On the minimum edge–Szeged index of fully–loaded unicyclic graphs

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Abstract

The edge–Szeged index of a connected graph $G$ is defined as the sum of products $m_u(e|G)m_v(e|G)$ over all edges $e = uv$ of $G$, where $m_u(e|G)$ (respectively, $m_v(e|G)$) is the number of those edges whose distance from the vertex $u$ (respectively, $v$) is smaller than the distance from the vertex $v$ (respectively, $u$). A fully–loaded unicyclic graph is a unicyclic graph having no vertex of degree less than 3 on its unique cycle. In this paper, we determine the first three minimum values of the edge–Szeged index of fully–loaded unicyclic graphs having a fixed order and characterize all the graphs attaining these values.

Keywords: edge–Szeged index; fully–loaded unicyclic graph; extremal value.

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1. Introduction

All graphs considered in this paper are finite, undirected and simple. We refer the reader to [1] for the notation and terminology that are used in this paper but not defined here.

Let $G = (V,E)$ be a connected graph with the vertex set $V(G)$ and edge set $E(G)$. For a vertex $u \in V(G)$, the degree of $u$, denoted by $d_G(u)$ (or simply $d(u)$), is the number of vertices adjacent to $u$. A vertex $u \in V(G)$ of degree 1 is called a pendant vertex. An edge $uv$ of $G$ is called a pendant edge if either $d(u) = 1$ or $d(v) = 1$. If $uv \in E(G)$ then by $G = uv$ we denote the graph obtained from $G$ by deleting the edge $uv$. Similarly, if $uv \notin E(G)$ then by $G + uv$ we denote the graph obtained from $G$ by adding an edge between $u$ and $v$. An edge $uv$ is called a cut edge of a connected graph $G$ if $G = uv$ is disconnect. The distance $d(u,v)(G)$ (or $d(u,v)$ for short) between the vertices $u$ and $v$ of $G$ is the length of a shortest $u-v$ path in $G$. Let $P_n$, $C_n$ and $S_n$ be the path, cycle and star graphs of order $n$, respectively.

Topological indices are the graph invariants used in theoretical chemistry to encode chemical compounds for predicting physicochemical properties or pharmacological and biological activities. Among them, distance-based indices have been of great interest and extensively studied.

Given an edge $e = uv \in E(G)$, the distance between the vertex $x$ and the edge $e$, denoted by $d(x,e)$, is defined as $d(x,e) = \min\{d(x,u),d(x,v)\}$. Denote $M_u(x|G) = \{e \in E(G) : d(u,e) < d(v,e)\}$ and $M_v(x|G) = \{e \in E(G) : d(v,e) < d(u,e)\}$. Let $m_u(e|G) = |M_u(e|G)|$ and $m_v(e|G) = |M_v(e|G)|$. Then, the edge–Szeged index [7] of $G$ is defined as

$$Sz_e(G) = \sum_{e \in E(G)} m_u(e|G)m_v(e|G).$$

The extremal values of the edge–Szeged index are of particular interest to us. In [2], Cai and Zhou determined the $n$-vertex unicyclic graphs with the largest, the second largest, the smallest and the second smallest edge–Szeged indices. Wang et al. [14] characterized the $n$-vertex unicyclic graphs with a given diameter having the minimum edge-Szeged index. They used a unified approach to identify the $n$-vertex unicyclic graphs with the minimum, second minimum, third minimum and fourth minimum edge-Szeged indices. Liu et al. [9,11] obtained the minimum value of Szeged index and revised edge–Szeged index among trees and unicyclic graphs with perfect matchings. For other relevant results, see [3,4,6,8,10,12,13] and the references cited therein.

Motivated by the above–mentioned results, we consider the extremal problem about the edge–Szeged index of fully–loaded unicyclic graphs, where a fully–loaded unicyclic graph is a unicyclic graph having no vertex of degree less than 3 on its unique cycle. In this paper, we determine the first three minimum values of the edge–Szeged index of fully–loaded unicyclic graphs having a fixed order and characterize all the graphs attaining these values.

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2. Preliminaries

Let \( G = (V, E) \) be a unicyclic graph of order \( n \) with its unique circuit \( C_g = v_1v_2 \cdots v_gv_1 \). Let \( E(C_g) \) be the set of edges of the circuit \( C_g \) and \( G \setminus E(C_g) \) be the graph obtained from \( G \) by removing all the edges of the circuit \( C_g \). For \( i = 1, 2, \ldots, g \), let \( T_i \) be the component of \( G \setminus E(C_g) \) that contains \( v_i \). Such a unicyclic graph is denoted by \( C_g(T_1, T_2, \ldots, T_g) \). Let \( n(T_i) = |T_i| = t_i \) for \( i = 1, 2, \ldots, g \), then \( \sum_{i=1}^g t_i = n \). Take \( D(u) = \sum_{v \in V(G)} d(u,v)G \).

Li [8] give an effective method for computing the edge–Szeged index of a unicyclic graph \( G = C_g(T_1, T_2, \ldots, T_g) \).

**Lemma 2.1.** [8] Let \( G = C_g(T_1, T_2, \ldots, T_g) \), \( D(v_i|T_i) = \sum_{u \in T_i} d(v_i, u|T_i) \) and \( \delta(g) = 0 \) for even \( g \), \( \delta(g) = 1 \) for odd \( g \).

\[
S_{ze}(G) = \sum_{i=1}^g W(T_i) + \sum_{i=1}^g (|G| - |T_i| + 1)D(v_i|T_i) + \sum_{i=1}^g \sum_{j=1}^g |T_i||T_j|d(v_i, v_j|C_g) - \delta(g) \sum_{i<j} |T_i||T_j| - |G|^2 + |G|^\delta(g)g.
\]

For convenience, we denote \( |T_i| = t_i (1 \leq i \leq g) \), \( d(v_i, v_j|C_g) = d_{ij} \) \( (1 \leq i, j \leq g) \) and take \( N_i = \sum_{j \neq i} t_jd_{ij} \) \( (1 \leq i, j \leq g) \).

3. Main result

Firstly, we give some elementary but useful results for our subsequent proofs.

**Lemma 3.1.** [5] Let \( T \) be an \( n \)-vertex tree, then \( (n - 1)^2 = W(S_n) \leq W(T) \leq W(P_n) = \frac{1}{3}n(n^2 - 1) \).

**Lemma 3.2.** [16] Let \( T \) be an \( n \)-vertex tree with \( u \in V(T) \), where \( n \geq 3 \). Let \( x \) and \( y \) be the center of the star \( S_n \) and a terminal vertex of the path \( P_n \). Then \( n - 1 = D(x|S_n) \leq D(u|T) \leq D(y|P_n) = \frac{1}{2}n(n - 1) \).

Let \( S'_n (n \geq 5) \) be the tree formed by attaching a pendant vertex to a pendant vertex of the star \( S_{n-1} \).

**Lemma 3.3.** [15] Among all \( n \)-vertex trees, \( S'_n \) \( (n \geq 5) \) are the unique tree with the second smallest Wiener index. And \( W(S'_n) = n^2 - n - 2 \).

**Lemma 3.4.** [15] Let \( T \) be an \( n \)-vertex tree with \( u \in V(T) \), where \( n \geq 5 \). \( T \not\cong S_n \). Let \( x \) be the vertex of maximal degree of \( S'_n \). Then \( D(u|T) \geq D(x|S'_n) = n \).

Let \( U_n (n \geq 6) \) be the set of \( n \)-vertex fully–loaded unicyclic graphs. Denote by \( U_{n,g} (3 \leq g \leq \lfloor \frac{n}{2} \rfloor) \) the set of all fully–loaded unicyclic graphs with \( n \) vertices and cycle \( C_g \).

Denote by \( S_n(t_1, t_2, \ldots, t_g) \) the set of \( n \)-vertex unicyclic graphs \( C_g(T_1, T_2, \ldots, T_g) \), where \( T_i \) is star on \( t_i \) vertices with center \( v_i (1 \leq i \leq g) \) and \( \sum_{i=1}^g t_i = n \). Also, let \( S_{n,g} = S_n(t_1, t_2, \ldots, t_g) \) with \( t_1 = n - 2g + 2 \) and \( t_2 = t_3 = \cdots = t_g = 2 \).

One can easily calculate the edge–Szeged index of \( S_{n,g} \) as given below

\[
S_{ze}(S_{n,g}) = \begin{cases} 
(g^2 - 2g - 1)n - n^3 + 2g^2 - g, & g \text{ is odd} \\
(g^2 - g)n - n^3 + g, & g \text{ is even}
\end{cases}
\]

By Lemmas 2.1, 3.1 and 3.2, we have

**Lemma 3.5.** Let \( G = C_g(T_1, T_2, \ldots, T_g) \) \( \in U_{n,g} \) with \( g \geq 3 \), \( t_i = |T_i| \geq 2 \). Then \( S_{ze}(G) \geq S_{ze}(S_n(t_1, t_2, \ldots, t_g)) \), with equality if and only if \( G \cong S_n(t_1, t_2, \ldots, t_g) \).

**Lemma 3.6.** Let \( G = S_n(t_1, t_2, \ldots, t_g) \). Suppose that \( t_k, t_l \geq 2 \) for \( 1 \leq k, l \leq g \) and \( k \neq l \). If \( N_k + \frac{1}{2}\delta(g)t_k \leq N_l + \frac{1}{2}\delta(g)t_l \), for \( G' = S_n(t'_1, t'_2, \ldots, t'_g) \), where \( t'_i = t_i (1 \leq i \leq g) \) with \( i \neq k, l \), and \( t'_k = t_k + 1, t'_l = t_l - 1 \), then \( S_{ze}(G') < S_{ze}(G) \).

**Proof.** Note that \( t'_k = t_k + 1, t'_l = t_l - 1 \), and by Lemma 2.1, we have that

\[
S_{ze}(G) - S_{ze}(G') = 2[t_k|t_l - (t_k + 1)(t_l - 1)]d_{kl} + 2 \sum_{i \neq k,l} [t_k|t_l - (t_k + 1)t_i]d_{ki} + 2 \sum_{i \neq k,l} [t_i|t_l - (t_k + 1)t_i]d_{li} - \delta(g)d_{kl} \sum_{i \neq k,l} t_i(t_k + t_l) - \sum_{i \neq k,l} t_i(t_k + 1 + t_l - 1) + t_k t_l - (t_k + 1)(t_l - 1)]
\]

\[
= 2[N_k + \frac{1}{2}\delta(g)t_k - (N_l + \frac{1}{2}\delta(g)t_l)] + 2d_{kl} - \delta(g) > 0.
\]

\[\square\]
By Lemmas 3.5 and 3.6, we have the next result.

**Lemma 3.7.** Let \( G \in \mathcal{U}_{n,g} \) \((3 \leq g \leq \left\lfloor \frac{n}{2} \right\rfloor)\), then \( Sz_e(G) \geq Sz_e(S_{n,g}) \) with equality if and only if \( G \cong S_{n,g} \).

Denote by \( F_n \) the set of graphs \( C_3(T_1, T_2, T_3) \) in \( \mathcal{U}_n \) with \( t_1 = t_2 = 2, \Phi_n \) the set of graphs \( C_3(T_1, T_2, T_3) \) in \( \mathcal{U}_n \) with \( t_3 \geq t_2 \geq \max\{3, t_1\} \), \( \Omega_n \) the set of graphs in \( \mathcal{U}_n \) with with cycle length \( g \geq 4 \). Then \( \mathcal{U}_n = F_n \cup \Phi_n \cup \Omega_n \).

![Figure 1: The graphs \( B'_n, G'_n \) and \( G''_n \).](image)

**Lemma 3.8.** Consider the graphs \( B'_n, G'_n \) and \( G''_n \) shown in Figure 1.

(i) Among the graphs in \( F_n \) \((n \geq 6)\), \( S_n(2, 2, n - 4) \) and \( B'_n \) are the unique graphs with the smallest and second smallest edge–Szeged index, respectively.

(ii) Among the graphs in \( \Phi_n \) \((n \geq 8)\), \( S_n(2, 3, n - 5) \) is the unique graph with the smallest edge–Szeged index. The graph \( G'_n \) for \( n = 8, S_9(3, 3, 3) \) for \( n = 9 \), and \( S_n(2, 4, n - 6) \) for \( n \geq 10 \) are the unique graphs with the second smallest edge–Szeged index.

(iii) Among the graphs in \( \Omega_n \) \((n \geq 8)\), \( S_{n,4} \) is the unique graph with the smallest edge–Szeged index.

**Proof.** (i) Let \( G \in F_n \), by Lemma 2.1, we have \( Sz_e(S_n) = -n^2 + 9n - 12 + W(T_3) + 5D(v_3 | T_3) \). Thus, by Lemmas 3.1, 3.2 and 3.7, we conclude that that \( S_n(2, 2, n - 4) \) and \( B'_n \) are the unique graphs with the smallest and second smallest edge–Szeged index, respectively.

(ii) Let \( G = C_3(T_1, T_2, T_3) \in \Phi_n \). Without loss of generality, we suppose that \( t_3 \geq t_2 \geq \max\{3, t_1\} \). If \( n = 8 \), the graphs in \( \Phi_8 \) are only \( S_8(2, 3, 3), G'_8 \) and \( C_3(P_2, P_3, P_3) \). But, we have \( Sz_e(S_8(2, 3, 3)) = 21 < Sz_e(G'_8) = 27 < Sz_e(C_3(P_2, P_3, P_3)) = 33 \).

If \( n = 9 \), by Lemmas 2.1, 3.1, 3.2 and 3.6, \( S_9(2, 3, 4) \) is the graph with the smallest edge–Szeged index. The graph in \( \Phi_n \) with the second smallest edge–Szeged index is one of the graphs \( S_9(3, 3, 3), G'_9 \) and \( G'_9 \). But, \( Sz_e(S_9(3, 3, 3)) = 27 < Sz_e(G'_9) = 33 < Sz_e(G''_9) \). Thus, \( S_9(3, 3, 3) \) is the graph with the second smallest edge–Szeged index.

If \( n \geq 10 \), we consider the two cases.

**Case 1.** \( G \cong S_n(t_1, t_2, t_3) \).

Suppose that \( G \not\cong S_n(2, 3, n - 5), S_n(2, 4, n - 6) \). Bearing in mind that \( N_i = \sum_{j \neq i} t_j d_{ij} \), we have \( N_1 = t_2 + t_3, N_2 = t_1 + t_3, N_3 = t_1 + t_2 \). Thus, we have \( N_3 + \frac{1}{2} t_3 \leq N_2 + \frac{1}{2} t_2 \leq N_1 + \frac{1}{2} t_1 \). By Lemmas 2.1 and 3.6, we have that.

**Subcase 1.1.** \( t_1 = 2 \).

Note that \( Sz_e(S_n(2, 3, n - 5)) = 5n - 19 < Sz_e(S_n(2, 4, n - 6)) = 6n - 28 < Sz_e(G'_n) = Sz_e(G''_n) = 6n - 21 \), and thus we have \( Sz_e(S_n(2, 2, t_3)) \geq Sz_e(S_n(2, 4, n - 6)) > Sz_e(S_n(2, 3, n - 5)) \).

**Subcase 1.2.** \( t_1 \geq 3 \).

In this case, we have \( Sz_e(S_n(t_1, t_2, t_3)) \geq Sz_e(S_n(3, 3, n - 6)) = 6n - 21 > 6n - 28 \).

**Case 2.** \( G \not\cong S_n(t_1, t_2, t_3) \).

By Lemmas 2.1, 3.1, 3.2, we have that.

**Subcase 2.1** \( t_1 = 2 \).

\( Sz_e(G) \geq Sz_e(G'_n) = Sz_e(G''_n) = 6n - 21 > 6n - 28 \).

**Subcase 2.2** \( t_1 \geq 3 \).

\( Sz_e(G) > Sz_e(S_n(t_1, t_2, t_3)) \geq Sz_e(S_n(3, 3, n - 6)) = 6n - 27 > 6n - 28 \).

Thus, for \( n \geq 10 \), \( S_n(2, 3, n - 5) \) and \( S_n(2, 4, n - 6) \) are the graphs with the smallest and second smallest edge–Szeged index, respectively.
(iii). Let $G \in \Omega_n$. If $g$ is odd, then $Sz_e(S_{n,g+2}) - Sz_e(S_{n,g}) = 4gn - 6g^2 - 4g - 2 \geq 4g([g+2]) - 6g^2 - 4g - 2 = 2g^2 + 20g - 2 > 0$. If $g$ is even, then $Sz_e(S_{n,g+2}) - Sz_e(S_{n,g}) = (4g+2)n - 6g^2 - 12g - 6 \geq (4g+2)[2(g+2)] - 6g^2 - 12g - 6 = 2g^2 + 8g + 2 > 0$. It means that $Sz_e(S_{n,g})$ is increasing for odd $g \in \{3, 5, \ldots, \lceil \frac{n}{2} \rceil \}$ and $Sz_e(S_{n,g})$ is increasing for even $g \in \{4, 6, \ldots, \lceil \frac{n}{2} \rceil \}$. Thus, we only need to compare the edge–Szeged index of $S_{n,4}$ and $S_{n,5}$. However, $Sz_e(S_{n,4}) = 12n - 60 < Sz_e(S_{n,5}) = 16n - 80 (n \geq 8)$. Thus, $S_{n,4}$ is the unique graph with the smallest edge–Szeged index in $\Omega_n$.

\[\square\]

**Theorem 3.1.** Among the graphs in $\mathcal{U}_n$,

(i). $S_{n,3}$ ($n \geq 6$) is the unique graph with the smallest edge–Szeged index.

(ii). $B_7' (n = 7)$ and $S_n(2, 3, n - 5)$ ($n \geq 8$) are the unique graphs with the second smallest edge–Szeged index.

(iii). $B'_8 (n = 8), S_9(3, 3, 3)$ ($n = 9), S_n(2, 4, n - 6)$ ($10 \leq n \leq 13), B'_14$ ($n = 14$) and $S_{14}(2, 4, 8)$ ($n = 14$), $B'_n$ ($n \geq 15$) are the unique graphs with the third smallest edge–Szeged index.

**Proof.** (i). By the proof of Lemma 3.8(iii), $Sz_e(S_{n,g})$ is increasing for odd $g \in \{3, 5, \ldots, \lceil \frac{n}{2} \rceil \}$ and $Sz_e(S_{n,g})$ is increasing for even $g \in \{4, 6, \ldots, \lceil \frac{n}{2} \rceil \}$. Thus, we only need to compare the edge–Szeged index of $S_{n,3}$ and $S_{n,4}$. Since $Sz_e(S_{n,3}) = 4n - 12$ and $Sz_e(S_{n,4}) = 12n - 60$. Thus, $S_{n,3}$ ($n \geq 6$) is the unique graph with the smallest edge–Szeged index.

(ii). The graphs in $\mathcal{U}_n$ with the second smallest edge–Szeged index are just the graphs in $\mathcal{U}_n \setminus \{S_{n,3}\} = (\mathcal{F}_n \setminus \{S_{n,3}\}) \cup \Phi_n \cup \Omega_n$ with the smallest edge–Szeged index. By Lemma 3.8, it holds that $\min \{Sz_e(B'_7), Sz_e(S_n(2, 3, n - 5)), Sz_e(S_{n,4})\} = \min \{5n - 14, 5n - 19, 12n - 60\} = 5n - 19$. It means that $B'_7$ ($n = 7$) and $S_n(2, 3, n - 5)$ ($n \geq 8$) are the unique graphs with the second smallest edge–Szeged index.

(iii). The graphs in $\mathcal{U}_n$ with the third smallest edge–Szeged index are just the graphs in $\mathcal{U}_n \setminus \{S_{n,3}, S_n(2, 3, n - 5)\} = (\mathcal{F}_n \setminus \{S_{n,3}\}) \cup \Phi_n \cup \Omega_n$ with the smallest edge–Szeged index.

If $n = 8$, then $\min \{Sz_e(B'_8), Sz_e(G'_8), Sz_e(S_{n,4})\} = \min \{26, 27, 36\} = 26$.

If $n = 9$, then $\min \{Sz_e(B'_9), Sz_e(S_9(3, 3, 3)), Sz_e(S_{9,4})\} = \min \{31, 27, 48\} = 27$.

If $n \geq 10$, then $\min \{Sz_e(B'_n), Sz_e(S_n(2, 4, n - 6)), Sz_e(S_{n,4})\} = \min \{5n - 14, 6n - 28, 12n - 60\}$, which is equal to $6n - 28$ for $10 \leq n \leq 13$, $56$ for $n = 14$, and $5n - 14$ for $n \geq 15$. This completes the proof.

\[\square\]

4. Conclusion

In this paper, we determine the first three minimum values of the edge–Szeged index of fully–loaded unicyclic graphs having a fixed order and characterize all the graphs attaining these values. It would be interesting to obtained the bounds of the edge–Szeged index for fully–loaded bicyclic graphs, and we intend to do it in the near future.

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