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# Edge Szeged Index of 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 $m_u(e|G)$ is the number of edges whose distance to vertex $u$ is smaller than the distance to vertex $v$, and $m_v(e|G)$ is the number of edges whose distance to vertex $v$ is smaller than the distance to vertex $u$. In this paper, we determine the $n$-vertex unicyclic graphs with the largest, the second largest, the smallest and the second smallest edge Szeged indices.

## 1. INTRODUCTION

Topological indices are numerical quantities associated with chemical structures via their hydrogen–depleted graphs, which are used in theoretical chemistry for design of chemical compounds with given physicochemical properties or given pharmacologic and biological activities. The Wiener index is one of the oldest and the most thoroughly studied topological indices [1–5]. The Szeged index is another such topological index which, in the case of trees, coincides with the Wiener index [6].

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Let $G$ be a connected graph with vertex set $V(G)$ and edge set $E(G)$. Suppose that $x$ and $y$ are vertices of $G$. The distance $d(x, y|G)$ between $x$ and $y$ is defined as the length of a shortest path between $x$ and $y$ in $G$. If $e$ is an edge of $G$ connecting the vertices $u$ and $v$, then we write $e = uv$ or $e = vu$. For $e = uv \in E(G)$, let $n_u(e|G)$ and $n_v(e|G)$ be 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 $u$. The Szeged index of the graph $G$ is defined as [6]

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

It has been studied extensively, see, e.g., [7–22], and has found applications in modelling physicochemical properties as well as physiological activities of organic compounds acting as drugs or possessing pharmacological activity, see [21].

If $e = uv$ is an edge of $G$ and $w$ is a vertex of $G$, then the distance between $e$ and $w$ is defined as $d(e, w|G) = \min\{d(u, w|G), d(v, w|G)\}$. For $e = uv \in E(G)$, let $m_u(e|G)$ be the number of edges whose distance to vertex $u$ is smaller than the distance to vertex $v$, and $m_v(e|G)$ the number of edges whose distance to vertex $v$ is smaller than the distance to vertex $u$. Recently, Gutman and Ashrafi [23] introduced an edge version of the Szeged index, named edge Szeged index. The edge Szeged index of the graph $G$ is defined as

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

In [23], some basic properties of the edge Szeged index were established (most of these are analogous to the properties of the ordinary Szeged index, but some remarkable differences are also recognized). Note that pendent edges make no contribution to $Sz_e$ and for a tree $T$ with $n$ vertices, $Sz_e(T) = Sz(T) - (n-1)^2$. In [24], the edge Szeged index of the Cartesian product of graphs was computed. Let $C_r$ be the cycle with $r$ vertices, where $r \geq 3$. Vukičević [25] determined the maximum value $\frac{1}{4}m(m-1)^2$ for odd $m$ and $\frac{1}{4}(m+2)(m-2)^2$ for even $m$ of the edge Szeged index for (not necessarily simple) graphs with $m \geq 5$ edges and the unique extremal graphs are respectively $C_m$ for odd $m$ and $C_{m-1}$ with one double edge for even $m$. Thus, for a simple graph $G$ with $m \geq 5$ edges, $Sz_e(G) \leq \frac{1}{4}m(m-1)^2$ with equality if and only if $G = C_m$ if $m$ is odd, while $Sz_e(G) < \frac{1}{4}(m+2)(m-2)^2$ if $m$ is even.

A unicyclic graph is a (simple) connected graph with a unique cycle. If $G$ is a unicyclic graph with $n \geq 5$ vertices, then by Vukičević's result, $Sz_e(G) \leq \frac{1}{4}n(n-1)^2$

with equality if and only if $G = C_n$ if $n$ is odd, while $Sz_e(G) < \frac{1}{4}(n+2)(n-2)^2$ if $n$ is even.

In this paper, we determine the $n$-vertex unicyclic graphs with the largest, the second largest, the smallest and the second smallest edge Szeged indices for $n \geq 5$, and compare the obtained results with the previous results [22] on the ordinary Szeged index.

## 2. PRELIMINARIES

For the graph $G$ with $e \in E(G)$, we also write $m(e)$ instead of $m_u(e|G)\, m_v(e|G)$, and then $Sz_e(G) = \sum\limits_{e \in E(G)} m(e)$. Recall that $m(e) = 0$ for a pendent edge $e$ of $G$.

For integers $n$ and $r$ with $3 \leq r \leq n$, let $S_{n,r}$ and $P_{n,r}$ be respectively the unicyclic graph obtained by attaching $n-r$ pendent vertices and $P_{n-r}$ to a vertex of the cycle $C_r$. In particular, $S_{n,n} = P_{n,n} = C_n$.

The number of vertices of a graph $G$ is denoted by $|G|$. Let $C_r(T_1, T_2, \ldots, T_r)$ be the graph constructed as follows. Let the vertices of the cycle $C_r$ be labelled consecutively by $v_1, v_2, \ldots, v_r$. Let $T_1, T_2, \ldots, T_r$ be vertex–disjoint trees such that $T_i$ and the cycle $C_r$ have exactly one vertex $v_i$ in common for $1 \leq i \leq r$. Then any $n$-vertex unicyclic graph $G$ with a cycle on $r$ vertices is of the form $C_r(T_1, T_2, \ldots, T_r)$, where $\sum\limits_{i=1}^{r} |T_i| = n$.

Note that for an edge $e = uv$ in an $n$-vertex graph $G$, $m_u(e|G) + m_v(e|G) \leq n-1$ and that for integers $k$ and $x$, the function $x(k-x)$ for $1 \leq x \leq \lfloor \frac{k}{2} \rfloor$ is increasing with $x$. These facts are used frequently.

## 3. UNICYCLIC GRAPHS WITH LARGE EDGE SZEGED INDICES

In this section, we determine the $n$-vertex unicyclic graphs with the largest and the second largest edge Szeged indices for $n \geq 5$. The obtained results are compared with the previous results for the ordinary Szeged index in [22].

**Proposition 1.** *For odd $n \geq 5$, let $G$ be an $n$-vertex unicyclic graph different from $C_n$ and $P_{n,n-2}$. Then*

$$Sz_e(G) < Sz_e(P_{n,n-2}) = \frac{n^3}{4} - n^2 + \frac{n}{4} + \frac{5}{2} < Sz_e(C_n) = \frac{1}{4}n(n-1)^2\,.$$

**Proof.** By the definition of the edge Szeged index, we have

$$\begin{aligned}
Sz_e(C_n) &= \sum_{e\in E(C_n)} m(e) = \sum_{e\in E(C_n)} \left(\frac{n-1}{2}\cdot\frac{n-1}{2}\right) = \frac{1}{4}n(n-1)^2,\\
Sz_e(P_{n,n-2}) &= \sum_{e\in E(C_{n-2})} m(e) + \sum_{e\in E(G)\setminus E(C_{n-2})} m(e)\\
&= \left[\frac{n-3}{2}\cdot\frac{n-3}{2} + \frac{n-3}{2}\cdot\frac{n+1}{2}\cdot(n-3)\right] + 0 + 1\cdot(n-2)\\
&= \frac{n^3}{4} - n^2 + \frac{n}{4} + \frac{5}{2}\\
&< Sz_e(C_n)\,.
\end{aligned}$$

Let $r$ be the cycle length of $G$, where $3 \le r \le n-1$. There are four cases.

**Case 1.** $r = n-1$. Then $G = P_{n,n-1}$. Obviously,

$$\begin{aligned}
Sz_e(G) &= Sz_e(P_{n,n-1}) = \sum_{e\in E(C_{n-1})} m(e)\\
&= \frac{n-3}{2}\cdot\frac{n-1}{2}\cdot(n-1)\\
&= \frac{n^3}{4} - \frac{5n^2}{4} + \frac{7n}{4} - \frac{3}{4} < Sz_e(P_{n,n-2})\,.
\end{aligned}$$

**Case 2.** $r = n-2$. Then $G = S_{n,n-2}$ or $G = C_{n-2}(T_1, T_2, \ldots, T_{n-2})$, where $|T_1| = |T_i| = 2$, $i \in \{2, 3, \ldots, \frac{n-1}{2}\}$, and $|T_j| = 1$ for all $j \ne 1, i$. In the former case, it is easily checked that $Sz_e(S_{n,n-2}) - Sz_e(P_{n,n-2}) = -(n-2)$ and then $Sz_e(S_{n,n-2}) < Sz_e(P_{n,n-2})$. In the latter case, $m(e_1) = m(e_2) = \frac{n-1}{2}\cdot\frac{n-3}{2}$ for $e_1 = v_{\frac{n-1}{2}}v_{\frac{n+1}{2}}$, $e_2 = v_{i+\frac{n-3}{2}}v_{i+\frac{n-1}{2}}$, where $v_{n-1} = v_1$, and then it is easily seen that

$$\begin{aligned}
Sz_e(G) &= m(e_1) + m(e_2) + \sum_{\substack{e\in E(C_{n-2})\\ e\ne e_1,e_2}} m\,(e)\\
&\le \frac{n-3}{2}\cdot\frac{n-1}{2}\cdot 2 + \frac{n-1}{2}\cdot\frac{n-1}{2}\cdot(n-4)\\
&= \frac{n^3}{4} - n^2 + \frac{n}{4} + \frac{1}{2} < Sz_e(P_{n,n-2})\,.
\end{aligned}$$

**Case 3.** $3 \le r \le n-4$ and $r$ is odd. Then $n \ge 7$. Note that $G$ may be written as $G = C_r(T_1, T_2, \ldots, T_r)$. Suppose first that all $T_i$ for $i = 1, 2, \ldots, r$ except one, say $T_1$ are trivial. Then $|T_1| = n - r + 1$. Let $e_1 = v_{\frac{r+1}{2}}v_{\frac{r+3}{2}}$. Then $m(e_1) = \frac{r-1}{2}\cdot\frac{r-1}{2}$. For $e = uv \in E(C_r)$ with $e \ne e_1$, we have $|m_u(e|G) - m_v(e|G)| = n - r \ge 4$, and then $m(e) \le \frac{n-5}{2}\cdot\frac{n+3}{2}$. If $r = n-4$, then by direct checking, we have

$$\sum_{e\in E(G)\setminus E(C_r)} m(e) \le 1\cdot(n-2) + 2\cdot(n-3) + 3\cdot(n-4)$$

and thus

$$\begin{aligned} Sz_e(G) &= m(e_1) + \sum_{\substack{e\in E(C_r)\\ e\neq e_1}} m(e) + \sum_{e\in E(G)\setminus E(C_r)} m(e) \\ &\leq \frac{r-1}{2}\cdot\frac{r-1}{2} + \frac{n-5}{2}\cdot\frac{n+3}{2}\cdot(r-1) \\ &\quad + [1\cdot(n-2) + 2\cdot(n-3) + 3\cdot(n-4)] \\ &= \frac{n^3}{4} - \frac{3n^2}{2} + \frac{9n}{4} + 5 < Sz_e(P_{n,n-2}). \end{aligned}$$

Suppose that $r < n-4$. We will show that

$$\begin{aligned} \sum_{e\in E(G)\setminus E(C_r)} m(e) &\leq \frac{n-1}{2}\cdot\frac{n-1}{2} + \frac{n+1}{2}\cdot\frac{n-3}{2}\cdot 2 \\ &\quad + \frac{n-5}{2}\cdot\frac{n+3}{2}\cdot(n-r-5) + 1\cdot(n-2). \end{aligned} \tag{1}$$

Let $E_1 = E(G)\setminus E(C_r)$, then $|E_1| = n-r$ and for any $e = uv \in E_1$, $m_u(e|G) + m_v(e|G) = n-1$. There are two edges $e_2$ and $e_3$ in $E_1$ (either two pendent edges or a pendent edge and a non-pendent edge adjacent) such that $m(e_2)+m(e_3) \leq 1\cdot(n-2)$. Let $E_2 = E_1\setminus\{e_2, e_3\}$. Consider the contributions of edges in $E_2$. If $m(e) \leq \frac{n+3}{2}\cdot\frac{n-5}{2}$ for any $e \in E_2$, then (1) follows easily. There are two other possibilities: (i) For some $e_4 \in E_2$, $m(e_4) = \frac{n-1}{2}\cdot\frac{n-1}{2}$. Let $G_1$ and $G_2$ be the two components of $G - e_4$. There is at most one edge, say $e_5$ in $E_2 \cap E(G_1)$ (resp. $e_6$ in $E_2 \cap E(G_2)$) if exists, such that $m(e_5) = \frac{n+1}{2}\cdot\frac{n-3}{2}$ (resp. $m(e_6) = \frac{n+1}{2}\cdot\frac{n-3}{2}$), and for any other edge $e \in E_2\setminus\{e_4\}$ (different from $e_5, e_6$ if exist), $m(e) \leq \frac{n+3}{2}\cdot\frac{n-5}{2}$. (ii) The maximum contribution of edges in $E_2$ is $m(e_4) = \frac{n+1}{2}\cdot\frac{n-3}{2}$ for some $e_4 \in E_2$. For one of the components $G_1$ and $G_2$ of $G - e_4$, say $G_1$, we have $|E(G_1)| = \frac{n-3}{2}$. Then for any edge $e \in E_2 \cap E(G_1)$, $m(e) \leq \frac{n+3}{2}\cdot\frac{n-5}{2}$. Note that for any edge $e \in E_2 \cap E(G_2)$, $m(e) \leq \frac{n+1}{2}\cdot\frac{n-3}{2}$. Suppose that there is an edge $e_5 \in E_2 \cap E(G_2)$ with $m(e_5) = \frac{n+1}{2}\cdot\frac{n-3}{2}$. Then for some edge $e_6 \in E_2 \cap E(G_2)$, the two components of $G - e_5$ are $G_1'$ and $G_2'$ with $E(G_1') = E(G_1)\cup\{e_4, e_6\}$ and $E(G_2') = E(G_2)\setminus\{e_5, e_6\}$. Thus $m(e_6) \leq \frac{n+1}{2}\cdot\frac{n-3}{2}$, and for any edge $e$ in $E_2 \cap E(G_2)\setminus\{e_5, e_6\} = E_2 \cap E(G_2')$, $m(e) \leq \frac{n+3}{2}\cdot\frac{n-5}{2}$. By combining (i) and (ii), we have (1). Then

$$\begin{aligned} Sz_e(G) &= m(e_1) + \sum_{\substack{e\in E(C_r)\\ e\neq e_1}} m(e) + \sum_{e\in E(G)\setminus E(C_r)} m(e) \\ &\leq \frac{r-1}{2}\cdot\frac{r-1}{2} + \frac{n-5}{2}\cdot\frac{n+3}{2}\cdot(r-1) + \Bigg[\frac{n-1}{2}\cdot\frac{n-1}{2} \\ &\quad + \frac{n+1}{2}\cdot\frac{n-3}{2}\cdot 2 + \frac{n-5}{2}\cdot\frac{n+3}{2}\cdot(n-r-5) + 1\cdot(n-2)\Bigg] \end{aligned}$$

$$\begin{aligned} &= \frac{n^3}{4} - \frac{5n^2}{4} - \frac{5n}{4} + \frac{39}{2} - \frac{r}{2} + \frac{r^2}{4} \\ &\leq \frac{n^3}{4} - n^2 - \frac{19n}{4} + \frac{63}{2} < Sz_e(P_{n,n-2}) . \end{aligned}$$

Now suppose that at least two of $T_i$ for $i = 1, 2, \ldots, r$, say $T_1$ and $T_i$ are nontrivial for some $i \in \{2, 3, \ldots, \frac{r+1}{2}\}$. Then with $e_1 = v_{\frac{r+1}{2}} v_{\frac{r+3}{2}}$ and $e_2 = v_{i+\frac{r-1}{2}} v_{i+\frac{r+1}{2}}$ where $v_{r+1} = v_1$, we have $m(e_1), m(e_2) \leq \frac{n-1}{2} \cdot \frac{n-3}{2}$ and thus

$$\begin{aligned} Sz_e(G) &= m(e_1) + m(e_2) + \sum_{\substack{e \in E(C_r) \\ e \neq e_1, e_2}} m(e) + \sum_{e \in E(G) \setminus E(C_r)} m(e) \\ &\leq \frac{n-1}{2} \cdot \frac{n-3}{2} \cdot 2 + \frac{n-1}{2} \cdot \frac{n-1}{2} \cdot (r-2) \\ &\quad + \frac{n-1}{2} \cdot \frac{n-1}{2} \cdot (n-r-3) + 1 \cdot (n-2) \\ &= \frac{n^3}{4} - \frac{5n^2}{2} + \frac{7n}{4} - \frac{7}{4} < Sz_e(P_{n,n-2}) . \end{aligned}$$

**Case 4.** $4 \leq r \leq n-3$ and $r$ is even. Then $n \geq 7$. Note that $G$ may be written as $G = C_r(T_1, T_2, \ldots, T_r)$. Suppose first that all $T_i$ for $i = 1, 2, \ldots, r$ except one, say $T_1$ are trivial. Then $|T_1| = n - r + 1$. For $e = uv \in E(C_r)$, $|m_u(e|G) - m_v(e|G)| \geq 3$ and then $m(e) \leq \frac{n-5}{2} \cdot \frac{n+1}{2}$, and thus

$$\begin{aligned} Sz_e(G) &= \sum_{e \in E(C_r)} m(e) + \sum_{e \in E(G) \setminus E(C_r)} m(e) \\ &\leq \frac{n-5}{2} \cdot \frac{n+1}{2} \cdot r \\ &\quad + \left[ \frac{n-1}{2} \cdot \frac{n-1}{2} \cdot (n-r-3) + 2 \cdot (n-3) + 1 \cdot (n-2) \right] \\ &= \frac{n^3}{4} - \frac{5n^2}{4} + \frac{19n}{4} - \frac{35}{4} - \frac{r}{2}(3+n) \\ &\leq \frac{n^3}{4} - \frac{5n^2}{4} + \frac{11n}{4} - \frac{59}{4} < Sz_e(P_{n,n-2}) . \end{aligned}$$

Now suppose that at least two of $T_i$ for $i = 1, 2, \ldots, r$, say $T_1$ and $T_i$ are nontrivial for some $i \in \{2, 3, \ldots, r\}$, then

$$\begin{aligned} Sz_e(G) &= \sum_{e \in E(C_r)} m(e) + \sum_{e \in E(G) \setminus E(C_r)} m(e) \\ &\leq \frac{n-1}{2} \cdot \frac{n-3}{2} \cdot r + \left[ \frac{n-1}{2} \cdot \frac{n-1}{2} \cdot (n-r-3) + 1 \cdot (n-2) \right] \\ &= \frac{n^3}{4} - \frac{5n^2}{4} + \frac{11n}{4} - \frac{11}{4} + \frac{r}{2}(1-n) \\ &\leq \frac{n^3}{4} - \frac{5n^2}{4} + \frac{3n}{4} - \frac{3}{4} < Sz_e(P_{n,n-2}) . \end{aligned}$$

By combining Cases 1–4, the result follows. ■

**Proposition 2.** *For even $n \geq 6$, let $G$ be an $n$-vertex unicyclic graph different from $P_{n,n-1}$ and $C_n$. Then*

$$Sz_e(G) < Sz_e(C_n) = \frac{n^3}{4} - n^2 + n < Sz_e(P_{n,n-1}) = \frac{n^3}{4} - \frac{3n^2}{4} + 1\,.$$

**Proof.** By the definition of edge Szeged index, we have

$$\begin{aligned} Sz_e(P_{n,n-1}) &= \sum_{e\in E(C_{n-1})} m(e) \\ &= \frac{n-2}{2}\cdot\frac{n-2}{2} + \frac{n}{2}\cdot\frac{n-2}{2}\cdot(n-2) \\ &= \frac{n^3}{4} - \frac{3n^2}{4} + 1 \\ Sz_e(C_n) &= \sum_{e\in E(C_n)} m(e) = \frac{n-2}{2}\cdot\frac{n-2}{2}\cdot n \\ &= \frac{n^3}{4} - n^2 + n < Sz_e(P_{n,n-1})\,. \end{aligned}$$

Let $r$ be the cycle length of $G$, where $3 \leq r \leq n-1$. Note that $G$ may be written as $G = C_r(T_1, T_2, \ldots, T_r)$. There are two cases.

**Case 1.** $3 \leq r \leq n-3$ and $r$ is odd. Suppose first that all $T_i$ for $i = 1, 2, \ldots, r$ except one, say $T_1$ are trivial. Then $|T_1| = n - r + 1$. Let $e_1 = v_{\frac{r+1}{2}} v_{\frac{r+3}{2}}$. Then $m(e_1) = \frac{r-1}{2}\cdot\frac{r-1}{2}$. For $e = uv \in E(C_r)$ with $e \neq e_1$, we have $|m_u(e|G) - m_v(e|G)| = n - r \geq 3$, and then $m(e) \leq \frac{n-4}{2}\cdot\frac{n+2}{2}$. It follows that

$$\begin{aligned} Sz_e(G) &= m(e_1) + \sum_{\substack{e\in E(C_r)\\ e\neq e_1}} m(e) + \sum_{e\in E(G)\setminus E(C_r)} m(e) \\ &\leq \frac{r-1}{2}\cdot\frac{r-1}{2} + \frac{n-4}{2}\cdot\frac{n+2}{2}\cdot(r-1) \\ &\quad + \left[\frac{n}{2}\cdot\frac{n-2}{2}\cdot(n-r-3) + 2\cdot(n-3) + 1\cdot(n-2)\right] \\ &= \frac{n^3}{4} - \frac{3n^2}{2} + 5n - \frac{23}{4} + \frac{r^2}{4} - \frac{5r}{2} \\ &\leq \max\left\{\frac{n^3}{4} - \frac{3n^2}{2} + +5n - 11, \frac{n^3}{4}\right\} - \frac{5n^2}{4} + n + 4 < Sz_e(C_n)\,. \end{aligned}$$

Suppose now that at least two of $T_i$ for $i = 1, 2, \ldots, r$, say $T_1$ and $T_i$ are nontrivial for some $i \in \{2, 3, \ldots, \frac{r+1}{2}\}$. Then with $e_1 = v_{\frac{r+1}{2}} v_{\frac{r+3}{2}}$ and $e_2 = v_{i+\frac{r-1}{2}} v_{i+\frac{r+1}{2}}$ where $v_{r+1} = v_1$, we have

$$Sz_e(G) = m(e_1) + m(e_2) + \sum_{\substack{e\in E(C_r)\\ e\neq e_1,e_2}} m(e) + \sum_{e\in E(G)\setminus E(C_r)} m(e)$$

$$\begin{aligned}
&\leq \frac{n-2}{2}\cdot\frac{n-2}{2}\cdot 2+\frac{n}{2}\cdot\frac{n-2}{2}\cdot(r-2)\\
&\quad+\left[\frac{n}{2}\cdot\frac{n-2}{2}\cdot(n-r-3)+1\cdot(n-2)\right]\\
&= \frac{n^3}{4}-\frac{5n^2}{4}+\frac{3n}{2}<Sz_e(C_n)\,.
\end{aligned}$$

**Case 2.** $4\leq r\leq n-2$ and $r$ is even. We can easily have

$$\begin{aligned}
Sz_e(G) &= \sum_{e\in E(C_r)} m\,(e)+\sum_{e\in E(G)\setminus E(C_r)} m(e)\\
&\leq \frac{n-2}{2}\cdot\frac{n-2}{2}\cdot r+\left[\frac{n}{2}\cdot\frac{n-2}{2}\cdot(n-r-2)+1\cdot(n-2)\right]\\
&= \frac{n^3}{4}-n^2+2n-2+r\left(1-\frac{n}{2}\right)\\
&\leq \frac{n^3}{4}-n+2<Sz_e(C_n)\,.
\end{aligned}$$

By combining Cases 1 and 2, the result follows. ■

By Propositions 1 and 2, for odd $n\geq 5$ the graphs $C_n$ and $P_{n,n-2}$ are respectively the unique $n$-vertex unicyclic graphs with the largest and the second largest edge Szeged indices, which are equal to $\frac{1}{4}n(n-1)^2$ and $\frac{n^3}{4}-n^2+\frac{n}{4}+\frac{5}{2}$ respectively, while for even $n\geq 6$ the graphs $P_{n,n-1}$ and $C_n$ are respectively the unique $n$-vertex unicyclic graphs with the largest and the second largest edge Szeged indices, which are equal to $\frac{n^3}{4}-\frac{3n^2}{4}+1$ and $\frac{n^3}{4}-n^2+n$ respectively. These should be compared with the corresponding results for the ordinary Szeged index [22]: For odd $n\geq 7$, $P_{n,n-1}$ is the unique $n$-vertex unicyclic graph with the largest Szeged index, which is equal to $\frac{1}{4}(n^3-n^2+3n-3)$, for $n=7,9,11$, the graph obtained by attaching a $P_2$ and a $P_1$ respectively to two vertices of distance $\frac{n-3}{2}$ in the cycle $C_{n-3}$ is the unique graph with the second largest Szeged index, which is equal to $\frac{1}{4}(n^3-3n^2+15n-21)$, for $n\geq 13$, $C_n$ is the unique graph with the second largest Szeged index, which is equal to $\frac{1}{4}(n^3-2n^2+n)$; for even $n\geq 6$, $C_n$, the graph obtained by attaching a pendent vertex to two vertices of distance $\frac{n-2}{2}$ in the cycle $C_{n-2}$ are respectively the unique graphs with the largest and the second largest Szeged indices, which are equal to $\frac{n^3}{4}$ and $\frac{1}{4}(n^3-2n^2+8n-8)$, respectively.

## 4. UNICYCLIC GRAPHS WITH SMALL EDGE SZEGED INDICES

In this section, we determine the $n$-vertex unicyclic graphs with the smallest and the second smallest edge Szeged indices for $n\geq 6$ and the results are compared with the

corresponding results for the ordinary Szeged index in [22].

Let $S_n(a,b,c)$ be the $n$-vertex unicyclic graph formed by attaching $a$, $b$, and $c$ pendent vertices to the three vertices of a triangle, respectively, where $a \geq b \geq c \geq 0$ and $a+b+c=n-3$. Obviously, $S_{n,3} = S_n(n-3,0,0)$.

**Lemma 1.** *For $n \geq 6$, let $G$ be an $n$-vertex unicyclic graph with cycle length 3 different from $S_{n,3}$ and $S_n(n-4,1,0)$. Then*

$$Sz_e(G) > Sz_e(S_n(n-4,1,0)) = 3n-7 > Sz_e(S_{n,3}) = 2n-3\,.$$

**Proof.** Note that $G$ may be written as $C_3(T_1,T_2,T_3)$ with $|T_1| = a+1$, $|T_2| = b+1$, and $|T_3| = c+1$, where $a \geq b \geq c \geq 0$ and $a+b+c=n-3$. It follows that

$$\begin{aligned} Sz_e(G) &\geq \sum_{e \in E(C_3)} m\,(e) \\ &= (a+1)(b+1) + (a+1)(c+1) + (b+1)(c+1) \\ &= ab+ac+bc+2(a+b+c)+3 \\ &= ab+ac+bc+2(n-3)+3, \end{aligned}$$

with equality if and only if any edge of $G$ outside the triangle is a pendent edge, i. e., $G = S_n(a,b,c)$. Let $f(a,b,c) = ab+ac+bc$, where $a,b,c$ are integers, $a \geq b \geq c \geq 0$ and $a+b+c=n-3$. It is easily seen that if $(a,b,c) \neq (n-3,0,0), (n-4,1,0)$, then $f(a,b,c) > f(n-4,1,0) > f(n-3,0,0)$. If $G$ is of the form $S_n(a,b,c)$, then

$$Sz_e(G) > Sz_e(S_n(n-4,1,0)) = 3n-7 > Sz_e(S_{n,3}) = 2n-3,$$

and if $G$ is not of the form $S_n(a,b,c)$, then

$$\begin{aligned} Sz_e(G) &= ab+ac+bc+2(n-3)+3+\sum_{i=1}^{3}\sum_{e \in E(T_i)} m(e) \\ &\geq 2(n-3)+3+1\cdot(n-2) \\ &= 3n-5 > 3n-7\,. \end{aligned}$$

The result follows. ■

**Proposition 3.** *For $n \geq 6$, let $G$ be an $n$-vertex unicyclic graph different from $S_{n,3}$ and $S_n(n-4,1,0)$. Then*

$$Sz_e(G) > Sz_e(S_n(n-4,1,0)) = 3n-7 > Sz_e(S_{n,3}) = 2n-3\,.$$

**Proof.** Let $r$ be the cycle length of $G$, where $3 \leq r \leq n$. If $r = 3$, then by Lemma 1, the result follows. Suppose that $r \geq 4$. It suffices to show that $Sz_e(G) > 3n - 7$.
**Case 1.** $r$ is odd. Then $r \geq 5$. Note that $G$ may be written as $G = C_r(T_1, T_2, \ldots, T_r)$. Let $|T_j| = i_j + 1$ for $j = 1, 2, \ldots, r$. If $T_j$ is a star with center $v_j$ for $j = 1, 2, \ldots, r$, then such a graph $G$ is denoted by $S_n(i_1, i_2, \ldots, i_r)$. Thus,

$$\begin{aligned} Sz_e(G) &\geq \sum_{e \in E(C_r)} m\,(e) = Sz_e(S_n(i_1, i_2, \ldots, i_r)) \\ &\geq \sum_{j=1}^{r} 2(n - 3 - i_j) \\ &= (2n - 6)r - 2(i_1 + i_2 + \cdots + i_r) \\ &= (2n - 4)r - 2n \geq 8n - 20, \end{aligned}$$

**Case 2.** $r$ is even. Then

$$\begin{aligned} Sz_e(G) &\geq \sum_{e \in E(C_r)} m\,(e) \\ &\geq 1 \cdot (n - 3) \cdot r \geq 4n - 12\,. \end{aligned}$$

By combining Cases 1 and 2, we have $Sz_e(G) > 3n - 7$. The result follows. ■

By Proposition 3, for $n \geq 6$ the graphs $S_{n,3}$ and $S_n(n - 4, 1, 0)$ are, respectively, the unique $n$-vertex unicyclic graphs with the smallest and the second smallest edge Szeged indices, which are equal to $2n - 3$ and $3n - 7$ respectively. We note that a similar result holds for the ordinary Szeged index [22]: $S_{n,3}$ and $S_n(n-4, 1, 0)$ are also respectively the $n$-vertex unicyclic graphs with the smallest and the second smallest Szeged indices, which are equal to $n^2 - 2n$ and $n^2 - n - 4$, respectively.

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