HK.NCCP

International Journal of Applied Mathematics and Soft Computing
Volume 3, Issue 3, October, 2017

Extremal Kirchhoff Index of a Class of Unicyclic Graphs

Xia Cai, Ting Zeng, Lihui Yang, Jianguang Yang, Zhijun Guo, Shubo Chen
College of Science, Hunan City University, Yiyang, 413000, China

Abstract: The resistance distance between two vertices of a connected graph G is defined as the effective resistance between them in the corresponding electrical network constructed from G by replacing each edge of G with a unit resistor. The Kirchhoff index Kf(G) is the sum of resistance distances between all pairs of vertices of the graph G. In this paper, we shall characterize a class of unicyclic graph with the extremal Kirchhoff index.

Keywords: Resistance distance; Kirchhoff index; Unicyclic graph

1. Introduction

For any $v \in V(G)$, $d(v) = d_G(v)$ is the degree of vertex v, the distance between vertices vi and vj, is denoted by $d(v_i, v_j) = d_G(v_i, v_j)$, is the length of a shortest path between them. Wiener index is the first recorded index, introduced by American chemist H. Wiener in [1], defined as

$$W(G) = \sum_{\{v_i, v_j \subseteq V(G)\}} d(v_i, v_j) \quad (1)$$

For the n vertices path Pn, one has $W(P_n) = \binom{n+1}{3}$.

In 1993, Klein and Randic [2] introduced resistance distance on the basis of electrical network theory. 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 the vertices vi and vj, are denoted by r(vi, vj)=rG(vi, vj), is defined to be the effective resistance between nodes $v_i, v_j \in N$. The Kirchhoff index Kf(G) of a graph G is defined as [2, 3]

$$Kf(G) = \sum_{\{v_i, v_j \subseteq V(G)\}} r(v_i, v_j) \quad (2)$$

If G is a tree, $d(v_i, v_j) = r(v_i, v_j)$ for any two vertices v_i and v_j. Consequently, the Kirchhoff and Wiener indices of trees coincide.

The Kirchhoff index is an important molecular structure descriptor [4], it has been well studied in both mathematical and chemical literatures. References to recent studies are available from [5-10].

A graph G is called a unicyclic graph if it contains exactly one cycle, the unique cycle Cg=v1v2⋯vgv1 in a unicyclic graphs, simply denoted as

G=U(Cg; T1, T2,⋯,Tg)

where Ti is the components of G. E(Cg) containing vi, 1≤i≤g, Ti is a tree rooted at vi. Let U(n; g) be the set of unicyclic graphs with n vertices and the unique cycle Cg, U(n) be the set of unicyclic graphs with n vertices. In [11], H. Zhang et al., determined unicyclic graphs with the maximal Kirchhoff index, and H. Deng et al. [12] obtained unicyclic graphs with the second maximal Kirchhoff index. X. Cai in [13] characterized unicyclic graphs with the second maximum Kirchhoff index.

In the paper we'll characterize a class unicyclic graphs Ug(k,i,l), depicted in Figure 1, with extremal Kirchhoff index. The paper is organized as follows, in Section 2 we state some preparatory results, whereas in Section 3 we state our main results.

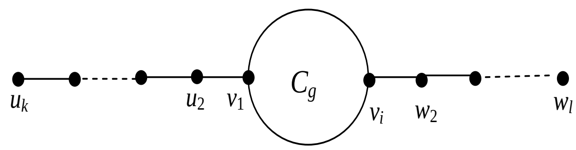

Figure 1. The graph Ug(k,i,l)

2. Preliminary Results

For a graph G with $v \in V(G)$, $G - v$ denotes the graph resulting from G by deleting v (and its incident edges). For an edge uv of the graph G (the complement of G, respectively), G-uv(G+uv, respectively) denotes the graph resulting from G by deleting (adding, respectively) uv.

Let $Kf_{v_i}(G) = \sum_{v_j \in V(G)} r(v_i, v_j)$, then

$$Kf(G) = \frac{1}{2} \sum_{u \in V(G)} Kf_u(G) \quad (3)$$

Let Cg be the cycle on k≥3 vertices, for any two vertices $v_i, v_j \in V(C_g)$ with i<j, by Ohm's law, we have $r(v_i, v_j) = \frac{(j-i)(g+i-j)}{g}$. For any vertex $v_i \in V(C_g)$,

it's suffice to see that $Kf_{v_i}(C_g)=\frac{k^2-1}{6}$, $Kf(C_g)=\frac{k^3-k}{12}$.

Lemma 2.1([2]). Let x be a cut vertex of a connected graph and a and b be vertices occurring in different components which arise upon deletion of x. Then

$$r_G(a,b)=r_G(a,x)+r_G(x,b) \quad (4)$$

Lemma 2.2([11]). Let G1 and G2 be two connected graphs with exactly one common vertex x, and $G=G_1\bigcup G_2$. Then

$$Kf(G)=Kf(G_1)+Kf(G_2)+(|V(G_1)|-1)Kf_x(G_2)+(|V(G_2)|-1)Kf_x(G_1) \quad (5)$$

3. Main Results

Let L(g,k) be the lollipop graph depicted in Figure 2.

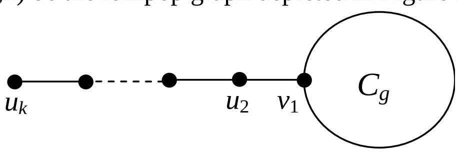

Figure 2. The lollipop graph L(g,k)

By Lemma 2.2, one has,

Theorem 3.1. Let L(g, k) be the graph depicted in Figure 2, then

$$Kf(L(g,k))=\frac{g^3}{12}+\frac{g^2}{6}(k-1)+\frac{g}{12}(6k^2-6k-1)+\frac{k^3-3k^2+k+1}{6}. \quad (6)$$

Proof. By the formula (2.3), one has,

$$\begin{aligned}Kf(L(g,k))&=Kf(C_g)+Kf(P_k)+(k-1)Kf_{v_1}(C_g)+(g-1)Kf_{v_1}(P_k)\\&=\frac{g^3-g}{12}+\frac{1}{6}k(k^2-1)+(k-1)\frac{g^2-1}{6}+(g-1)\frac{1}{2}k(k+1)\\&=\frac{g^3-g}{12}+\frac{g^2(k-1)}{6}+\frac{g(6k^2-6k-1)}{12}+\frac{k^3-3k^2+k+1}{6}\end{aligned} \quad (7)$$

The proof is completed.

In the following, we'll investigate the extremal Kirchhoff index of $U_g(k,i,l)$.

Theorem 3.2. Let $G\in U_g(k,i,l), 2\le i\le l-1$ be the graph depicted in Figure 1,

(i) If g is even, then

$Kf(U_g(k,i,l))\le Kf(U_g(l+k,\frac{g}{2}+1,0))$ or

$Kf(U_g(k,i,l))\le Kf(U_g(0,\frac{g}{2}+1,l+k))$.

(ii) If g is odd, then

$Kf(U_g(k,i,l))\le Kf(U_g(l+k,\frac{g+1}{2}+1,0))$ or

$Kf(U_g(k,i,l))\le Kf(U_g(0,\frac{g+1}{2}+1,l+k))$.

Proof. By Theorem 3.1 and Lemma 2.2, one has,

$$\begin{aligned}Kf(U_g(k,i,l))&=Kf(L(g,k))+Kf(P_l)+(g+k-2)Kf_{v_i}(P_l)+(l-1)Kf_{v_i}(L(g,k))\\&=\frac{g}{12}+\frac{g^2(k-1)}{6}+\frac{g(6k^2-6k-1)}{12}+\frac{k^3-3k^2+k+1}{6}+\binom{l+1}{3}+\\&\quad(g+k-2)\frac{l(l-1)}{2}+(l-1)[Kf_{v_i}(C_g)+(k-1)r(v_1,v_i)+\frac{k(k-1)}{2}]\end{aligned} \quad (8)$$

where $r(v_1,v_i)=\frac{(i-1)(g+1-i)}{g}\le\begin{cases}\frac{g}{4}, & if\ g\ is\ even;\\ \frac{g^2-1}{4g}, & if\ g\ is\ odd.\end{cases}$

with the equality if and only if $i=\left[\frac{g}{2}\right]+1$ or $i=\left[\frac{g+1}{2}\right]+1$.

(i) If g is even, then $g\ge 4$ and $r(v_1,v_i)\le r(v_1,v_{\frac{g}{2}+1})=\frac{g}{4}$, then

$$\begin{aligned}Kf(U_g(k,i,l))&\le\frac{g}{12}+\frac{g^2(k-1)}{6}+\frac{g(6k^2-6k-1)}{12}+\frac{k^3-3k^2+k+1}{6}+\binom{l+1}{3}+\\&\quad(g+k-2)\frac{l(l-1)}{2}+(l-1)[Kf_{v_i}(C_g)+(k-1)\frac{g}{4}+\frac{k(k-1)}{2}]\\&=Kf(U_g(k,\frac{g}{2}+1,l))\end{aligned} \quad (9)$$

Supposing that $k\ge l+1$, then

$$Kf(U_g(k,\frac{g}{2}+1,l))-Kf(U_g(k-1,\frac{g}{2}+1,l+1))=\left(\frac{3g}{4}-1\right)(k-l-1)\ge 0 \quad (10)$$

Thus, we have

$Kf(U_g(k,i,l))\le Kf(U_g(l+k,\frac{g}{2}+1,0))$ or

$Kf(U_g(k,i,l))\le Kf(U_g(0,\frac{g}{2}+1,l+k))$.

(ii) If g is odd, then $g\ge 3$ and $r(v_1,v_i)\le r(v_1,v_{\frac{g+1}{2}+1})=\frac{g^2-1}{4g}<\frac{g+1}{4}$, then

$$\begin{aligned}Kf(U_g(k,i,l))&\le\frac{g^3}{12}+\frac{g^2(k-1)}{6}+\frac{g(6k^2-6k-1)}{12}+\frac{k^3-3k^2+k+1}{6}+\binom{l+1}{3}+\\&\quad(g+k-2)\frac{l(l-1)}{2}+(l-1)[Kf_{v_i}(C_g)+(k-1)\frac{g^2-1}{4g}+\frac{k(k-1)}{2}]\\&=Kf(U_g(k,\frac{g+1}{2}+1,l))\end{aligned} \quad (11)$$

Supposing that $k\ge l+1$ again, then

$$Kf(U_g(k,\frac{g+1}{2}+1,l))-Kf(U_g(k-1,\frac{g+1}{2}+1,l+1))=\frac{k-l-1}{4}\left(3g-4+\frac{1}{g}\right)\ge 0 \quad (12)$$

Thus, one has

$Kf(U_g(k,i,l))\le Kf(U_g(l+k,\frac{g+1}{2}+1,0))$ or

$Kf(U_g(k,i,l)) \le Kf(U_g(0,\frac{g+1}{2}+1,l+k))$.

This completes the proof.

Theorem 3.3. Let $G \in U_g(k,i,l)$, then

$$Kf(U_g(k,i,l)) \le \frac{g^3}{12} + \frac{g^2(k+l-2)}{6} + \frac{g[6(k+l)^2-18(k+l)+11]}{12} + \frac{(k+l)^3-6(k+l)^2+10(k+l)-4}{6} \qquad (13)$$

the equality holds if and only if $G \cong U_g(k+l,i,0)$ or $G \cong U_g(0,i,k+l)$.

Finally, we'll investigate graphs in $U_g(k,i,l)$ with the minimal Kirchhoff index.

By the same reasons as those used in Theorem 3.2 and Theorem 3.3, we'll arrives at following result.

Theorem 3.4. Let $G \in U_g(k,i,l)$ for $2 \le i \le g$, then

$$Kf(U_g(k,i,l)) \ge \begin{cases} \frac{g^3}{12} + \frac{g^2(t-1)}{6} + \frac{g(12t^2-12t-1)}{12} + \frac{t^3-6t^2-2t+4}{3} - \frac{(t-1)^2}{g}, & \text{if } k+l=2t; \\ \frac{g^3}{12} + \frac{g^2(t-1)}{6} + \frac{g(12t^2-1)}{12} + \frac{8t^3-10t+1}{6} - \frac{t^2-t}{g}, & \text{if } k+l=2t+1. \end{cases} \qquad (14)$$

The equality holds if and only if $G \cong U_g(t,2,t)$ for $k+l=2t$ or $G \cong U_g(t+1,2,t)$ for $k+l=2t+1$.

Proof. By Theorem 3.1, one has,

$$\begin{aligned} Kf(U_g(k,i,l)) &= \frac{g^3}{12} + \frac{g^2(k-1)}{6} + \frac{g(6k^2-6k-1)}{12} + \frac{k^3-3k^2+k+1}{6} + \binom{l+1}{3} + \\ &\quad (g+k-2)\frac{l(l-1)}{2} + (l-1)[Kf_{v_i}(C_g) + (k-1)r(v_1,v_i) + \frac{k(k-1)}{2}] \\ &= Kf(U_g(k,\frac{g+1}{2}+1,l)) \end{aligned} \qquad (15)$$

where

$$r(v_1,v_i) = \frac{(i-1)(g+1-i)}{g} \ge \frac{(2-1)(g+1-2)}{g} = \frac{g-1}{g},$$

with the equality if and only if i=2 or i=g.

It's noted that,

$$Kf\left(U_g\left(\left\lceil \frac{k+l}{2} \right\rceil, 2, \left\lfloor \frac{k+l}{2} \right\rfloor\right)\right) = Kf\left(U_g\left(\left\lceil \frac{k+l}{2} \right\rceil, g, \left\lfloor \frac{k+l}{2} \right\rfloor\right)\right) \qquad (16)$$

Then,

$$\begin{aligned} Kf(U_g(k,i,l)) &\ge \frac{g^3}{12} + \frac{g^2(k-1)}{6} + \frac{g(6k^2-6k-1)}{12} + \frac{k^3-3k^2+k+1}{6} + \binom{l+1}{3} + \\ &\quad (g+k-2)\frac{l(l-1)}{2} + (l-1)[Kf_{v_i}(C_g) + (k-1)\frac{g-1}{g} + \frac{k(k-1)}{2}] \\ &= Kf(U_g(k,2,l)) \end{aligned} \qquad (17)$$

Supposing that $k \ge l+1$, then

$$Kf(U_g(k,2,l)) - Kf(U_g(k-1,2,l+1)) = (k-l-1)\left(g+\frac{1}{g}-2\right) \ge 0. \qquad (18)$$

This completes the proof.

By a simple calculation, we'll arrive at the desired result.

4. Acknowledgment

Projects supported by NSFC(Grant no. 11401192), Natural Science Foundation of Hunan Province(Grant no. 2015JJ3031), Scientific Research Fund of Hunan Provincial Education Department (Grant no. 15C0248, 14A026).

References

[1] H. Wiener, Structural determination of paraffinboiling points, J. Amer. Chem. Soc. 69 (1947) 17-20.

[2] D. J. Klein and M. Randic, Resistance distance, J. Math. Chem. 12 (1993) 81-95.

[3] D. Bonchev, A. T. Balaban, X. Liu, D. J. Klein, Molecular cyclicity and centricity of polycyclic graphs—I. Cyclicity based on resistance distances or reciprocal distances, Int. J. Quantum Chem. 50 (1994) 1-20.

[4] J. L. Palacios, Foster's Formulas via Probability and the Kirchhoff index, Methodology and Computing in Applied Probability. 6 (2004) 381-387.

[5] H. Zhang, X. Jiang, Y. Yang, Bicyclic graphs with extremal Kirchhoff index, MATCH Commun. Math. Comput. Chem. 61(2009) 697-712.

[6] J. L. Palacios, Resistance distance in graphs and random walks, Int. J. Quantum Chem. 81 (2001) 29-33.

[7] Q. Guo, H. Deng, D. Chen, The extremal Kirchhoff index of a class of unicyclic graphs, MATCH Commun. Math. Comput. Chem. 61 (2009) 713-722.

[8] I. Lukovits, S. Nikolic, N. Trinajstic, Resistance distance in regular graphs, Int. J. Quantum Chem. 71(1999) 217-225.

[9] H. Deng, On the minimum Kirchhoff index of graphs with a given number of cut-edges, MATCH Commun. Math. Comput. Chem. 63 (2010) 171-180.

[10] R. Li, Lower bounds for the Kirchhoff index, MATCH Commun. Math. Comput. Chem., 70 (2013) 163-174.

[11] Y. Yang, H. Zhang, Unicyclic graphs with extremal Kirchhoff index, MATCH Commun. Math. Comput. Chem. 60 (2008) 107-120.

[12] W. Zhang, H. Deng, The second maximal and minimal Kirchhoff indices of unicyclic graphs, MATCH Commun. Math. Comput. Chem. 61 (2009) 683-695.

[13] X. Cai, Z. Guo, S. Wu, L. Yang, Unicyclic graphs with the second maximum Kirchhoff index, South Asian J. Math., 4(2014) 181-184.

Subscriptions and Individual Articles:

User	**Hard copy:**
Institutional:	800 (HKD/year)
Individual:	500 (HKD/year)
Individual Article:	20 (HKD)