A note on the Kirchhoff index of bicyclic graphs *

Lihua Feng[a,b]†, Guihai Yu[b], Kexiang Xu[c], Zhengtao Jiang[d]
[a]Department of Mathematics, Central South University
Railway Campus, Changsha, Hunan, 410075, P.R. China.
[b]School of Mathematics, Shandong Institute of Business and Technology
191 Binhaizhong Road, Yantai, Shandong, 264005, P.R. China.
[c]College of Science, Nanjing University of Aeronautics & Astronautics,
Nanjing, 210016, P.R. China
[d]School of Computer Science, Communication University of China
Beijing 100024, P.R. China.
e-mail: `fenglh@163.com`

Abstract

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 pairs of vertices. In this paper, we determine the bicyclic graph of order $n \geq 8$ with maximal Kirchhoff index. This improves and extends an earlier result by Zhang et al. [19].

1 Introduction

Let G be a connected graph with vertices labeled as $v_1, v_2, \ldots, v_n$. The 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. The famous Wiener index $W(G)$ [14] is the sum of distances between all pairs of vertices, that is, $W(G) = \sum_{i<j} d_G(v_i, v_j)$.

In 1993, Klein and Randić [7] introduced a new distance function named resistance distance based on electrical network theory. They viewed G as an electrical network N by replacing each edge of G with a unit resistor, the

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resistance distance between v_i and v_j, denoted by $r_G(v_i, v_j)$, is defined to be the effective resistance between them 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 and physical interpretations [7, 8], but with a substantial potential for chemical applications.

In fact, 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 the chemical communication in molecules is rather wavelike suggests the utility of this concept in chemistry. So in recent years, the resistance distance was well studied in mathematical and chemical literatures [1, 2, 3, 4, 21].

Analogue to Wiener index, the Kirchhoff index (or resistance index) [3] is defined as

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

As a useful structure-descriptor, the computation of Kirchhoff index is a hard problem [1], but one may compute the specific classes of graphs. Since for trees, the Kirchhoff index and the Wiener index coincide. It is possible to study the Kirchhoff index of topological structures containing cycles. Let P_n (resp. C_n) denote the path (resp. cycle) on n vertices. For a general graph G, Lukovits et al. [10] 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 [11] 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, it is showed in [20] that $n-1 \leq Kf(G) \leq \frac{1}{12}(n^3 - n)$, 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 [17], Yang et al studied the Kirchhoff index of unicyclic graphs with given girth and determined the extremal graphs. In [15], the authors studied the Kirchhoff index of linear hexagonal chains. In [18], Deng et al obtained the second maximal and minimal Kirchhoff index of unicyclic graphs. Deng also studied the Kirchhoff index of full loaded unicyclic graphs [6] and graphs with many cut edges [5]. Zhou [22] obtained the extremal graphs with given matching number, connectivity and minimal Kirchhoff index. Wang et al [13] obtained the first three minimal Kirchhoff indices among cacti.

In [19], the authors studied the Kirchhoff index of bicyclic graphs with exactly two cycles. Motivated by this result, in this paper, we further study the Kirchhoff index of general bicyclic graphs and determine the extremal graphs of order $n \geq 8$ with maximal Kirchhoff index. This improves and extends the result obtained by Zhang et al. [19].

2 Preliminaries

Lemma 2.1 *[7] 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 $r_G(a,b) = r_G(a,x) + r_G(x,b)$.*

It is well known that [7] $d_G(v_i, v_j) \geq r_G(v_i, v_j)$ with equality if and only if there is one unique path linking v_i and v_j. Therefore,

Lemma 2.2 *[7] Let G be a connected graph. Then we have $W(G) \geq Kf(G)$, with equality if and only if G is a tree.*

For a vertex v in G, we define $D_G(v) = \sum_{u \neq v} d_G(u,v)$, $Kf_v(G) = \sum_{u \neq v} r_G(u,v)$. Obviously, $D_G(v) \geq Kf_v(G)$.

Lemma 2.3 *Let G be a connected graph with a pendent vertex v with its unique neighbor w. Then $Kf_v(G) = Kf_w(G-v) + n - 1$.*

Proof. From the definition and Lemma 2.1, we have

$$\begin{aligned} Kf_v(G) &= \sum_{x \in G-v} r_G(v,x) = r_G(v,w) + \sum_{x \in G-v-w} r_G(v,x) \\ &= d_G(v,w) + \sum_{x \in G-v-w} (d_G(v,w) + r_G(w,x)) \\ &= 1 + n - 2 + \sum_{x \in G-v-w} r_G(w,x) = Kf_w(G-v) + n - 1. \end{aligned}$$

The result follows. ■

Lemma 2.4 *Let G be a connected bicyclic graph of order n and $v \in V(G)$. Then $Kf_v(G) \leq \frac{n^2}{2} - \frac{n}{2} - \frac{15}{4}$.*

Proof. If $n = 4$, then G is obtained from K_4 by deleting one edge, so the result holds. We assume $n \geq 5$ in the sequel.

Case 1. v is a pendent vertex. Let w be its neighbor. We shall prove the conclusion by induction on n. Clearly $G - v$ satisfies the induction hypothesis, and therefore together with Lemma 2.3, we have

$$\begin{aligned} Kf_v(G) &= Kf_w(G-v) + n - 1 \leq \left(\frac{(n-1)^2}{2} - \frac{n-1}{2} - \frac{15}{4}\right) + n - 1 \\ &= \frac{n^2}{2} - \frac{n}{2} - \frac{15}{4}. \end{aligned}$$

Case 2. v is not a pendent vertex. Then, the degree of v, $\deg_G(v)$, is at least 2. It follows that there are at least 2 vertices at resistance distance 1 from v, and the remaining vertices have resistance distance at most $2, 3, \ldots n-4, n-4+\frac{2}{3}, n-4+\frac{2}{3}$ from v, with equality if and only if G is the graph obtained from a triangle by attaching a path (at this moment, G is not bicyclic, but we just need one bound here). Note that for a graph, if we add one edge, the Kirchhoff index decreases [22]. Hence

$$\begin{aligned} Kf_v(G) &\leq 1+1+2+3+\ldots+(n-4)+(n-4+\frac{2}{3})+(n-4+\frac{2}{3}) \\ &= \frac{n^2}{2}-\frac{3}{2}n+\frac{1}{3}<\frac{n^2}{2}-\frac{n}{2}-\frac{15}{4}. \end{aligned}$$

This yields the result. ■

Lemma 2.5 *Let G be a connected graph, v a pendent vertex of G and w its neighbor. Then $Kf(G) = Kf(G-v) + Kf_w(G-v) + n - 1$.*

Proof. From the definition, we have

$$Kf(G) = \sum_{x,y\in G-v} r(x,y) + \sum_{x\in G-v} r(x,v) = \sum_{x,y\in G-v} r(x,y) + \sum_{x\in G-v}(r(x,w)+1) = Kf(G-v) + Kf_w(G-v) + n - 1,$$

and the result follows. ■

Lemma 2.6 *[18] Let G be a connected graph with a cut-vertex v such that G_1 and G_2 are two connected subgraphs of G having v as the only common vertex and $G_1 \cup G_2 = G$. Let $n_1 = |V(G_1)|$ and $n_2 = |V(G_2)|$. Then*

$$Kf(G) = Kf(G_1) + Kf(G_2) + (n_1-1)Kf_v(G_2) + (n_2-1)Kf_v(G_1).$$

For the cycle C_k, $Kf(C_k)$ (see [17]), $Kf_v(C_k)$ where $v \in V(C_k)$ (see [17]) are computed as follows.

$$Kf_v(C_k) = \tfrac{1}{6}(k^2-1), \quad Kf(C_k) = \tfrac{1}{12}(k^3-k).$$

Lemma 2.7 *Let H be connected graph of order $h \geq 2$ and C_k be a cycle of order $k \geq 4$. Let F be the graph of order k obtained from C_3 by attaching one pendent path of order $k-3$ to one vertex of C_3. Further suppose G_1 is the graph obtained from H and C_k by identifying one vertex in H and one vertex in C_k; G_2 is the graph obtained from H and F by identifying one vertex in H and the pendent vertex in F. Then we have $Kf(G_1) < Kf(G_2)$.*

Proof. Suppose $V(H) \cap V(C_k) = V(H) \cap V(F) = \{v\}$. From Lemma 2.6, we have

$$Kf(G_1) = Kf(C_k) + Kf(H) + (k-1)Kf_v(H) + (h-1)Kf_v(C_k),$$
$$Kf(G_2) = Kf(F) + Kf(H) + (k-1)Kf_v(H) + (h-1)Kf_v(F).$$

Therefore, it follows that

$$Kf(G_1) - Kf(G_2) = Kf(C_k) - Kf(F) + (h-1)\big(Kf_v(C_k) - Kf_v(F)\big).$$

A straightforward calculation [17] shows that

$Kf_v(F) = 1+2+\ldots+(k-3)+(k-3+\frac{2}{3})+(k-3+\frac{2}{3}) = \frac{1}{6}(3k^2-3k-10)$.

$Kf(F) = \frac{1}{6}(k^3 - 11k + 18)$.

Therefore,

$Kf(C_k) - Kf(F) = \frac{1}{12}(k^3 - k) - \frac{1}{6}(k^3 - 11k + 18) = -\frac{1}{12}(k-3)(k^2 + 3k - 12) < 0$,

$Kf_v(C_k) - Kf_v(F) = \frac{1}{6}(k^2-1) - \frac{1}{6}(3k^2-3k-10) = \frac{1}{6}(-2k^2+3k+9) < 0$.

We get finally that $Kf(G_1) < Kf(G_2)$.■

3 Main results

In this section, we characterize bicyclic graphs of order at least 8 with maximal Kirchhoff index and determine bounds for Kirchhoff index of bicyclic graphs.

Let G be a bicyclic graph. The base of G, denoted by $\widehat{G}$, is the (unique) minimal bicyclic subgraph of G. It is easy to see that $\widehat{G}$ is the unique bicyclic subgraph of G containing no pendent vertices, while G can be obtained from $\widehat{G}$ by attaching trees to some vertices of $\widehat{G}$.

It is well known that there are the following three types of bicyclic graphs containing no pendent vertices:

Let $B(p, q)$ be the bicyclic graph obtained from two vertex-disjoint cycles C_p and C_q by identifying vertices u of C_p and v of C_q

Let $B(p, l, q)$ be the bicyclic graph obtained from two vertex-disjoint cycles C_p and C_q by joining vertices u of C_p and v of C_q by a new path $uu_1u_2\ldots u_{l-1}v$ with length l ($l \geq 1$).

Let $B(P_k, P_l, P_m)$, $1 \leq m \leq \min\{k, l\}$ be the bicyclic graph obtained from three pairwise internal disjoint paths from a vertex x to a vertex y. These three paths are $xv_1v_2\ldots v_{k-1}y$ with length k, $xu_1u_2\ldots u_{l-1}y$ with length l, and $xw_1w_2\ldots w_{m-1}y$ with length m.

Let B_n be the graph of order n obtained from two triangles linked by a path (for example, B_{10} is shown in Fig. 1). It is known that [19]

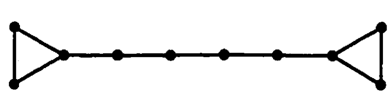

Figure 1: *The bicyclic graph B_{10}.*

$Kf(B_n) = \frac{1}{6}(n^3-21n+36)$. It is well known that $W(P_k) = \frac{1}{6}k(k-1)(k+1)$. For a pendent vertex u of P_k, we have $D_{P_k}(u) = \frac{(k-1)k}{2}$.

Let D_n be the graph obtained from $B(P_2, P_2, P_1)$ (which is just $K_4 - e$) by attaching one path of order $n-4$ to a vertex of degree 2 in $B(P_2, P_2, P_1)$. Let v be the vertex with degree 3 in D_n, at which the pendent path P_{n-3} is attached. From [16], one has $Kf(K_4 - e) = 4$ and $Kf_v(K_4 - e) = \frac{9}{4}$. From Lemma 2.6 and Lemma 2.2, it follows that

$$\begin{aligned} Kf(D_n) &= Kf(K_4 - e) + Kf(P_{n-3}) + 3Kf_v(P_{n-3}) + (n-4)Kf_v(K_4 - e) \\ &= 4 + \frac{1}{6}(n-4)(n-3)(n-2) + 3 \cdot \frac{1}{2}(n-4)(n-3) + \frac{9}{4}(n-4) \\ &= \frac{n^3}{6} - \frac{47n}{12} + 9. \end{aligned}$$

A straight forward calculation shows that $Kf(B_n) - Kf(D_n) = \frac{5n-36}{12}$, which is positive if $n \geq 8$.

Theorem 3.1 *Let G be a bicyclic graph of order $n \geq 8$. Then $Kf(G) \leq Kf(B_n)$. The equality holds if and only if $G \cong B_n$.*

Proof. We now distinguish the following cases.

Case 1. G has a pendent vertex. We prove this case by induction. Let v be a pendent vertex of G and let w be its neighbor. Clearly $G - v$ satisfies the induction hypothesis, and so by Lemma 2.4, Lemma 2.5, we have

$$\begin{aligned} Kf(G) &= Kf(G-v) + Kf_w(G-v) + n - 1 \\ &\leq \left(\frac{n^3}{6} - \frac{n^2}{2} - \frac{41n}{12} + \frac{51}{4}\right) + \left(\frac{(n-1)^2}{2} - \frac{n-1}{2} - \frac{15}{4}\right) + n - 1 \\ &= \frac{n^3}{6} - \frac{47n}{12} + 9 = Kf(D_n). \end{aligned}$$

Case 2. G has no pendent vertex. From the description at the beginning of this section, there are three types of bicyclic graphs with no pendent vertices, and we consider the following cases.

Subcase 2.1. G is of the form $B(p, l, q)$. By Lemma 2.7, we can get that $Kf(G) \leq Kf(B_n)$ holds, we get the result.

Subcase 2.2. G is of the form $B(P_k, P_l, P_m)$, i.e., G is 2-connected. Let v be an arbitrary vertex. It is well known that [12] $D_G(v) \leq \frac{1}{4}n^2$ with equality holding if and only if G is an even cycle, then it follows that $Kf_v(G) \leq D_G(v)$ and

$$\begin{aligned} Kf(G) &= \frac{1}{2}\sum_{x \in G} Kf_x(G) \leq \frac{1}{2}\sum_{x \in G} D_G(x) \leq \frac{1}{2} \cdot \frac{1}{4}n^2 \cdot n \\ &< \frac{1}{6}(n^3 - 21n + 36) = Kf(B_n). \end{aligned}$$

Subcase 2.3. G is of the form $B(p,q)$. By Lemma 2.7, we can get $Kf(G) \leq Kf(B_n)$.

Combining the above cases, the result follows. ■

Remark. In [19], the authors obtained that among bicyclic graphs with exactly two cycles, the graph B_n has the maximal Kirchhoff index. Based on Theorem 3.1, we find that the result also holds for all bicyclic graphs of order at least 8.

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