l, u) + \sum\nolimits_{u\in V(G)} r(v_k, u) + \sum\nolimits_{u\in V_{P_l}} r(w_l, u) = \frac{l(l-1)}{2} + \sum\nolimits_{u\in V(G)} [l + r(w_0, u)] + \sum\nolimits_{i=1}^{k} [l + r(v_0, w_0) + i]$$

$$= \frac{l(l-1)}{2} + l|V(G)| + Kf_{w_0}(G) + kl + \frac{k(k+1)}{2} + kr(w_0, v_0)$$

So $Kf_{w_l}(G_1) - Kf_{v_k}(G_1) = (l-k)(|V(G)| - r(v_0, w_0) - 1)$. Since $|V(G)| - 1 \ge d(v_0, w_0) \ge r(v_0, w_0)$, and $l - k \ge 0$. Then $Kf_{v_k}(G_1) \le Kf_{w_l}(G_1)$. Thus $Kf_{v_k}(G_2) = Kf_{w_l}(G_1) - r_{G_1}(w_l, v_k) + |V(G)| - 1 > Kf_{w_l}(G_1)$. Therefore $Kf_{v_k}(G_2) > Kf_{v_k}(G_1)$. Since $Kf(G_2) - Kf(G_1) = Kf_{v_k}(G_2) - Kf_{v_k}(G_1)$, then we get $Kf(G_2) > Kf(G_1)$.

Theorem 2.3 $G_0 \in \Theta_n$ is the graph with the maximal Kirchhoff index, then there must be a vertex of G_0 with only one vertex hanging path.

Proof. The result can be obtained by Theorem 2.1 and Theorem 2.2 easily.

Theorem 2.4

The graph G is a graph depicted in Fig.1(2), $i<j<t$, $G_1 = G - e_{l,l+1}$, $G_2 = G \setminus e_{l,l+1} (1 \le l \le i-1)$, then $Kf_{v_{\frac{i+1}{2}}}(G)$ is the maximal amongst all vertices of G when i is odd, $Kf_{v_{\frac{i}{2}}}(G) = Kf_{v_{\frac{i}{2}+1}}(G)$ are the maximal when i is even.

Proof. $\forall q \in V(G)$, by Lemma 1.8 $r_G(l,q) = [1 - r_G(l,l+1)] r_{G_1}(l,q) + r_G(l,l+1) r_{G_2}(l,q)$,

$$r_G(l+1,q) = [1 - r_G(l,l+1)] r_{G_1}(l+1,q) + r_G(l,l+1) r_{G_2}(l+1,q)$$

If we want to compare $Kf_{v_l}(G)$ with $Kf_{v_{l+1}}(G)$, we are sufficient to compare $Kf_{v_l}(G_1)$ with $Kf_{v_{l+1}}(G_1)$. And $Kf_{v_l}(G_1) = \sum_{1 \le q \le t, q \ne l} r_{G_1}(l,q)$, $Kf_{v_{l+1}}(G_1) = \sum_{1 \le q \le t, q \ne l+1} r_{G_1}(l+1,q)$, so if $1 \le l \le [\frac{i}{2}]$, $Kf_{v_l}(G_1) \le Kf_{v_{l+1}}(G_1)$, $Kf_{v_l}(G) \le Kf_{v_{l+1}}(G)$; if $[\frac{i}{2}] < l \le i$, $Kf_{v_l}(G_1) \ge Kf_{v_{l+1}}(G_1)$, $Kf_{v_l}(G) \ge Kf_{v_{l+1}}(G)$. Thus we complete the proof.

Theorem 2.5 If $G_0 \in \Theta_n^t$ is the graph with the maximal Kirchhoff index, then $G_0 \cong G_1$ when i is odd, and $G_0 \cong G_2, G_3$ when i is even.(see Fig.1(3)).

Proof. The result is obtained from Theorem 2.4.

2.2. The maximal Kirchhoff index and the corresponding graph

In this section we consider $G \in \Theta_n^t$ such that $t = j-1$, i and j are both odd,

Theorem 2.6

The graph $G_1 \in \Theta_n^{j-1}$ and $v_{\underline{i+1}}$ with hanging path P_{n-j+1}, the graph $G_2 \in \Theta_n^{j-2}$ and $v_{\underline{i+1}}$ with hanging path P_{n-j+2}, then $Kf(G_1) < Kf(G_2)$. (see Fig.1(4))

Proof. Suppose $G_1' \cong G_1 - e_{1i}$ and $G_2' \cong G_2 - e_{1i}$, by Lemma 1.7,

$$Kf(G_1) = Kf(G_1') - \frac{n\sum_{k=1}^n [r_{G_1'}(1,k) - r_{G_1'}(i,k)]^2 - [\sum_{k=1}^n r_{G_1'}(1,k) - \sum_{k=1}^n r_{G_1'}(i,k)]^2}{4[1 + r_{G_1'}(1,\mathrm{i})]}.$$

$$Kf(G_2) = Kf(G_2') - \frac{n\sum_{k=1}^n [r_{G_2'}(1,k) - r_{G_2'}(i,k)]^2 - [\sum_{k=1}^n r_{G_2'}(1,k) - \sum_{k=1}^n r_{G_2'}(i,k)]^2}{4[1 + r_{G_2'}(1,\mathrm{i})]}.$$

As $\sum_{k=1}^n r_{G_1'}(1,k) = \sum_{k=1}^{j-1} r_{G_1'}(1,k) + \sum_{k=j}^n r_{G_1'}(1,k) = \sum_{k=1}^{j-1} r_{G_1'}(1,k) + \sum_{k=j}^n (\mathrm{d}_{G_1'}(l,k) + r_{G_1'}(l,1))$,

$\sum_{k=1}^n r_{G_1'}(\mathrm{i},k) = \sum_{k=1}^{j-1} r_{G_1'}(\mathrm{i},k) + \sum_{k=j}^n (\mathrm{d}_{G_1'}(l,k) + r_{G_1'}(l,\mathrm{i}))$, and $r_{G_1'}(l,1) = r_{G_1'}(l,i)$, $\sum_{k=1}^{j-1} r_{G_1'}(1,k) = \sum_{k=1}^{j-1} r_{G_1'}(i,k)$,

so $\sum_{k=1}^{n} r_{G_1'}(1,k) = \sum_{k=1}^{n} r_{G_1'}(i,k)$. Similarly, $\sum_{k=1}^{n} r_{G_2'}(1,k) = \sum_{k=1}^{n} r_{G_2'}(i,k)$. As G_1' and G_2' are both bicycle graphs, by the result of [11], we have $Kf(G_1') < Kf(G_2')$. Thus,

$$\frac{\sum_{k=1}^n [r_{G_1'}(1,k) - r_{G_1'}(i,k)]^2}{1 + r_{G_1'}(1,\mathrm{i})} - \frac{\sum_{k=1}^n [r_{G_2'}(1,k) - r_{G_2'}(i,k)]^2}{1 + r_{G_2'}(1,\mathrm{i})} = \frac{(i-1)^2(i+1)(i^2-2i+3) - (i-1)^2(2i^2-i+2)j + i(i-1)^2 j^2}{3(1+i^2-ij)(1-i+i^2-ij)}$$

As $i \ge 3$, $j \ge 5$, $j \ge i+2$, $1+i^2-ij \le 1-2i < 0$, $1-i+i^2-ij \le 1-3i < 0$, then $3(1+i^2-ij)(1-i+i^2-ij) > 0$.

And suppose that the function $f(j) = (i-1)^2(i+1)(i^2-2i+3) - (i-1)^2(2i^2-i+2)j + i(i-1)^2 j^2$, $i(i-1)^2 > 0$, $(i-1)^2(i+1)(i^2-2i+3) > 0$, $-(i-1)^2(2i^2-i+2) < 0$, so if $j \ge 5$, $f(j) > 0$. Thus $Kf(G_1) < Kf(G_2)$.

3. Conclusion

We have studied the case that i and j are both odd and $t = j-1$ and the corresponding theta shape graph with the maximal Kirchhoff index is also obtained. Now we haven't good method to solve other cases, they are also open.

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