ARTICLE IN PRESS
Discrete Applied Mathematics ▮ (▮▮▮▮) ▮▮▮–▮▮▮
Contents lists available at ScienceDirect
Discrete Applied Mathematics
journal homepage: www.elsevier.com/locate/dam

On the Szeged index of unicyclic graphs with given diameter ☆

Yan Liu [a], Aimei Yu [a,*], Mei Lu [b], Rong-Xia Hao [a]

[a] Department of Mathematics, Beijing Jiaotong University, Beijing 100044, China
[b] Department of Mathematical Sciences, Tsinghua University, Beijing 100084, China

ARTICLE INFO

Article history:
Received 30 July 2016
Received in revised form 31 July 2017
Accepted 27 August 2017
Available online xxxx

Keywords:
Szeged index
Wiener index
Unicyclic graph
Diameter

ABSTRACT

The Szeged index of a connected graph G is defined as

$$S_z(G) = \sum_{e=uv\in E(G)} n_u(e|G)n_v(e|G),$$

where $E(G)$ is the edge set of G, and for any $e = uv \in E(G)$, $n_u(e|G)$ is the number of vertices of G lying closer to vertex u than to v, and $n_v(e|G)$ is the number of vertices of G lying closer to vertex v than to u. In this paper, we characterize the graph with minimum Szeged index among all the unicyclic graphs with given order and diameter.

1. Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$, and let $|G| = |V(G)|$. The distance between two vertices u and v of G, denoted by $d(u, v|G)$, is the length of a shortest path connecting them. The diameter of a graph G is the maximum distance between any two vertices of G. We use C_n, S_n and P_n to denote a cycle, a star and a path, respectively, each on n vertices.

For any $e = uv \in E(G)$, $n_u(e|G)$ is the number of vertices of G lying closer to vertex u than to v, and $n_v(e|G)$ is the number of vertices of G lying closer to vertex v than to u. The Szeged index of the graph G is defined as

$$S_z(G) = \sum_{e=uv\in E(G)} n_u(e|G)n_v(e|G).$$

The Szeged index coincides with the Wiener index on trees [3]. The Szeged index has received much attention for both its mathematical properties and chemical applications, see [4,7]. In particular, Khadikar et al. [6] described various applications of Szeged index for modeling physicochemical properties as well as physiological activities of organic compounds acting as drugs or possessing pharmacological activity.

A (n, m)-graph is a connected graph with n vertices and m edges. Obviously, a $(n, n-1)$-graph is a tree. A connected graph is said to be unicyclic (resp., bicyclic, tricyclic) if it is a (n, n)-graph (resp., $(n, n+1)$-graph, $(n, n+2)$-graph). Dobrynin [2] showed that $K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$ is the unique graph with maximum Szeged index in the set of all connected graphs with n vertices. Gutman [3] determined the n-vertex unicyclic graphs with maximum and minimum Szeged indices, respectively. Simić et al. [11] determined the n-vertex bicyclic and tricyclic graphs with maximum and minimum Szeged indices, respectively.

☆ This work is partially supported by National Natural Science Foundation of China (Nos. 11371193, 11371052, 11731002), the Beijing Higher Education Young Elite Teacher Project (No. YETP0573), Fundamental Research Funds for the Central Universities of China (No. 2015JBM107).

* Corresponding author.
E-mail addresses: 13121534@bjtu.edu.cn (Y. Liu), yuaimeimath@163.com (A. Yu), mlu@math.tsinghua.edu.cn (M. Lu), rxhao@bjtu.edu.cn (R.-X. Hao).

http://dx.doi.org/10.1016/j.dam.2017.08.009
0166-218X/

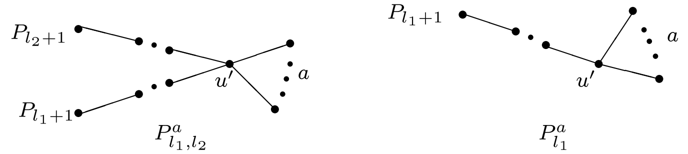

Fig. 1. The graphs $P^a_{l_1,l_2}$ and $P^a_{l_1}$.

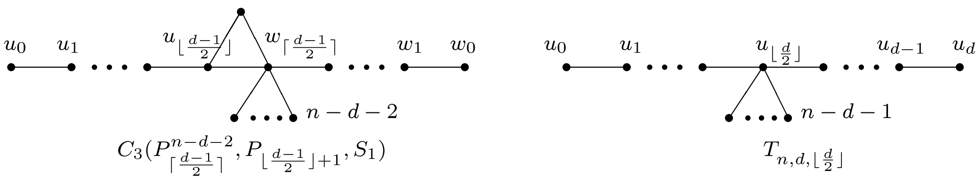

Fig. 2. The graphs $C_3(P^{n-d-2}_{\lceil \frac{d-1}{2} \rceil}, P_{\lfloor \frac{d-1}{2} \rfloor+1}, S_1)$ and $T_{n,d,\lfloor \frac{d}{2} \rfloor}$.

Zhou et al. [14] characterized the n-vertex unicyclic graphs of cycle length g ($3 \le g \le n$) with maximum and minimum Szeged indices, respectively. For other results on the Szeged index, we refer to [1,5,8,13].

Liu and Pan [9] determined the graph with minimum Wiener index among the n-vertex trees with given diameter. Ren and Shi [10] and Tan [12] independently determined the graph with minimum Wiener index among the n-vertex unicyclic graphs with given diameter. In this paper, we characterize the graph with minimum Szeged index among the n-vertex unicyclic graphs with given diameter.

Let G be a unicyclic graph of order n with diameter d. Then $1 \le d \le n-2$. If $d = 1$, then $G \cong C_3$. Hence throughout the paper, we assume that $2 \le d \le n-2$. Our main result is the theorem below. In order to state our result, we need more notations.

Let l_1, l_2 and a be three nonnegative integers. Let P_{l_1+1} be a path on l_1+1 vertices with terminal vertex u and P_{l_2+1} be a path on l_2+1 vertices with terminal vertex v. Let S_{a+1} be a star on $a+1$ vertices with center vertex w. We denote by $P^a_{l_1,l_2}$ the tree obtained from P_{l_1+1}, P_{l_2+1} and S_{a+1} by identifying u, v and w to u', and call u' the root vertex of $P^a_{l_1,l_2}$ (see Fig. 1). For convenience, we write $P^a_{l_1}$ for $P^a_{l_1,0}$ (see Fig. 1). Note that $P^a_{0,0} \cong S_{a+1}$.

Let $C_3(P^{n-d-2}_{\lceil \frac{d-1}{2} \rceil}, P_{\lfloor \frac{d-1}{2} \rfloor+1}, S_1)$ be the graph obtained from cycle $C_3 = v_1v_2v_3v_1$ by identifying the root vertex of $P^{n-d-2}_{\lceil \frac{d-1}{2} \rceil}$ with v_1, and identifying one end vertex of $P_{\lfloor \frac{d-1}{2} \rfloor+1}$ with v_2 (see Fig. 2).

Theorem 1.1. *Among the unicyclic graphs of order n with diameter $2 \le d \le n-2$, $C_3(P^{n-d-2}_{\lceil \frac{d-1}{2} \rceil}, P_{\lfloor \frac{d-1}{2} \rfloor+1}, S_1)$ is the unique graph with minimum Szeged index.*

The rest of this paper is organized as follows. In Section 2, we introduce some useful lemmas. In Section 3, we present some transformations of graphs which keep the diameter and order of the graphs, but decrease the Szeged index of the graphs. In Section 4, Theorem 1.1 is proved.

2. Useful lemmas

Recall that the Wiener index of a graph G is defined as

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u, v|G), \tag{2.1}$$

and that if G is a tree, then

$$W(G) = Sz(G). \tag{2.2}$$

By (2.1) and (2.2), the lemma below holds immediately.

Lemma 2.1. *Let $|P^a_{l_1,l_2}| = n$. Then $W(P^a_{l_1,l_2}) = a(n-1) + \sum_{j=0}^{l_1} j(n-j) + \sum_{j=0}^{l_2} j(n-j)$.*

In the following, we present some useful results on the Wiener index.

Lemma 2.2 ([14]). *Let T be a n-vertex tree different from S_n and P_n. Then*

$$(n-1)^2 = W(S_n) < W(T) < W(P_n) = \frac{n^3-n}{6}.$$

Please cite this article in press as: Y. Liu, et al., On the Szeged index of unicyclic graphs with given diameter, Discrete Applied Mathematics (2017), http://dx.doi.org/10.1016/j.dam.2017.08.009.