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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 pendent vertex. An edge uv of G is called a pendent 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 $M_u(e|G) = \{e \in E(G) : d(u, e) < d(v, e)\}$ and $M_v(e|G) = \{e \in E(G) : d(v, e) < d(u, e)\}$. 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

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

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 $C_g = v_1 v_2 \cdots v_g v_1$. 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 $C_g(T_1, T_2, \cdots, T_g)$. Let $n(T_i) = |T_i| = t_i$ for $i = 1, 2, \cdots, g$, then $\sum_{i=1}^{g} t_i = n$. Take $D(u|G) = \sum_{u \in V(G)} d(u, v|G)$.

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

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

$$\begin{aligned} Sz_e(G) = &\sum_{i=1}^{g} W(T_i) + \sum_{i=1}^{g} (|G| - |T_i| + 1) D(v_i|T_i) + \sum_{i=1}^{g}\sum_{j=1}^{g} |T_i||T_j| d(v_i, v_j|C_g) \\ &- \delta(g) \sum_{i<j} |T_i||T_j| - |G|^2 + |G|^{\delta(g)} g. \end{aligned}$$

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

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

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

Let S_n' $(n \ge 5)$ be the tree formed by attaching a pendent vertex to a pendent vertex of the star S_{n-1}.

Lemma 3.3. [15] *Among all n-vertex trees, S_n' $(n \ge 5)$ 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 $n \ge 5$. $T \ncong S_n$. Let x be the vertex of maximal degree of S_n'. Then $D(u|T) \ge D(x|S_n') = n$.*

Let $\mathcal{U}_n$ $(n \ge 6)$ be the set of n-vertex fully–loaded unicyclic graphs. Denote by $\mathcal{U}_{n,g}$ $(3 \le g \le \lfloor \frac{n}{2} \rfloor)$ the set of all fully–loaded unicyclic graphs with n vertices and cycle C_g.

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

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

By Lemmas 2.1, 3.1 and 3.2, we have

Lemma 3.5. *Let $G = C_g(T_1, T_2, \cdots, T_g) \in \mathcal{U}_{n,g}$ with $g \ge 3$, $t_i = |T_i| \ge 2$. Then $Sz_e(G) \ge Sz_e(S_n(t_1, t_2, \cdots, t_g))$, with equality if and only if $G \cong S_n(t_1, t_2, \cdots, t_g)$.*

Lemma 3.6. *Let $G = S_n(t_1, t_2, \cdots, t_g)$. Suppose that $t_k, t_l \ge 2$ for $1 \le k, l \le g$ and $k \ne l$. If $N_k + \frac{1}{2}\delta(g) t_k \le N_l + \frac{1}{2}\delta(g) t_l$, for $G' = S_n(t_1', t_2', \cdots, t_g')$, where $t_i' = t_i$ $(1 \le i \le g)$ with $i \ne k, l$, and $t_k' = t_k + 1$, $t_l' = t_l - 1$, then $Sz_e(G') < Sz_e(G)$.*

Proof. Note that $t_k' = t_k + 1$, $t_l' = t_l - 1$, and by Lemma 2.1, we have that

$$\begin{aligned} Sz_e(G) - Sz_e(G') = &\, 2[t_k t_l - (t_k + 1)(t_l - 1)] d_{kl} + 2 \sum_{i \ne k,l} [t_k t_i - (t_k + 1) t_i] d_{ki} + 2 \sum_{i \ne k,l} [t_l t_i \\ &- (t_l - 1) t_i] d_{li} - \delta(g) [\sum_{i \ne k,l} t_i (t_k + t_l) - \sum_{i \ne k,l} t_i (t_k + 1 + t_l - 1) + t_k t_l \\ &- (t_k + 1)(t_l - 1)] \\ = &\, 2[(N_l + \frac{1}{2}\delta(g) t_l) - (N_k + \frac{1}{2}\delta(g) t_k)] + 2 d_{kl} - \delta(g) > 0\,. \end{aligned}$$

$\square$

By Lemmas 3.5 and 3.6, we have the next result.

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

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

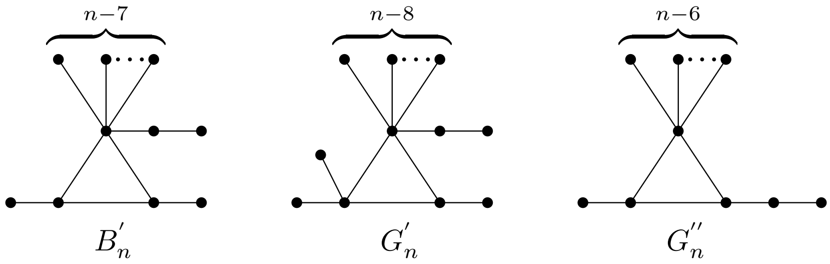

Figure 1: The graphs $B_n^{'}$, $G_n^{'}$ and $G_n^{''}$.

Lemma 3.8. *Consider the graphs $B_n^{'}$, $G_n^{'}$ and $G_n^{''}$ shown in Figure 1.*

(i). *Among the graphs in $\mathcal{F}_n$ $(n \geq 6)$, $S_n(2, 2, n-4)$ and $B_n^{'}$ are the unique graphs with the smallest and second smallest edge–Szeged index, respectively.*

(ii). *Among the graphs in Φ_n $(n \geq 8)$, $S_n(2, 3, n-5)$ is the unique graph with the smallest edge–Szeged index. The graph $G_8^{'}$ 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 Ω_n $(n \geq 8)$, $S_{n,4}$ is the unique graph with the smallest edge–Szeged index.*

Proof. (i). Let $G \in \mathcal{F}_n$, by Lemma 2.1, we have $Sz_e(G) = -n^2 + 9n - 12 + W(T_3) + 5D(v_3|T_3)$. 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 Φ_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 Φ_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 $G \ncong S_n(2, 3, n-5), S_n(2, 4, n-6)$. 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 $Sz_e(S_n(2, t_2, t_3)) > Sz_e(S_n(2, 4, n-6)) > Sz_e(S_n(2, 3, n-5))$.

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. $G \ncong S_n(t_1, t_2, t_3)$.
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 $Sz_e(S_{n,g+2}) - Sz_e(S_{n,g}) = 4gn - 6g^2 - 4g - 2 \geq 4g[2(g+2)] - 6g^2 - 4g - 2 = 2g^2 + 20g - 2 > 0$. 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 $g \in \{3, 5, \cdots, \lfloor \frac{n}{2} \rfloor\}$ and $Sz_e(S_{n,g})$ is increasing for even $g \in \{4, 6, \cdots, \lfloor \frac{n}{2} \rfloor\}$. 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 Ω_n.

□

In the following theorem, we determine the first three minimum values of edge–Szeged index from the class $\mathcal{U}_n$ of fully–loaded unicyclic graphs of order n.

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 $g \in \{3, 5, \cdots, \lfloor \frac{n}{2} \rfloor\}$ and $Sz_e(S_{n,g})$ is increasing for even $g \in \{4, 6, \cdots, \lfloor \frac{n}{2} \rfloor\}$. 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 $\min\{Sz_e(B_n'), Sz_e(S_n(2,3,n-5)), Sz_e(S_{n,4})\} = min\{5n - 14, 5n - 19, 12n - 60\} = 5n - 19$. 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 $\mathcal{U}_n \setminus \{S_{n,3}, S_n(2, 3, n-5)\} = (\mathcal{F}_n \setminus \{S_{n,3}\}) \cup (\Phi_n \setminus S_n(2, 3, n-5)) \cup \Omega_n$ with the smallest edge–Szeged index.

If $n = 8$, then $\min\{Sz_e(B_8'), Sz_e(G_8'), Sz_e(S_{8,4})\} = \min\{26, 27, 36\} = 26$.

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.

□

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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