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ON SZEGED INDICES OF UNICYCLIC GRAPHS

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Abstract

The Szeged index of a connected graph G is defined as

$$Sz(G) = \sum_{e \in E(G)} n_1(e|G) n_2(e|G),$$

where $E(G)$ is the edge set of G, and for the edge $e = uv \in E(G)$, $n_1(e|G)$ and $n_2(e|G)$ 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. Gutman has determined the n-vertex unicyclic graphs with the smallest and the largest Szeged indices. Now we determine the n-vertex unicyclic graphs of cycle length r with the smallest and the largest Szeged indices for $3 \le r \le n$, the n-vertex unicyclic graphs with the second, the third and the fourth smallest Szeged indices, and the n-vertex unicyclic graphs with the kth largest Szeged indices for all k up to $\frac{n}{2} + 2$ if $n \ge 6$ is even, to four if $n = 7$, to five if $n = 9$, to $\frac{n+13}{4}$ if $n \equiv 3 \pmod 4$ with $n \ge 11$, and to $\frac{n+15}{4}$ if $n \equiv 1 \pmod 4$ with $n \ge 13$.

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1. INTRODUCTION

Topological indices 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 coincides to the Wiener index on trees [6].

Let G be a simple connected (molecular) graph with vertex set $V(G)$ and edge set $E(G)$. If e is an edge of G connecting the vertices u and v, then we write $e = uv$ or $e = vu$. The number of vertices of G is denoted by $|G|$.

Let $e = uv \in E(G)$. Let $n_1(e|G)$ and $n_2(e|G)$ 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]

$$Sz(G) = \sum_{e \in E(G)} n_1(e|G) n_2(e|G).$$

It has received much attention for both its mathematical properties and its chemical applications, see, e.g., [7–21]. In particular, Khadikar *et al.* [21] described various applications of Szeged index for modeling physicochemical properties as well as physiological activities of organic compounds acting as drugs or possessing pharmacological activity.

A unicyclic graph is a connected graph with a unique cycle. Let C_n be the n-vertex cycle. Let $S_{n,r}$ be the unicyclic graph obtained by attaching $n-r$ pendent vertices to a vertex of the cycle C_r, where $3 \le r \le n$. In particular, $S_{n,n} = C_n$. Let $Q_n = C_n$ if n is even and $Q_n = S_{n,n-1}$ if n is odd. The n-vertex unicyclic graphs with the smallest and the largest Szeged indices have been known [6]: $S_{n,3}$ and Q_n are respectively the unique n-vertex unicyclic graphs with the smallest and the largest Szeged indices. In this paper, we determine the n-vertex unicyclic graphs of cycle length r with the smallest and the largest Szeged indices for $3 \le r \le n$, the n-vertex unicyclic graphs with the second, the third and the fourth smallest Szeged indices, and the n-vertex unicyclic graphs with the kth largest Szeged indices for all k up to $\frac{n}{2} + 2$ if $n \ge 6$ is even, to four if $n = 7$, to five if $n = 9$, to $\frac{n+13}{4}$ if $n \equiv 3 \pmod 4$ with $n \ge 11$, and to $\frac{n+15}{4}$ if $n \equiv 1 \pmod 4$ with $n \ge 13$.

2. PRELIMINARIES

The distance between the vertices u and v of a connected graph G, denoted by $d(u,v|G)$, is equal to the length (number of edges) of a shortest path connecting them. Let $D(u|G) = \sum_{v \in V(G)} d(u,v|G)$. Recall that the Wiener index of the graph G is defined as [3]

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v|G) = \frac{1}{2} \sum_{u \in V(G)} D(u|G),$$

and that if G is a tree then $W(G) = Sz(G)$.

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 $i = 1, 2, \ldots, r$. 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 $\sum_{i=1}^{r} |T_i| = n$.

Let $\delta(n) = 0$ if n is even and $\delta(n) = 1$ if n is odd. Gutman *et al.* [13] showed that

Proposition 1. [13] *Let $G = C_r(T_1, T_2, \ldots, T_r)$. Then*

$$\begin{aligned} Sz(G) &= \sum_{i=1}^{r} W(T_i) + \sum_{i=1}^{r} (|G| - |T_i|) D(v_i|T_i) \\ &\quad + \sum_{i=1}^{r} \sum_{j=1}^{r} |T_i||T_j| d(v_i, v_j|C_r) - \delta(r) \sum_{i<j} |T_i||T_j|. \end{aligned}$$

Let S_n and P_n be respectively the n-vertex star and path.

Lemma 1. [3] *Let T be an n-vertex tree different from S_n and P_n. Then $(n-1)^2 = W(S_n) < W(T) < W(P_n) = \frac{n^3-n}{6}$.*

The following lemma is obvious.

Lemma 2. [22] *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, respectively. Then $n - 1 = D(x|S_n) \leq D(u|T) \leq D(y|P_n) = \frac{n(n-1)}{2}$. Left equality holds exactly when $T = S_n$ and $u = x$, and right equality holds exactly when $T = P_n$ and u is a terminal vertex.*

For $n \geq 5$, let S'_n be the tree formed by attaching a pendent vertex to a pendent vertex of the star S_{n-1}, and S''_n the tree formed by attaching two pendent vertices to a pendent vertex of the star S_{n-2}.

Lemma 3. [22] *Among the n-vertex trees with $n \geq 6$, S'_n and S''_n are respectively the unique trees with the second and the third smallest Wiener indices, which are equal to $n^2 - n - 2$ and $n^2 - 7$, respectively.*

We will also use the following lemma.

Lemma 4. [22] *Let T be an n-vertex tree with $n \geq 6$, $u \in V(T)$, $T \neq S_n$, where u is not the vertex of maximal degree if $T = S'_n$. Let x and y be the vertex of maximal degree in S'_n and S''_n, respectively. Then $n = D(x|S'_n) < D(y|S''_n) \leq D(u|T)$.*

For the graph $G = C_r(T_1, T_2, \ldots, T_r)$, let $d_{ij} = d(v_i, v_j|C_r)$ and $t_i = |T_i|$ for $i = 1, 2, \ldots, r$.

Let $\mathbb{U}_{n,r}$ be the set of n-vertex unicyclic graphs with cycle length r, where $3 \leq r \leq n$, and $\mathcal{U}_n$ the set of n-vertex unicyclic graphs, where $n \geq 3$.

3. UNICYCLIC GRAPHS WITH SMALL SZEGED INDICES

Proposition 2. *Let $G \in \mathbb{U}_{n,r}$, where $3 \leq r \leq n$. Then $Sz(G) \geq Sz(S_{n,r})$ with equality if and only if $G = S_{n,r}$, where*

$$Sz\left(S_{n,r}\right) = \begin{cases} (n-1)(n-r) + \frac{r^2}{4}(2n-r) & \text{if } r \text{ is even,} \\ n(n-1) + \frac{1}{4}(r-1)^2(2n-r) - (n-1)r & \text{if } r \text{ is odd.} \end{cases}$$

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

$$\begin{aligned} Sz\left(S_{n,r}\right) &= 1 \cdot (n-1) \cdot (n-r) + \frac{r}{2} \cdot \left(n - \frac{r}{2}\right) \cdot r \\ &= (n-1)(n-r) + \frac{r^2}{4}(2n-r) \end{aligned}$$

if r is even, and

$$\begin{aligned} Sz\left(S_{n,r}\right) &= 1 \cdot (n-1) \cdot (n-r) + \frac{r-1}{2} \cdot \frac{r-1}{2} \\ &\quad + \frac{r-1}{2} \cdot \left(n - \frac{r+1}{2}\right) \cdot (r-1) \end{aligned}$$

$$= \quad n(n-1)+\frac{1}{4}(r-1)^2(2n-r)-(n-1)r$$

if r is odd.

The cases $r = n-1, n$ are obvious. Suppose that $r \le n-2$.

Assume that $G = C_r(T_1, T_2, \dots, T_r)$ is a graph in $\mathbb{U}_{n,r}$ with the smallest Szeged index. By Proposition 1 and Lemmas 1 and 2, T_i is a star with center v_i for $i = 1, 2, \dots, r$. Then

$$\begin{aligned} Sz(G) &= \sum_{i=1}^{r}(t_i-1)^2+\sum_{i=1}^{r}(n-t_i)(t_i-1) \\ &\quad +\sum_{i=1}^{r}\sum_{j=1}^{r}t_it_jd_{ij}-\delta(r)\sum_{i<j}t_it_j \\ &= (n-1)(n-r)+\sum_{i=1}^{r}\sum_{j=1}^{r}t_it_jd_{ij} \\ &\quad -\delta(r)\sum_{i<j}t_it_j. \end{aligned}$$

Let $N_s = \sum_{i \neq s} t_i d_{si}$. Suppose that there exist k and l with $1 \le k < l \le r$ such that $t_k, t_l \ge 2$.

Case 1. r is even. Assume that $N_l \ge N_k$. For a pendent vertex w in T_l, consider $G' = G - v_l w + v_k w \in \mathbb{U}_{n,r}$. We have

$$\begin{aligned} \frac{Sz(G)-Sz(G')}{2} &= [t_kt_l-(t_k+1)(t_l-1)]\,d_{kl}+\sum_{i\neq k,l}[t_kt_i-(t_k+1)t_i]\,d_{ki} \\ &\quad +\sum_{i\neq k,l}[t_lt_i-(t_l-1)t_i]\,d_{li} \\ &= d_{kl}-N_k+N_l>0, \end{aligned}$$

which is a contradiction. Thus $r-1$ of $t_1, t_2, \dots, t_r$ are equal to 1 and the remaining one is equal to $n-(r-1)$, i.e., $G = S_{n,r}$.

Case 2. r is odd. Assume that $N_l + \frac{1}{2}t_l \ge N_k + \frac{1}{2}t_k$. For a pendent vertex w in T_l, consider $G' = G - v_l w + v_k w \in \mathbb{U}_{n,r}$. We have

$$\begin{aligned} \frac{Sz(G)-Sz(G')}{2} &= d_{kl}-N_k+N_l-\frac{1}{2}\Bigg[\sum_{i\neq k,l}t_i(t_k+t_l)-\sum_{i\neq k,l}t_i(t_k+1+t_l-1) \\ &\quad +t_kt_l-(t_k+1)(t_l-1)\Bigg] \\ &= d_{kl}-N_k+N_l+\frac{1}{2}\left(-t_k+t_l-1\right) \end{aligned}$$

$$= d_{kl} - \frac{1}{2} - \left(N_k + \frac{1}{2}t_k\right) + \left(N_l + \frac{1}{2}t_l\right) > 0,$$

which is a contradiction. Thus $r-1$ of $t_1, t_2, \ldots, t_r$ are equal to 1 and the remaining one is equal to $n-(r-1)$, i.e., $G = S_{n,r}$.

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

For fixed n, from the expression above, $Sz\,(S_{n,r})$ is increasing for even r and odd r, respectively, where $3 \le r \le n$. Note that $Sz(S_{n,4}) = n^2+3n-12 > Sz(S_{n,3}) = n^2-2n$ for $n \ge 4$. By Proposition 2, we have: $S_{n,3}$ is the unique n-vertex unicyclic graph for $n \ge 3$ with the smallest Szeged index, which is equal to n^2-2n (see [6]), and $S_{n,4}$ is the unique n-vertex bipartite unicyclic graph for $n \ge 4$ with the smallest Szeged index, which is equal to $n^2+3n-12$.

Let $\Phi_n = \bigcup_{r=4}^{n} \mathbb{U}_{n,r}$. Let Γ_n be the set of graphs $C_3(T_1, T_2, T_3)$ in $\mathbb{U}_{n,3}$ with $|T_2| = |T_3| = 1$. Let Ψ_n be the set of graphs $C_3(T_1, T_2, T_3)$ in $\mathbb{U}_{n,3}$ with $|T_1| \ge |T_2| \ge \max\{|T_3|, 2\}$. Then $\mathcal{U}_n = \Phi_n \cup \Gamma_n \cup \Psi_n$.

For $n \ge 5$, let B'_n be the n-vertex unicyclic graph formed by attaching $n-5$ pendent vertices and a path P_2 to one vertex of a triangle. For $n \ge 6$, let B''_n be the n-vertex unicyclic graph formed by attaching $n-6$ pendent vertices and the star S_3 at its center to one vertex of a triangle. Evidently, B'_n, $B''_n \in \Gamma_n$.

Lemma 5. *Among the graphs in Γ_n with $n \ge 6$, B'_n and B''_n are respectively the unique graphs with the second and the third smallest Szeged indices, which are equal to n^2-n-3 and n^2-8, respectively.*

Proof. The result holds trivially for $n = 6, 7$. Suppose that $n \ge 8$. Let $G = C_3(T_1, T_2, T_3) \in \Gamma_n$. Note that $|T_1| = n-2 \ge 6$ and $W(T_2) = W(T_3) = 0$. By Proposition 1, we have

$$Sz(G) = W(T_1) + 2D(v_1|T_1) + 2(n-2) + 1$$

which, together with Lemmas 3 and 4, implies that B'_n and B''_n are respectively the unique graphs in Γ_n with the second and the third smallest Szeged indices, where

$$\begin{aligned} Sz(B'_n) &= W(S'_{n-2}) + 2(n-3+1) + 2n-3 = n^2-n-3, \\ Sz(B''_n) &= W(S''_{n-2}) + 2(n-3+2) + 2n-3 = n^2-8. \end{aligned}$$

This proves the result. ■

Let $S_n(a,b,c)$ be the n-vertex unicyclic graph formed by attaching $a-1$, $b-1$ and $c-1$ pendent vertices to the three vertices of a triangle, respectively, where $a,b,c \geq 1$ and $a+b+c=n$.

Lemma 6. *Among the graphs in Ψ_n with $n \geq 6$, if $n=6$ then $S_n(n-3,2,1)$ and $S_n(n-4,2,2)$ are respectively the unique graphs with the first and the second smallest Szeged indices, which are equal to $n^2-n-4=26$ and $n^2-9=27$, respectively, and if $n \geq 7$ then $S_n(n-3,2,1)$ and $S_n(n-4,3,1)$ are respectively the unique graphs with the first and the second smallest Szeged indices, which are equal to n^2-n-4 and n^2-10, respectively.*

Proof. The case $n=6$ may be checked easily. Suppose that $n \geq 7$. Let $G = C_3(T_1,T_2,T_3) \in \Psi_n$ with $a \geq b \geq \max\{c,2\}$ and $a+b+c=n$, where $a=|T_1|$, $b=|T_2|$ and $c=|T_3|$.

Suppose first that $G = S_n(a,b,c)$. Then $Sz(G) = n^2-4n+3+ab+bc+ca$. If $c=1$ and $(a,b,c) \neq (n-3,2,1)$, $(n-4,3,1)$, then from $Sz(G) = n^2-4n+3+ab+n-1$ and $a+b=n-1$ we have

$$\begin{aligned} Sz(G) &> Sz(S_n(n-4,3,1)) = n^2-10 \\ &> Sz(S_n(n-3,2,1)) = n^2-n-4. \end{aligned}$$

If $c \geq 2$, then

$$\begin{aligned} Sz(G) &= -c^2+nc+n^2-4n+3+ab \\ &\geq -c^2+nc+n^2-4n+3+(n-2c)c \\ &= -3c^2+2nc+n^2-4n+3 \\ &\geq -3\cdot 2^2+2n\cdot 2+n^2-4n+3 \\ &= n^2-9 > n^2-10. \end{aligned}$$

If $G \neq S_n(a,b,c)$, then by Proposition 1 and Lemmas 1–4, we have either $Sz(G) \geq Sz(C_3(S'_{n-3},P_2,P_1)) = n^2-7 > n^2-10$ for $(b,c)=(2,1)$ or $Sz(G) > Sz(S_n(a,b,c)) \geq Sz(S_n(n-4,3,1)) = n^2-10$ otherwise. ■

Proposition 3. *For $n \geq 6$, $S_n(n-2,1,1)$ and $S_n(n-3,2,1)$ are respectively the unique graphs in $\mathcal{U}_n$ with the first and the second smallest Szeged indices, which are equal to n^2-2n and n^2-n-4, respectively. Furthermore,*

(i) *$S_6(2,2,2)$ and B'_6 are the unique graphs in $\mathcal{U}_6$ with the third smallest Szeged index, which is equal to 27, while B''_6 is the unique graph in $\mathcal{U}_6$ with the fourth smallest Szeged index, which is equal to 28;*

(ii) *B'_7 and $S_7(3,3,1)$ are the unique graphs in $\mathcal{U}_7$ with the third smallest Szeged index, which is equal to 39, while $S_7(3,2,2)$ is the unique graph in $\mathcal{U}_7$ with the fourth smallest Szeged index, which is equal to 40;*

(iii) *if $n \geq 8$, then B'_n and $S_n(n-4,3,1)$ are respectively the unique graphs in $\mathcal{U}_n$ with the third and the fourth smallest Szeged indices, which are equal to n^2-n-3 and n^2-10, respectively.*

Proof. From the discussion above, the Szeged indices of graphs in Φ_n are at least $\min\{Sz(S_{n,5}), Sz(S_{n,4})\} = n^2+2n-15$.

By Lemma 5, $S_{n,3} = S_n(n-2,1,1)$, B'_n and B''_n are respectively the unique graphs in Γ_n with the first, the second and the third smallest Szeged indices, which are equal to n^2-2n, n^2-n-3 and n^2-8, respectively.

By Lemma 6, for $n \geq 7$, $S_n(n-3,2,1)$ and $S_n(n-4,3,1)$ are respectively the unique graphs in Ψ_n with the first and the second smallest Szeged indices, which are equal to n^2-n-4 and n^2-10, respectively, while $S_n(n-3,2,1)$ and $S_n(n-4,2,2)$ are respectively the unique graphs in Ψ_6 with the first and the second smallest Szeged indices, which are equal to $n^2-n-4=26$ and $n^2-9=27$, respectively.

Note that $\mathcal{U}_n = \Phi_n \cup \Gamma_n \cup \Psi_n$. Then the Szeged indices of the graphs in $\mathcal{U}_n$ may be ordered as:

$$\begin{aligned} Sz\left(S_n(n-2,1,1)\right) = n^2-2n \quad &< \quad Sz(S_n(n-3,2,1)) = n^2-n-4 \\ &< \quad Sz(B'_n) = n^2-n-3 \\ &< \quad Sz(S_n(n-4,3,1)) = n^2-10 \\ &< \quad \cdots \end{aligned}$$

for $n \geq 8$,

$$Sz\left(S_n(n-2,1,1)\right) = n^2-2n \quad < \quad Sz(S_n(n-3,2,1)) = n^2-n-4$$

$$
\begin{aligned}
&< Sz(B'_n) = n^2 - n - 3 \\
&= Sz(S_n(n-4,3,1)) = n^2 - 10 \\
&< \cdots
\end{aligned}
$$

for $n = 7$, and

$$
\begin{aligned}
Sz\left(S_n(n-2,1,1)\right) = n^2 - 2n &< Sz(S_n(n-3,2,1)) = n^2 - n - 4 = n^2 - 10 \\
&< Sz(S_n(n-4,2,2)) = n^2 - 9 \\
&= Sz(B'_n) = n^2 - n - 3 \\
&< \cdots
\end{aligned}
$$

for $n = 6$.

To complete the proof, we need only to determine the graphs in $\mathcal{U}_n$ for $n = 6, 7$ with the fourth smallest Szeged indices. As $Sz(G) \geq n^2 + 2n - 15$ for $G \in \Phi_n$, these graphs are just the graphs in $\mathcal{U}_n$ of cycle length 3 for $n = 6, 7$ with the fourth smallest Szeged indices, which may be checked directly. ■

4. UNICYCLIC GRAPHS WITH LARGE SZEGED INDICES

Let $P(r, l, a, b)$ be the unicyclic graph obtained by attaching a path P_a at one terminal vertex to v_1 and a path P_b at one terminal vertex to v_l of the cycle C_r, where $l = 1, 2, \ldots, \lfloor \frac{r}{2} \rfloor + 1$. If $a = 0$ or $b = 0$, then no path is attached to v_1 or v_l. Let $P_{n,r} = P\left(r, \frac{r}{2}+1, \lceil \frac{n-r}{2} \rceil, \lfloor \frac{n-r}{2} \rfloor\right)$ if r is even, and $P_{n,r} = P(r, 1, n-r, 0)$ if r is odd. Obviously, $P_{n,r} \in \mathbb{U}_{n,r}$, $P(r, 1, 1, 1) = S_{r+2,r}$, and if r is odd then $P(r, l, n-r, 0) = P_{n,r}$ for any l.

Proposition 4. *Let $G \in \mathbb{U}_{n,r}$, where $3 \leq r \leq n$. Then $Sz(G) \leq Sz(P_{n,r})$ with equality if and only if $G = P_{n,r}$, where*

$$
Sz(P_{n,r}) = \begin{cases}
\frac{(n-r)(n-r+2)(2n+r-1)}{12} + \frac{rn^2}{4} & \text{if } n \text{ and } r \text{ are even,} \\
\frac{(n-r-1)(n-r+1)(2n+r)}{12} + \frac{(r+1)n^2-r^2+r-1}{4} & \text{if } n \text{ is odd and } r \text{ is even,} \\
\frac{(n-r)(n-r+1)(n+2r-1)}{6} + \frac{(r-1)^2(2n-r)}{4} & \text{if } r \text{ is odd.}
\end{cases}
$$

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

$$
Sz\left(P_{n,r}\right) = 2 \sum_{i=1}^{(n-r)/2} i(n-i) + \frac{rn^2}{4}
$$

$$= \frac{(n-r)(n-r+2)(2n+r-1)}{12} + \frac{rn^2}{4}$$

if n and r are even,

$$\begin{aligned} Sz\left(P_{n,r}\right) &= 2\sum_{i=1}^{(n-r-1)/2} i(n-i) + \frac{n-r+1}{2}\left(n - \frac{n-r+1}{2}\right) + \frac{r(n^2-1)}{4} \\ &= \frac{(n-r-1)(n-r+1)(2n+r)}{12} + \frac{(r+1)n^2 - r^2 + r - 1}{4} \end{aligned}$$

if n is odd and r is even, and

$$\begin{aligned} Sz\left(P_{n,r}\right) &= \sum_{i=1}^{n-r} i(n-i) + (r-1)\frac{r-1}{2}\left(n - 1 - \frac{r-1}{2}\right) + \frac{(r-1)^2}{4} \\ &= \frac{(n-r)(n-r+1)(n+2r-1)}{6} + \frac{(r-1)^2(2n-r)}{4} \end{aligned}$$

if r is odd.

The cases $r = n, n-1$ are obvious. Suppose that $r \leq n-2$.

Assume that $G = C_r(T_1, T_2, \ldots, T_r)$ is a graph in $\mathbb{U}_{n,r}$ with the largest Szeged index. By Proposition 1 and Lemmas 1 and 2, T_i is a path with one terminal vertex v_i for $i = 1, 2, \ldots, r$. Then

$$\begin{aligned} Sz(G) &= \sum_{i=1}^{r} \frac{1}{6}\left(t_i^3 - t_i\right) + \sum_{i=1}^{r} \frac{1}{2}(n-t_i)t_i(t_i-1) \\ &\quad + \sum_{i=1}^{r}\sum_{j=1}^{r} t_i t_j d_{ij} - \delta(r)\sum_{i<j} t_i t_j \\ &= -\frac{1}{3}\sum_{i=1}^{r} t_i^3 + \frac{1}{2}(n+1)\sum_{i=1}^{r} t_i^2 - \frac{1}{2}n^2 - \frac{1}{6}n \\ &\quad + \sum_{i=1}^{r}\sum_{j=1}^{r} t_i t_j d_{ij} - \delta(r)\sum_{i<j} t_i t_j . \end{aligned}$$

Let $N_s = \sum_{i \neq s} t_i d_{si}$. Suppose that there exist distinct k, l, m with $1 \leq k, l, m \leq r$, such that $t_k, t_l, t_m \geq 2$ and $t_m \geq \max\{t_k, t_l\}$.

Case 1. r is even. Assume that $t_k^2 + nt_l + 2N_l \leq t_l^2 + nt_k + 2N_k$. Let G' be the graph formed from G by deleting the pendent vertex in T_l and attaching it to the pendent vertex in T_k. Obviously, $G' \in \mathbb{U}_{n,r}$. Then

$$\begin{aligned} Sz(G) - Sz(G') &= -\frac{1}{3}\left[t_k^3 + t_l^3 - (t_k+1)^3 - (t_l-1)^3\right] \\ &\quad + \frac{n+1}{2}\left[t_k^2 + t_l^2 - (t_k+1)^2 - (t_l-1)^2\right] \end{aligned}$$

$$
\begin{aligned}
& +2\left[t_k t_l-(t_k+1)(t_l-1)\right] d_{kl} \\
& +2 \sum_{i \neq k, l}\left[t_k t_i-(t_k+1) t_i\right] d_{ki} \\
& +2 \sum_{i \neq k, l}\left[t_l t_i-(t_l-1) t_i\right] d_{li} \\
= & \; t_k^2-n t_k-t_l^2+(n+2) t_l-(n+1)+2 d_{kl} \\
& -2 \sum_{i \neq k} t_i d_{ki}+2 \sum_{i \neq l} t_i d_{li} \\
= & \;(t_k^2+n t_l+2 N_l)-(t_l^2+n t_k+2 N_k) \\
& +2 t_l+2 d_{kl}-n-1 .
\end{aligned}
$$

Note that $2t_l + 2d_{kl} \leq t_l + t_m + r \leq n+1$. If $2t_l + 2d_{kl} < n+1$, then $Sz(G) < Sz(G')$, which is a contradiction. Suppose that $2t_l + 2d_{kl} = n+1$. Then $d_{kl} = \frac{r}{2}$, $d_{ml} < \frac{r}{2}$ and $t_m = t_l \geq t_k = 2$. Assume that $t_m^2 + nt_l + 2N_l \leq t_l^2 + nt_m + 2N_m$. Let G'' be the graph formed from G by deleting the pendent vertex in T_l and attaching it to the pendent vertex in T_m. Obviously, $G'' \in \mathbb{U}_{n,r}$. Since $2t_l + 2d_{ml} - n - 1 < 0$, we have

$$
\begin{aligned}
& Sz(G)-Sz(G'') \\
= & \;(t_m^2+n t_l+2 N_l)-(t_l^2+n t_m+2 N_m)+2 t_l+2 d_{ml}-n-1<0,
\end{aligned}
$$

and then $Sz(G) < Sz(G'')$, which is a contradiction again. Thus, $r-2$ of $t_1, t_2, \ldots, t_r$ are equal to 1, say $t_i = 1$ for $i \neq k, l$. Let $t_k = a$ and $t_l = b$, where $a, b \geq 1$. Suppose without loss of generality that $k = 1$ and $l \leq \frac{r}{2} + 1$. We write $G = G_l$. If $l \leq \frac{r}{2}$, then by Proposition 1 or the expression for $Sz(G)$ given above, for $a, b > 1$, we have

$$
\begin{aligned}
& Sz(G_l)-Sz(G_{l+1}) \\
= & \;2\left[a b d_{1l}-a b d_{1, l+1}+a d_{1, l+1}-a d_{1, l}+(b-1) \sum_{j \neq 1, l, l+1}(d_{lj}-d_{l+1, j})\right] \\
= & \;2\left[a b d_{1l}-a b d_{1, l+1}+a d_{1, l+1}-a d_{1, l}+(b-1)(d_{1, l+1}-d_{1, l})\right] \\
= & -2(a-1)(b-1)<0,
\end{aligned}
$$

and then $Sz(G_l) < Sz(G_{l+1})$, a contradiction. Thus, if $a, b > 1$ then $l = \frac{r}{2} + 1$. We write $G = G_{a,b}$, where $a, b \geq 1$ and $a + b + r - 2 = n$. If $a + 2 \leq b$, then

$$
\begin{aligned}
& Sz\left(G_{a, b}\right)-Sz\left(G_{a+1, b-1}\right) \\
= & \;a^2+n b+(2 a-2) d_{lk}-b^2-n a-(2 b-2) d_{lk}+2 b+2 d_{lk}-n-1
\end{aligned}
$$

$$= \quad (r-1-2d_{lk})(b-a-1) = -(b-a-1) < 0,$$

and thus $Sz(G_{a,b})$ for $a+b=n-r+2$ is maximum if and only if $|a-b| \le 1$. It follows that $G = P\left(r, \frac{r}{2}+1, \lceil \frac{n-r}{2} \rceil, \lfloor \frac{n-r}{2} \rfloor\right) = P_{n,r}$.

Case 2. r is odd. Assume that $t_k^2 + (n+1)t_l + 2N_l \le t_l^2 + (n+1)t_k + 2N_k$. Let G' be the graph formed from G by deleting the pendent vertex in T_l and attaching it to the pendent vertex in T_k. Obviously, $G' \in \mathbb{U}_{n,r}$. Then

$$\begin{aligned} Sz(G) - Sz(G') &= (t_k^2 + nt_l + 2N_l) - (t_l^2 + nt_k + 2N_k) \\ &\quad + 2t_l + 2d_{kl} - n - 1 + (-t_k + t_l - 1) \\ &= \left[t_k^2 + (n+1)t_l + 2N_l\right] - \left[t_l^2 + (n+1)t_k + 2N_k\right] \\ &\quad + 2t_l + 2d_{kl} - n - 2 < 0. \end{aligned}$$

Note that $2t_l + 2d_{kl} \le t_l + t_m + r \le n+1$. Thus, $Sz(G) < Sz(G')$, which is a contradiction. Thus $r-2$ of $t_1, t_2, \ldots, t_r$ are equal to 1, say $t_i = 1$ for $i \ne k, l$. Let $t_k = a$ and $t_l = b$. We write $G = G_{a,b}$, where $a, b \ge 1$ and $a+b+r-2 = n$. If $a \ge b \ge 2$, then

$$\begin{aligned} Sz(G_{a,b}) - Sz(G_{a+1,b-1}) &= (r-1-2d_{lk})(b-a-1) + b - a - 1 \\ &= -(r-2d_{lk})(a+1-b) < 0, \end{aligned}$$

and thus $Sz(G_{a,b})$ is maximum for $a+b=n-r+2$ and $a \ge b$ if and only if $a = n-(r-1)$ and $b=1$. It follows that $G = P(r,1,n-r,0) = P_{n,r}$.

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

For odd $n \ge 7$, let $\mathcal{H}_n$ be the set of graphs $C_{n-3}(T_1, T_2, \ldots, T_{n-3})$ with $t_1 = t_j = t_s = 2$, $t_i = 1$ for $i \ne 1, j, s$, and either $1 < j \le \lfloor \frac{n+1}{4} \rfloor < \frac{n-1}{2} \le s \le \frac{n-5}{2} + j$ or $n-2-s \ge s-j \ge j-1 \ge \lfloor \frac{n+1}{4} \rfloor$. In the former case, there are

$$\sum_{j=2}^{\lfloor (n+1)/4 \rfloor} (j-1) = \frac{1}{2} \left\lfloor \frac{n-3}{4} \right\rfloor \cdot \left\lfloor \frac{n+1}{4} \right\rfloor = \begin{cases} \frac{(n-3)(n+1)}{32} & \text{if } n \equiv 3 \pmod 4 \\ \frac{(n-5)(n-1)}{32} & \text{if } n \equiv 1 \pmod 4 \end{cases}$$

(non-isomorphic) graphs. In the latter case, there are

$$p\left(n-3-3\left\lfloor \frac{n-3}{4} \right\rfloor, 3\right) = \begin{cases} \left\lfloor \frac{(n-3)^2}{192} + \frac{1}{4} \right\rfloor & \text{if } n \equiv 3 \pmod 4 \\ \left\lfloor \frac{(n+3)^2}{192} + \frac{1}{4} \right\rfloor & \text{if } n \equiv 1 \pmod 4 \end{cases}$$

(non-isomorphic) graphs, where $p(m,3)$ is the number of partitions of m into exactly three parts, and from [23], with $A(3,m) = 1$ for $m \equiv 0 \pmod 3$ and $A(3,m) = 0$ otherwise,

$$p(m,3) = \frac{2m^2 + 12m + 13 + 3(-1)^m + 8A(3,m)}{24} - \left\lfloor \frac{m+1}{2} \right\rfloor = \left\lfloor \frac{m^2+3}{12} \right\rfloor.$$

Thus,

$$|\mathcal{H}_n| = \begin{cases} \frac{(n-3)(n+1)}{32} + \left\lfloor \frac{(n-3)^2}{192} + \frac{1}{4} \right\rfloor & \text{if } n \equiv 3 \pmod 4, \\ \frac{(n-5)(n-1)}{32} + \left\lfloor \frac{(n+3)^2}{192} + \frac{1}{4} \right\rfloor & \text{if } n \equiv 1 \pmod 4. \end{cases}$$

In particular, $|\mathcal{H}_7| = 1$, $|\mathcal{H}_9| = 2$ and $|\mathcal{H}_{11}| = 3$.

Lemma 7. *For odd $n \geq 7$, let $G = C_{n-3}(T_1, T_2, \ldots, T_{n-3})$, where $t_1 = t_j = t_s = 2$, $t_i = 1$ for $i \neq 1, j, s$, and $1 < j < s$. Then*

$$Sz(G) \leq \frac{n^3 - 3n^2 + 11n - 9}{4}$$

with equality if and only if G is isomorphic to a graph in $\mathcal{H}_n$.

Proof. By the definition of the Szeged index,

$$\begin{aligned} Sz(G) &\leq 1 \cdot (n-1) \cdot 3 + \left(\frac{n-3}{2} + 1\right) \cdot \left(\frac{n-3}{2} + 2\right) \cdot (n-3) \\ &= \frac{n^3 - 3n^2 + 11n - 9}{4} \end{aligned}$$

with equality if and only if for every edge on the cycle, its contribution to $Sz(G)$ is maximal, which is equal to $\left(\frac{n-3}{2} + 1\right) \cdot \left(\frac{n-3}{2} + 2\right)$, i.e., any vertex of v_1, v_j, v_s lies outside a shortest path connecting the other two vertices in the cycle of G. Suppose that the equality holds. By possible relabeling vertices on the cycle, we may suppose that $j - 1 \leq s - j \leq n - 2 - s$. Then $d_G(v_1, v_j) = j - 1$ and $d_G(v_j, v_s) = s - j$. Since v_j lies outside a shortest path connecting v_1 and v_s, we have $d_G(v_1, v_s) = \min\{n-2-s, s-1\} = n - 2 - s$, and then $s \geq \frac{n-1}{2}$. If $s = \frac{n-1}{2}$, then $s - j < n - 2 - s = \frac{n-3}{2}$. If $s > \frac{n-1}{2}$, then $s - j \leq n - 2 - s \leq \frac{n-5}{2}$. In either case, we have $s \leq j + \frac{n-5}{2}$. Now there are two possibilities: (1) $j \leq \lfloor \frac{n+1}{4} \rfloor$ and then $1 < j \leq \lfloor \frac{n+1}{4} \rfloor < \frac{n-1}{2} \leq s \leq \frac{n-5}{2} + j$, implying that $G \in \mathcal{H}_n$; (2) $j - 1 \geq \lfloor \frac{n+1}{4} \rfloor$ and then obviously $G \in \mathcal{H}_n$. Conversely, it is easily seen that the bound for $Sz(G)$ is attained for any graph $G \in \mathcal{H}_n$. ■

For even integer $r \geq 4$, let $S(r, l, 2, 1)$ be the unicyclic graph obtained by attaching two pendent vertices to v_1 and a pendent vertex to v_l of the cycle C_r, where $l = 1, 2, \ldots, \frac{r}{2} + 1$.

Proposition 5. *Among graphs in $\mathcal{U}_n$ with $n \geq 6$,*

(i) *if n is even, then C_n, $P\left(n-2, \frac{n}{2}, 1, 1\right)$ and $P(n-2, 1, 2, 0)$ are respectively the unique graphs with the first, the second and the third largest Szeged indices, which are equal to $\frac{n^3}{4}$, $\frac{1}{4}(n^3-2n^2+8n-8)$ and $\frac{1}{4}(n^3-2n^2+8n-12)$ respectively, $P\left(n-2, \frac{n}{2}-(l-3), 1, 1\right)$ for $l = 4, \ldots, \frac{n+4}{2}$, is the unique graph with the lth largest Szeged index, which is equal to $\frac{1}{4}(n^3-2n^2+8n-8)-2(l-3)$;*

(ii) *if n is odd, then $P_{n,n-1}$ is the unique graph with the largest Szeged index, which is equal to $\frac{1}{4}(n^3-n^2+3n-3)$,*

(a) *for $n = 7, 9, 11$, $P\left(n-3, \frac{n-1}{2}, 2, 1\right)$ and $P(n-3, 1, 3, 0)$ are respectively the unique graphs with the second and the third largest Szeged indices, which are equal to $\frac{1}{4}(n^3-3n^2+15n-21)$ and $\frac{1}{4}(n^3-3n^2+15n-29)$ respectively, for $n = 7$, $P\left(n-3, \frac{n-3}{2}, 2, 1\right)$, $S\left(n-3, \frac{n-1}{2}, 2, 1\right)$ and graphs in $\mathcal{H}_7$ are the unique graphs with the fourth largest Szeged index, which is equal to $\frac{1}{4}(n^3-3n^2+11n-9)$, for $n = 9$, $P\left(n-3, \frac{n-3}{2}, 2, 1\right)$ is the unique graph with the fourth largest Szeged index, which is equal to $\frac{1}{4}(n^3-3n^2+15n-37)$, while C_n, $S\left(n-3, \frac{n-1}{2}, 2, 1\right)$ and graphs in $\mathcal{H}_9$ are the unique graphs with the fifth largest Szeged index, which is equal to $\frac{1}{4}(n^3-3n^2+11n-9)$, and for $n = 11$, C_n and $P\left(n-3, \frac{n-3}{2}, 2, 1\right)$ are respectively the unique graphs with the fourth and the fifth largest Szeged indices, which are equal to $\frac{1}{4}(n^3-2n^2+n)$ and $\frac{1}{4}(n^3-3n^2+15n-37)$, respectively, while $P\left(n-3, \frac{n-5}{2}, 2, 1\right)$, $S\left(n-3, \frac{n-1}{2}, 2, 1\right)$ and graphs in $\mathcal{H}_{11}$ are the unique graphs with the sixth largest Szeged index, which is equal to $\frac{1}{4}(n^3-3n^2+11n-9)$,*

(b) *for $n \geq 13$, C_n, $P\left(n-3, \frac{n-1}{2}, 2, 1\right)$ and $P\left(n-3, 1, 3, 0\right)$ are respectively the unique graphs with the second, the third and the fourth largest Szeged indices, which are equal to $\frac{1}{4}(n^3-2n^2+n)$, $\frac{1}{4}(n^3-3n^2+15n-21)$ and $\frac{1}{4}(n^3-3n^2+15n-29)$ respectively, $P\left(n-3, \frac{n-1}{2}-(l-4), 2, 1\right)$ for $l = 5, \ldots, \lceil \frac{n+9}{4} \rceil$ is the unique graph with the lth largest Szeged index, which is equal to $\frac{1}{4}(n^3-3n^2+15n-21)-4(l-4)$, for $l = \frac{n+13}{4}$ with $n \equiv 3 \pmod 4$, $P\left(n-3, \frac{n-1}{2}-(l-4), 2, 1\right)$, $S\left(n-3, \frac{n-1}{2}, 2, 1\right)$ and graphs in $\mathcal{H}_n$ are the unique graphs with the lth largest Szeged index, which is equal to $\frac{1}{4}(n^3 -$*

$3n^2+11n-9)$, and for $l=\frac{n+15}{4}$ with $n\equiv 1\,(\mathrm{mod}\,4)$, $S\left(n-3,\frac{n-1}{2},2,1\right)$ and graphs in $\mathcal{H}_n$ are the unique graphs with the lth largest Szeged index, which is equal to $\frac{1}{4}(n^3-3n^2+11n-9)$.

Proof. Let $f_1(r)=Sz(P_{n,r})$ if n and r are even, $f_2(r)=Sz(P_{n,r})$ if n is odd and r is even, $f_3(r)=Sz(P_{n,r})$ if r is odd. For fixed n, taking the derivatives for $f_i(r)$ where $i=1,2,3$ whose expressions are given in Proposition 4, we get

$$f_1'(r)=f_2'(r)=\frac{r^2}{4}-\frac{r}{2}+\frac{1}{6}>0,$$
$$f_3'(r)=\frac{r^2}{4}-\frac{n}{2}-\frac{1}{12},$$

and $f_3'(r)>0$ if and only if $r>\sqrt{2n+\frac{1}{3}}$. Hence $f_1(r)$ and $f_2(r)$ are increasing for r, $f_3(r)$ is decreasing for $r<\sqrt{2n+\frac{1}{3}}$ and increasing for $r>\sqrt{2n+\frac{1}{3}}$, where $3\le r\le n$. Let $G\in\mathcal{U}_n$.

Case 1. n is even. Note that $3<\sqrt{2n+\frac{1}{3}}<n-3$ for $n\ge 8$. If the cycle length of G is at most $n-3$, then by Proposition 4,

$$Sz(G)\le Sz(P_{n,r})=f_3(3)=\frac{n^3-7n+12}{6}=31<42=\frac{n^3-2n^2+4n}{4}$$

for $n=6$, and

$$\begin{aligned}
Sz(G) &\le Sz(P_{n,r})\le \max\{f_1(n-4),f_3(n-3),f_3(3)\}\\
&= \max\left\{\frac{n^3-4n^2+24n-40}{4},\frac{n^3-5n^2+16n-8}{4},\frac{n^3-7n+12}{6}\right\}\\
&< \frac{n^3-2n^2+4n}{4}
\end{aligned}$$

for $n\ge 8$. Suppose that the cycle length of G is at least $n-2$. Then $G=C_n$ and $Sz(G)=\frac{n^3}{4}$, or $G=P_{n,n-1}$ and $Sz(G)=\frac{1}{4}(n^3-3n^2+4n)<\frac{1}{4}(n^3-2n^2+4n)$, or the cycle length of G is $n-2$, then by Propositions 2 and 4,

$$\begin{aligned}
&Sz\left(P(n-2,1,1,1)\right)=\frac{n^3-2n^2+4n}{4}\\
\le\ &Sz(G)\\
\le\ &Sz\left(P\left(n-2,\frac{n}{2},1,1\right)\right)=\frac{n^3-2n^2+8n-8}{4}
\end{aligned}$$

and from the arguments of Proposition 4, we have

$$Sz\left(P(n-2,l+1,1,1)\right)-Sz\left(P(n-2,l,1,1)\right)=2$$

for $l = 2, 3, \ldots, \frac{n-2}{2}$. Note that if the cycle length of G is $n-2$, then either $G = P(n-2, l, 1, 1)$ for $l = 1, 2, \ldots, \frac{n}{2}$ or $G = P(n-2, 1, 2, 0)$ and $Sz\left(P(n-2, 1, 2, 0)\right) = \frac{1}{4}(n^3 - 2n^2 + 8n - 12)$. Now the result in (i) follows easily.

Case 2. n is odd. If the cycle length of G is at most $n-4$, then by Proposition 4,

$$Sz(G) \le Sz(P_{n,r}) = f_3(3) = \frac{n^3 - 7n + 12}{6} = 51 < 66 = \frac{n^3 - 3n^2 + 11n - 9}{4}$$

for $n = 7$, and

$$\begin{aligned} Sz(G) &\le Sz(P_{n,r}) \le \max\{f_3(n-4), f_3(3), f_2(n-5)\} \\ &= \max\left\{\frac{n^3 - 6n^2 + 25n - 20}{4}, \frac{n^3 - 7n + 12}{6}, \frac{n^3 - 5n^2 + 35n - 71}{4}\right\} \\ &< \frac{n^3 - 3n^2 + 11n - 9}{4} \end{aligned}$$

for $n \ge 9$. If the cycle length of G is $n-2$, then by Proposition 4,

$$Sz(G) \le Sz\left(P(n-2, 1, 2, 0)\right) = \frac{n^3 - 4n^2 + 9n - 2}{4} < \frac{n^3 - 3n^2 + 11n - 9}{4}.$$

If the cycle length of G is n or $n-1$, then $G = C_n$ and $Sz(G) = \frac{1}{4}(n^3 - 2n^2 + n)$, or $G = P_{n,n-1}$ and $Sz(G) = \frac{1}{4}(n^3 - n^2 + 3n - 3)$. Suppose that the cycle length of G is $n-3$, then by Propositions 2 and 4,

$$\begin{aligned} Sz\left(S_{n,n-3}\right) &= \frac{n^3 - 3n^2 + 3n + 15}{4} \\ &\le Sz(G) \\ &\le Sz\left(P\left(n-3, \frac{n-1}{2}, 2, 1\right)\right) = \frac{n^3 - 3n^2 + 15n - 21}{4}. \end{aligned}$$

It follows that in $\mathcal{U}_n$, $P_{n,n-1}$ is the unique graph with the largest Szeged index, which is equal to $\frac{1}{4}(n^3 - n^2 + 3n - 3)$.

To prove (ii), we need to consider the case when the cycle length of G is $n-3$ in more detail. In this case, G may be of five types:

(1) $G = P(n-3, l, 2, 1)$ for some $l = 1, 2, \ldots, \frac{n-1}{2}$, and from the arguments of Proposition 4,

$$Sz\left(P\left(n-3, l+1, 2, 1\right)\right) - Sz\left(P\left(n-3, l, 2, 1\right)\right) = 4 \text{ for } l = 2, 3, \ldots, \frac{n-3}{2}.$$

(2) $G = S(n-3, l, 2, 1)$ for some $l = 1, 2, \ldots, \frac{n-1}{2}$, and from the arguments of Proposition 2 with $N_l - N_1 = l - 1$ for $l > 1$,

$$Sz(G) = Sz\left(S_{n,n-3}\right) + 4(l-1)$$

$$\leq \frac{n^3-3n^2+3n+15}{4}+4\cdot\frac{n-3}{2}=\frac{n^3-3n^2+11n-9}{4}$$

with equality if and only if $l=\frac{n-1}{2}$.

(3) $G=P(n-3,1,3,0)$, for which

$$Sz(G)=1\cdot(n-1)+2\cdot(n-2)+3\cdot(n-3)+\frac{n-3}{2}\cdot\frac{n+3}{2}\cdot(n-3)=\frac{n^3-3n^2+15n-29}{4}.$$

(4) G is formed by attaching a star S_3 at its center to a cycle of length $n-3$, for which

$$\begin{aligned} Sz(G) &= 1\cdot(n-1)\cdot 2+3\cdot(n-3)+\frac{n-3}{2}\cdot\frac{n+3}{2}\cdot(n-3) \\ &= \frac{n^3-3n^2+11n-17}{4}<\frac{n^3-3n^2+11n-9}{4}. \end{aligned}$$

(5) G is formed by attaching three pendent vertices, each to a vertex of the cycle of length $n-3$, say $G=C_{n-3}(T_1,T_2,\ldots,T_{n-3})$, where $t_1=t_j=t_s=2$, $t_i=1$ for $i\neq 1,j,s$, and $1<j<s$, and by Lemma 7,

$$Sz(G)\leq\frac{n^3-3n^2+11n-9}{4}$$

with equality if and only if G is isomorphic to a graph in $\mathcal{H}_n$.

It is easily seen that

$$\begin{aligned} &\frac{n^3-3n^2+11n-9}{4} \\ \leq\ &\frac{n^3-3n^2+15n-37}{4}=Sz\left(P\left(n-3,\frac{n-3}{2},2,1\right)\right) \\ <\ &\frac{n^3-3n^2+15n-29}{4}=Sz(P(n-3,1,3,0)) \\ <\ &\frac{n^3-3n^2+15n-21}{4}=Sz\left(P\left(n-3,\frac{n-1}{2},2,1\right)\right) \end{aligned}$$

with equality in the first inequality if and only if $n=7$.

First we consider the cases when $n=7,9,11$. Note that $Sz(C_n)=\frac{n^3-2n^2+n}{4}$ and that

$$\frac{n^3-2n^2+n}{4}<\frac{n^3-3n^2+11n-9}{4}=\frac{n^3-3n^2+15n-37}{4}\text{ if } n=7,$$

$$\frac{n^3-2n^2+n}{4}=\frac{n^3-3n^2+11n-9}{4}<\frac{n^3-3n^2+15n-37}{4}\text{ if } n=9,$$

$$\frac{n^3-3n^2+11n-9}{4}<\frac{n^3-3n^2+15n-37}{4}$$

$$< \frac{n^3-2n^2+n}{4} < \frac{n^3-3n^2+15n-29}{4} \text{ if } n=11.$$

If $n = 7, 9, 11$, then $P\left(n-3, \frac{n-1}{2}, 2, 1\right)$ and $P(n-3, 1, 3, 0)$ are respectively the unique graphs with the second and the third largest Szeged indices, which are equal to $\frac{1}{4}(n^3-3n^2+15n-21)$ and $\frac{1}{4}(n^3-3n^2+15n-29)$ respectively. If $n = 7$, then $P\left(n-3, \frac{n-3}{2}, 2, 1\right)$, $S\left(n-3, \frac{n-1}{2}, 2, 1\right)$ and graphs in $\mathcal{H}_7$ are the unique graphs with the fourth largest Szeged index, which is equal to $\frac{1}{4}(n^3-3n^2+11n-9)$. If $n = 9$, then $P\left(n-3, \frac{n-3}{2}, 2, 1\right)$ is the unique graph with the fourth largest Szeged index, which is equal to $\frac{1}{4}(n^3-3n^2+15n-37)$, while C_n, $S\left(n-3, \frac{n-1}{2}, 2, 1\right)$ and graphs in $\mathcal{H}_9$ are the unique graphs with the fifth largest Szeged index, which is equal to $\frac{1}{4}(n^3-3n^2+11n-9)$. If $n = 11$, then C_n and $P\left(n-3, \frac{n-3}{2}, 2, 1\right)$ are respectively the unique graphs with the fourth and the fifth largest Szeged indices, which are equal to $\frac{1}{4}(n^3-2n^2+n)$ and $\frac{1}{4}(n^3-3n^2+15n-37)$, respectively, while $P\left(n-3, \frac{n-5}{2}, 2, 1\right)$, $S\left(n-3, \frac{n-1}{2}, 2, 1\right)$ and graphs in $\mathcal{H}_{11}$ are the unique graphs with the sixth largest Szeged index, which is equal to $\frac{1}{4}(n^3-3n^2+11n-9)$.

Now suppose that $n \geq 13$. Note that

$$\frac{n^3-3n^2+15n-21}{4} < Sz(C_n) = \frac{n^3-2n^2+n}{4}$$

and that

$$\frac{n^3-3n^2+15n-21}{4} - 4(l-4) \geq \frac{n^3-3n^2+11n-9}{4} \Leftrightarrow l \leq \frac{n+13}{4}.$$

Thus, C_n, $P\left(n-3, \frac{n-1}{2}, 2, 1\right)$ and $P\left(n-3, 1, 3, 0\right)$ are respectively the unique graphs with the second, the third and the fourth largest Szeged indices, which are equal to $\frac{1}{4}(n^3-2n^2+n)$, $\frac{1}{4}(n^3-3n^2+15n-21)$ and $\frac{1}{4}(n^3-3n^2+15n-29)$ respectively. Moreover, if $\frac{n+13}{4}$ is an integer, then $P\left(n-3, \frac{n-1}{2}-l+4, 2, 1\right)$ is the unique graph with the lth largest Szeged index, which is equal to $\frac{1}{4}(n^3-3n^2+15n-21)-4(l-4)$ for $l = 5, \ldots, \frac{n+9}{4}$, and for $l = \frac{n+13}{4}$, $P\left(n-3, \frac{n-1}{2}-l+4, 2, 1\right)$, $S\left(n-3, \frac{n-1}{2}, 2, 1\right)$ and graphs in $\mathcal{H}_n$ are the unique graphs with the lth largest Szeged index, which is equal to $\frac{1}{4}(n^3-3n^2+11n-9)$, while if $\frac{n+13}{4}$ is not an integer, then $P\left(n-3, \frac{n-1}{2}-l+4, 2, 1\right)$ is the unique graph with the lth largest Szeged index, which is equal to $\frac{1}{4}(n^3-3n^2+15n-21)-4(l-4)$ for $l = 5, \ldots, \frac{n+11}{4}$, and for $l = \frac{n+15}{4}$, $S\left(n-3, \frac{n-1}{2}, 2, 1\right)$ and graphs in $\mathcal{H}_n$ are the unique graphs with the lth largest Szeged index, which is equal to $\frac{1}{4}(n^3-3n^2+11n-9)$. ■

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