HK.NCCP

International Journal of Applied Mathematics and Soft Computing
Volume 3, Issue 2, August, 2017

A Class of Unicyclic Graphs With The Extremal Kirchhoff Index

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

Abstract: The Kirchhoff index Kf(G) is the sum of resistance distances between all pairs of vertices of the graph G, where 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. In this paper, we shall determine a class unicyclic graph with extremal Kirchhoff index.

Keywords: Resistance distance; Kirchhoff index; Unicyclic graph

1. Introduction

All graphs in this paper are connected simple graphs. For any $v \in V(G)$, $d(v) = d_G(v)$ is the degree of vertex v, the distance between vertices u and v, is denoted by $d(u,v) = d_G(u,v)$, is the length of a shortest path between them. Wiener index is the first recorded index, introduced by America chemist Harold Wiener in [1], defined as

$$W(G) = \sum_{\{u,v \subseteq V(G)\}} d(u,v) \qquad (1)$$

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 u and v, are denoted by r(u,v)=rG(u,v), is defined to be the effective resistance between nodes $u, v \in N$. The Kirchhoff index Kf(G) of a graph G is defined as [2, 3]

$$Kf(G) = \sum_{\{u,v \subseteq V(G)\}} r(u,v) \qquad (2)$$

If G is a tree, then r(u, v)=d(u, v) for any two vertices u and v. 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 Ck=v1v2⋯vkv1 in a unicyclic graphs, simply denoted as

G=U(Ck; T1, T2,⋯,Tk),

where Ti is the components of G. E(Ck) containing vi, 1≤i≤k, Ti is a tree rooted at vi. Let U(n; k) be the set of unicyclic graphs with n vertices and the unique cycle Ck, 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 determine a class unicyclic graphs U(k,l,i), 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.

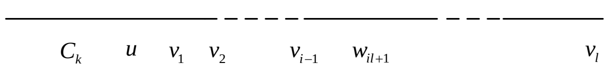

Figure .1. The Graph U(K,L,I).

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.

$$\text{Let, } Kf_v(G) = \sum_{u \in V(G)} r(u,v) \text{ then}$$
$$Kf(G) = \frac{1}{2}\sum_{v \in V(G)} Kf_v(G) \qquad (3)$$

Let Ck be the cycle on k≥3 vertices, for any two vertices $v_i, v_j \in V(C_k)$ with i<j, by Ohm's law, we have $r(v_i, v_j) = \frac{(j-i)(k+i-j)}{k}$. For any vertex $v \in V(C_k)$, it's suffice to see that $Kf_v(C_k) = \frac{k^2-1}{6}$, $Kf(C_k) = \frac{k^3-k}{12}$.

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:

$$r_G(a,b) = r_G(a,x) + r_G(x,b) \tag{4}$$

Let G1 and G2 be two connected graphs with exactly one common vertex x, and $G = G_1 \cup G_2$. Then

$$Kf(G) = Kf(G_1) + Kf(G_2) + (|G_1|-1)Kf_x(G_2) + (|G_2|-1)Kf_x(G_1) \tag{5}$$

Let T(l,i) be a tree depicted in Figure 2.

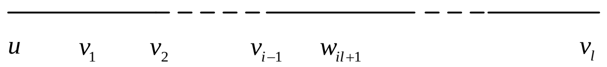

Figure .2. The Tree T(L,I)

As we'll need the Wiener index of both the star Sn and the path Pn on several occasions, we list the results in advance,

$W(S_n) = (n-1)^2$, $W(P_n) = \binom{n+1}{3} = \frac{1}{6}n(n^2-1)$ T(l,i) be the tree depicted in Figure 2, it's suffice to see that

$$Kf(T(l,i)) = \binom{l+2}{3} + i^2 - li + \frac{1}{2}(l^2+3l+2) = \frac{(l+1)(l+2)(l+3)}{6} + i^2 - li$$

3. Main Results

Firstly, by Lemma 2.1, one has,

Theorem 3.1. Let U(k,l,i) be the graph depicted in Figure 1, then

$$Kf(U(k,l,i)) = \frac{k^3-k}{12} + \frac{1}{6}(l+1)[(l+2)(l+3)+k^2-1] + i^2 - il + (k-1)[\frac{1}{2}l(l+1)+i+1]$$

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

$$Kf(U(k,l,i)) = Kf(C_k) + Kf(T(l,i)) + (k-1)Kf_u(T(l,i)) + (l+1)Kf_u(C_k)$$

$$= \frac{k^3-k}{12} + \frac{1}{6}(l+1)[(l+2)(l+3)+k^2-1] + i^2 - il + (k-1)[\frac{1}{2}l(l+1)+i+1]$$

This completes the proof.

Nextly, we'll investigate the extremal Kirchhoff index of U(k,l,i).

Theorem 3.2. Let $G \in U(k,l,i)$, for the fixed k and l, where k≥3, one has,

(i) If $k \geq l+1$, then $Kf(U(k,l,1)) \leq Kf(G) \leq Kf(U(k,l,l-1))$. (ii) If $l-1 \leq k \leq l+1$, then $Kf(U(k,l,1)) \leq Kf(G) \leq Kf(U(k,l,l-1))$. (iii) If $k \leq l-1$, then $Kf(G) \leq Kf(U(k,l,l-1))$ Proof. By Theorem 3.1, one has,

$$Kf(U(k,l,i)) = i^2 - i(l+1-k) + \frac{k^3-k}{12} + \frac{1}{6}(l+1)[(l+2)(l+3)+k^2-1] + (k-1)[\frac{1}{2}l(l+1)+1]$$

For $2 \leq i \leq l-1$, let $f(i) = i^2 - i(l+1-k) + a$,By a simple reasoning, Theorem 3.2 holds.

It's easy to see that,

Corollary 3.1. Let $G \in U(k,l,i)$, for the fixed k and l, where k≥3, one has,

$$Kf(G) \leq \frac{k^3-k}{12} + \frac{(l+1)k^2}{6} + \frac{k(6l^2+18l-1)}{12} + \frac{l^3}{6} + \frac{l^2}{2} - \frac{5l}{6} + \frac{11}{6}$$

with the equality holds if and only if $G \cong U(k,l,l-1)$.

Theorem 3.3[13]. Let $G \in U(k,l,l-1)$ and $k \geq 3$, then $Kf(G) \leq \frac{1}{6}(l^3+12l^2+31l+32)$ the equality holds if and only if $G \cong U(3,l,l-1)$.

4. Acknowledgment

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

References

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

[2] D. J. Klein and M. Randc, 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] I. Lukovits, S. Nikolic, N. Trinajstic, Resistance distance in regular graphs, Int. J. Quantum Chem. 71(1999) 217-225.

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

[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.