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On the edge-Szeged index of unicyclic graphs with given diameter☆

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A B S T R A C T

Given a connected graph G, the edge-Szeged index $Sz_e(G)$ is defined as $Sz_e(G) = \sum_{e=uv\in E} m_u(e)m_v(e)$, where $m_u(e)$ and $m_v(e)$ are, respectively, the number of edges of G lying closer to vertex u than to vertex v and the number of edges of G lying closer to vertex v than to vertex u. In this paper, some extremal problems on the edge-Szeged index of unicyclic graphs are considered. All the n-vertex unicyclic graphs with a given diameter having the minimum edge-Szeged index are identified. Using a unified approach we identify the n-vertex unicyclic graphs with the minimum, second minimum, third minimum and fourth minimum edge-Szeged indices.

1. Introduction

In this paper, we consider connected simple and finite graphs, and refer to Bondy and Murty [2] for notations and terminologies used but not defined here.

Let $G = (V_G, E_G)$ be a graph with vertex set $V_G = \{v_1, v_2, \dots, v_n\}$ and edge set E_G. We call $n := |V_G|$ the *order* of G and $|E_G|$ the *size* of G. Denote by P_n, C_n and K_n a path, a cycle and a complete graph of order n, respectively. The set of neighbors of a vertex v in G is denoted by $N_G(v)$ or simply $N(v)$. The *degree* $d_G(v)$ of a vertex v is equal to the number of neighbors of v. An edge uv is called a *pendant edge* if one of its endpoints is of degree 1. By $G - uv$ we denote the graph obtained from G by deleting an edge $uv \in E_G$. (This notation is naturally extended if more than one edge are deleted.) Similarly, $G + uv$ is obtained from G by adding an edge $uv \notin E_G$. The *distance*, $d_G(u, v)$ (or $d(u, v)$ for short), between vertices u and v of G is the length of a shortest u, v-path in G.

Recently, in organic chemistry, topological indices have been found to be useful in chemical documentation, structure–property relationships, structure–activity relationships and pharmaceutical drug design. These indices include Wiener index [43], Randić index [28,29], Hosoya index [17,18], graph energy [36], matching energy [15,16,27], the HOMO-LUMO index [32] and Zagreb index [8] and so on.

Among all the topological indices, the most well-known is the Wiener index and it was studied extensively. The *Wiener index* (or *transmission*) $W(G)$ of G is the sum of distances between all pairs of vertices of G, that is,

$$W(G) = \sum_{\{u,v\}\subseteq V_G} d_G(u, v)\,. \tag{1.1}$$

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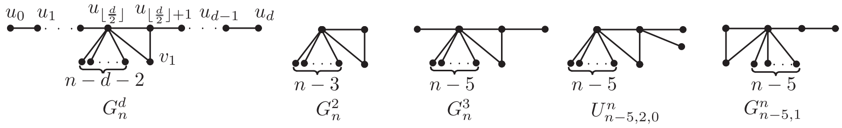

Fig. 1. Graphs $G_n^d, G_n^2, G_n^3, U_{n-5,2,0}^n$ and $G_{n-5,1}^n$.

This distance-based graph invariant was in chemistry introduced back in 1947 [43] and in mathematics about 30 years later [12]. Nowadays, the Wiener index is an extensive studied graph invariant; see the surveys [7,10]. A collection of recent papers dedicated to the investigations of the Wiener index [23,25,31].

Given an edge $e = uv$ of a graph G, the sets $N_0(e)$, $N_u(e)$ and $N_v(e)$ are defined to be the set of vertices equidistant from u and v, the set of vertices whose distance to vertex u is smaller than the distance to vertex v and the set of vertices closer to v than u, respectively. Put $n_u(e) = |N_u(e)|$, $n_v(e) = |N_v(e)|$ and $n_0(e) = |N_0(e)|$. Obviously, $N_u(e) \cup N_v(e) \cup N_0(e)$ is a partition of V_G with respect to e, where $N_0(e) = \emptyset$ if G is bipartite. Thus, one has $n_u(e) + n_v(e) + n_0(e) = |V_G|$.

Gutman [14] introduced the *Szeged index* $Sz(G)$ of a graph G as

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

Furthermore, in order to involve also those vertices that are at equal distance from the endpoints of an edge, Randić [37] proposed the *revised Szeged index* $Sz^*(G)$ of a graph G as follows:

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

For more detailed information on Szeged index and revised Szeged index, one may be referred to the recent work [40,41] and the references therein.

Since $Sz(T) = W(T)$ holds for any tree T, a lot of research has been done on the relation between the (revised) Szeged index and the Wiener index on general graphs. On the one hand, the difference between $Sz(G)$ and $W(G)$ was investigated systematically in [1,4,5,9,20–22,34,35,47]; On the other hand, the quotient between (revised) Szeged index and the Wiener index was also studied in [26,46].

Given an edge $e = uv \in E_G$, the distance between the edge e and the vertex w, denoted by $d(e, w)$, is defined as

$$d(w, e) = \min\{d(u, w), d(v, w)\}.$$

Then, let

$$M_u(e|G) = \{x \in E_G : \ d(u, x) < d(v, x)\}, \quad M_v(e|G) = \{x \in E_G : \ d(v, x) < d(u, x)\},$$
$$M_0(e|G) = \{x \in E_G : \ d(u, x) = d(v, x)\}.$$

For simplicity, let $M_u(e) = M_u(e|G)$, $M_v(e) = M_v(e|G)$ and $M_0(e) = M_0(e|G)$. Put $m_u(e) = |M_u(e)|$, $m_v(e) = |M_v(e)|$ and $m_0(e) = |M_0(e)|$. Then, the *edge-Szeged index* [15] of G is defined as

$$Sz_e(G) = \sum_{e=uv \in E_G} m_u(e) m_v(e).$$

In the case of trees, in view of Gutman and Ashrafi [15], we know that $Sz_e(T) = W(T) - (n-1)^2$. Note that the Wiener index of trees with some given parameters have been studied extensively. Hence, it is interesting for us to study the edge-Szeged index of connected graphs with cycles.

The edge-Szeged index is also a distance-based graph invariant, it attracts more and more researchers' attention. On the one hand, one focuses on finding method to compute the edge-Szeged index of some type of graphs; see [13,33,42,45]; On the other hand, the researchers are also interested in determining the graph with the maximum or minimum edge-Szeged index among some type of graphs; see [3,6,30,38,39,44]. Furthermore, some relation between the edge-Szeged index and other graph invariants were studied; see [11,19,24,32]. Cai and Zhou [3] identified the n-vertex unicyclic graphs with the largest, the second largest, the smallest and the second smallest edge-Szeged indices.

In this paper, we continue the above direction of research by considering the extremal problems on the edge-Szeged index of unicyclic graphs. In the next section, we recall some known results and prove new results that are needed for the proofs of the main results. In Section 3, we determine the sharp lower bounds on the edge-Szeged index of n-vertex unicyclic graphs with diameter d. Some further discussions are given in the last section, which identify the unicyclic graphs with the minimum, second minimum, third minimum and the fourth minimum edge-Szeged indices.

2. Main results

A *unicyclic graph* is a (simple) connected graph with a unique cycle. The greatest distance between any two vertices in G is the *diameter* of G. For convenience, let $\mathcal{G}_n$ be the set of all n-vertex unicyclic graphs, $\mathcal{G}_n^d$ be the set of all n-vertex unicyclic graphs with diameter d.