Applied Mathematics and Computation 309 (2017) 85–92

Contents lists available at ScienceDirect

Applied Mathematics and Computation

journal homepage: www.elsevier.com/locate/amc

On extremal cacti with respect to the Szeged index

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ARTICLE INFO

MSC:
05C69
05C05

Keywords:
Szeged index
Cactus
Pendent vertex

ABSTRACT

The Szeged index of a graph G is defined as $Sz(G) = \sum_{e=uv\in E} n_u(e)n_v(e)$, where $n_u(e)$ and $n_v(e)$ are, respectively, the number of vertices of G lying closer to vertex u than to vertex v and the number of vertices of G lying closer to vertex v than to vertex u. A cactus is a graph in which any two cycles have at most one common vertex. Let $\mathcal{C}(n, k)$ denote the class of all cacti with order n and k cycles, and $\mathcal{C}_n^t$ denote the class of all cacti with order n and t pendant vertices. In this paper, a lower bound of the Szeged index for cacti of order n with k cycles is determined, and all the graphs that achieve the lower bound are identified. As well, the unique graph in $\mathcal{C}_n^t$ with minimum Szeged index is characterized.

1. Introduction

In this paper we are concerned with simple finite graphs. Undefined notation and terminology can be found in [2]. Let G be a connected graph with vertex set $V(G)$ and edge set $E(G)$. For $v \in V(G)$, let $N_G(v)$ (or $N(v)$ for short) denote the set of all the adjacent vertices of v in G and $d_G(v) = |N_G(v)|$, the degree of v in G. Call u a *pendant vertex* in G, if $d_G(u) = 1$ and call uv a *pendant edge* in G, if $d_G(u) = 1$ or $d_G(v) = 1$. Denote by P_n, S_n, C_n and K_n the path, star, cycle and complete graph on n vertices, respectively. One of the oldest and well-studied topological indices is the *Wiener index*, defined as the sum of distances over all unordered vertex pairs in a graph G [34] and denoted by

$$W(G) = \sum_{\{u,v\}\subset V} d_G(u, v)$$

where $d_G(u, v)$ denotes the distance between u and v in G.

This topological index has been extensively studied in the mathematical literature, many papers have contributed to the Wiener index and these studies mainly focused on determining the lower and upper bounds on Wiener index; see, e.g., [7,9,11,14,15,22,24,25,31,33,37]. Also in [34], another topological index was also introduced by Wiener, called the *Wiener polarity index* $W_p(G)$, which is defined as the number of unordered pairs of vertices that are at distance 3 in G. For some properties and applications of the Wiener polarity index one may be referred to those in [3,20,26].

Let $e = uv$ be an edge of G, and define three sets as follows:

$$N_u(e) = \{w \in V : d(u, w) < d(v, w)\}, \quad N_v(e) = \{w \in V : d(v, w) < d(u, w)\},$$
$$N_0(e) = \{w \in V : d(u, w) = d(v, w)\}.$$

Thus, $[N_u(e), N_v(e), N_0(e)]$ is a partition of the vertices of G with respect to e. The number of vertices of $N_u(e), N_v(e)$ and $N_0(e)$ are denoted by $n_u(e), n_v(e)$ and $n_0(e)$, respectively. A long time known property of the Wiener index is the formula

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http://dx.doi.org/10.1016/j.amc.2017.03.036

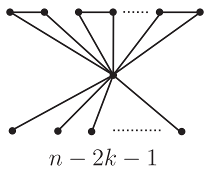

Fig. 1. The graph $C_0(n, k)$.

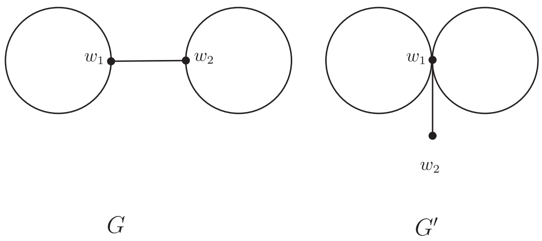

Fig. 2. G and G' in Lemma 2.1.

[15,34]:

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

which is applicable for trees. Using the above formula, Gutman [13] introduced a graph invariant named the *Szeged index* as an extension of the Wiener index and defined it by

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

Randić [31] observed that the Szeged index does not take into account the contributions of the vertices at equal distances from the endpoints of an edge, and so he conceived a modified version of the Szeged index which is named the *revised Szeged index*. The revised Szeged index of a connected graph G is defined as

$$Sz^*(G) = \sum_{e=uv \in E} \left(n_u(e) + \frac{n_0(e)}{2} \right) \left(n_v(e) + \frac{n_0(e)}{2} \right).$$

There are several results on the difference (resp. quotient) between the Szeged index (resp. revised Szeged index) and Wiener index; see, e.g., [4,5,9,10,17–19,27,28,36]. For some properties and applications of the Szeged index and the revised Szeged index one may be referred to those in [1,6,12,16,21,23,29,30,32,35].

In [8], Dobrynin proved that $K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$ is the unique graph with maximal Szeged index in the set of all connected graphs with n vertices. In [13], Gutman characterized the extremal trees and unicyclic graphs that have minimum (resp. maximum) Szeged index, respectively. In [32], Simić, Gutman and Baltić identified those graphs whose Szeged index is extremal (minimal and maximal) among bicyclic and tricyclic graphs.

A cactus is a graph that any block is either a cut edge or a cycle. It is also a graph in which any two cycles have at most one common vertex. A cycle in a cactus is called *end-block* if all but one vertex of this cycle have degree 2. A cut edge is said to be *nontrivial* if it is not a pendent edge. If all the cycles in a cactus have exactly one common vertex, then they form a bundle. Let $\mathcal{C}(n, k)$ be the class of all cacti of order n with k cycles and $\mathcal{C}_n^t$ be the class of all cacti of order n with t pendant vertices. In this paper, we give a lower bound of the Szeged index for cacti of order n with k cycles, and also characterize those graphs that achieve the lower bound. We also determine the unique graph in $\mathcal{C}_n^t$ with minimum Szeged index. Let $C_0(n, k) \in \mathcal{C}(n, k)$ be a bundle of k triangles with $n - 2k - 1$ pendant vertices attached at the common vertex; see Fig. 1.

2. Preliminaries

In this section, we give some preliminary results which will be used in the subsequent sections.

Lemma 2.1. *Let G be a graph with a cut edge $e' = w_1w_2$, and G' be the graph obtained from G by contracting the edge e' and adding a pendant edge attaching at the contracting vertex; see Fig. 2. If $d_G(w_i) \geq 2$ for $i = 1, 2$, we have that $Sz(G') < Sz(G)$.*

Proof. Let G_1 and G_2 be the component of $G - w_1w_2$ that contains w_1 and w_2, respectively. One can see that for any $e = xy \in E(G_1)$, if $w_1 \in N_x(e), N_y(e)$ or $N_0(e)$ respectively, then $V(G_2) \subseteq N_x(e)$, $N_y(e)$ or $N_0(e)$ respectively. Similarly, for any $e =$