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SZEGED INDEX OF A CLASS OF UNICYCLIC GRAPHS

XULI QI

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Abstract. The Szeged index is a modification of the Wiener index to cyclic molecules. 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 any $e = uv \in E(G)$, $n_1(e|G)$ is the number of vertices of G lying closer to vertex u than to vertex v, and $n_2(e|G)$ is the number of vertices of G lying closer to vertex v than to vertex u. In this paper, we determine the n-vertex unicyclic graphs whose vertices on the unique cycle have degree at least three with the first, the second and the third smallest as well as largest Szeged indices for $n \geq 6$, $n \geq 7$ and $n \geq 8$, respectively.

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1. INTRODUCTION

A topological index is a numerical quantity derived from the hydrogen-depleted graph of a molecule as a tool for compact and effective description of structural formula which allows one to study and predict the structure-property correlations of organic compounds. The Wiener index is one of the oldest topological indices, which was introduced by Wiener [17] in 1947 to study boiling points of paraffins. Since then, it has been used to explain various chemical and physical properties of molecules and to correlate the structure of molecules to their biological activity.

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. Let $d_G(x,y)$ be the distance between vertices x and y in G. Recall that the Wiener index of G is defined as $W(G) = \sum_{\{x,y\} \subseteq V(G)} d_G(x,y)$ [5,8].

If e is an edge of G connecting the vertices u and v, then we write $e = uv$ or $e = vu$.

Let $e = uv \in E(G)$. Let $n_1(e|G)$ be the number of vertices of G lying closer to vertex u than to vertex v, and $n_2(e|G)$ be the number of vertices of G lying closer to vertex v than to vertex u, i.e.,

$$n_1(e|G) = |\{x \in V(G) : d_G(x,u) < d_G(x,v)\}|$$

and

$$n_2(e|G) = |\{x \in V(G) : d_G(x,v) < d_G(x,u)\}|.$$

If T is a tree, then $W(T) = \sum\limits_{e \in E(T)} n_1(e|T)n_2(e|T)$, see [5, 8]. Motivated by this equality for Wiener index of trees, Gutman [7] put forward to the Szeged index. For a connected graph G, it is defined as [7]

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

The Szeged index found applications for modeling physicochemical properties as well as physiological activities of organic compounds acting as drugs or possessing pharmacological activity [11], and its mathematical properties may be found, e.g.,[1–4, 6, 9, 12–16, 19].

A unicyclic graph is a connected graph with a unique cycle. The n-vertex unicyclic graphs with the smallest and the largest Szeged indices have been determined [7, 16]. Zhou *et al.* [19] determined the n-vertex unicyclic graphs of cycle length r with the smallest and the largest Szeged indices for $3 \leq r \leq n$, 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 $n \geq 6$ is even, to four if $n = 7$, to five if $n = 9$, to $\frac{n+13}{4}$ if $n \equiv 3 \pmod 4$ with $n \geq 11$, and to $\frac{n+15}{4}$ if $n \equiv 1 \pmod 4$ with $n \geq 13$.

A unicyclic graph is fully loaded if vertices on its unique cycle all have degree at least three. In the present paper, in continuation of the study on the Szeged index, we determine the n-vertex fully loaded unicyclic graphs with the first, the second and the third smallest as well as largest Szeged indices for $n \geq 6$, $n \geq 7$ and $n \geq 8$, respectively.

2. Preliminaries

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

Lemma 1 ([5, 8])**.** *Let T be an n-vertex tree different from S_n and P_n. Then*

$$(n-1)^2 = W(S_n) < W(T) < W(P_n) = \frac{n^3 - n}{6}.$$

For a connected graph G with $u \in V(G)$, let $W_u(G) = \sum\limits_{v \in V(G)} d_G(u, v)$.

Lemma 2 ([18])**.** *Let T be an n-vertex tree with $u \in V(T)$, where u is not the center if $T = S_n$ and u is not a terminal vertex if $T = P_n$. Let x and y be the center of the star S_n and a terminal vertex of the path P_n, respectively. Then*

$$n - 1 = W_x(S_n) < W_u(T) < W_y(P_n) = \frac{n(n-1)}{2}.$$

Let S'_n be the graph formed by attaching a pendent vertex to one pendent vertex of S_{n-1} for $n \geq 4$. Let P'_n be the graph formed by attaching a pendent vertex to the neighbor of a terminal vertex of P_{n-1} for $n \geq 4$.

Lemma 3 ([10, 18]). *Among the n-vertex trees with $n \geq 4$, S'_n is the unique graph with the second smallest Wiener index, which is equal to $n^2 - n - 2$, and P'_n is the unique graph with the second largest Wiener index, which is equal to $\frac{1}{6}(n^3 - 7n + 18)$.*

The following lemma may be easily checked.

Lemma 4. *Let T be an n-vertex tree with $n \geq 5$, $u \in V(T)$, $T \neq S_n, P_n$, where u is not a vertex of maximal degree if $T = S'_n$, and not the terminal vertex whose neighbor has degree two if $T = P'_n$. Let x be the vertex of maximal degree of S'_n, and y be the terminal vertex whose neighbor has degree two in P'_n. Then $n = W_x(S'_n) < W_u(T) < W_y(P'_n) = \frac{(n+1)(n-2)}{2}$.*

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 labeled 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 share exactly one common vertex v_i for $i = 1, 2, \ldots, r$. Denote $|G| = |V(G)|$ for a graph G. 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 $\sum_{i=1}^{r} |T_i| = n$. For the graph $G = C_r(T_1, T_2, \ldots, T_r)$, let $d_{ij} = d_{C_r}(v_i, v_j)$ and $t_i = |T_i|$ for $i = 1, 2, \ldots, r$. Then let $N_s = \sum_{i \neq s} t_i d_{is}$.

For a subset M of $E(G)$, $G - M$ denotes the graph obtained from G by deleting the edges in M. For a subset M^* of the edge set of the complement of G, $G + M^*$ denotes the graph obtained from G by adding the edges in M^*.

Lemma 5 ([19]). *Let $G = C_r(T_1, T_2, \ldots, T_r)$ and T_i be a star with center v_i for $i = 1, 2, \ldots, r$. Suppose that trees T_k and T_l are nontrivial. Let $w \in V(T_l)$ with $w \neq v_l$. If r is odd and $N_k + \frac{1}{2}t_k \leq N_l + \frac{1}{2}t_l$, or r is even and $N_k \leq N_l$, then $Sz(G - \{v_l w\} + \{v_k w\}) < Sz(G)$.*

Let $\varepsilon_n = 1$ if n is odd and $\varepsilon_n = 0$ if n is even.

Lemma 6 ([9]). *Let $G = C_r(T_1, T_2, \ldots, T_r)$. Then*

$$Sz(G) = \sum_{i=1}^{r} W(T_i) + \sum_{i=1}^{r} (|G| - t_i) W_{v_i}(T_i) + \sum_{i=1}^{r} \sum_{j=1}^{r} t_i t_j d_{ij} - \varepsilon_r \sum_{i<j} t_i t_j.$$

For $3 \leq r \leq \lfloor \frac{n}{2} \rfloor$, let $\mathbb{U}_{n,r}$ be the set of all fully loaded unicyclic graphs with n vertices and unique cycle C_r. For $n \geq 6$, let $\mathbb{U}_n$ be the set of n-vertex fully loaded unicyclic graphs.

3. Fully loaded unicyclic graphs with small Szeged indices

For $3 \leq r \leq \lfloor \frac{n}{2} \rfloor$, let $S_{n,r} = C_r(T_1, T_2, \ldots, T_r)$ with $T_1 = \cdots = T_{r-1} = P_2$ and $T_r = S_{n-2(r-1)}$ with center v_r.

Proposition 1. *Let $G \in \mathbb{U}_{n,r}$ with $3 \leq r \leq \lfloor \frac{n}{2} \rfloor$. Then*

$$Sz(G) \geq \begin{cases} n^2+(r^2-3r)n-r^3+2r^2 & \text{if } r \text{ is odd} \\ n^2+(r^2-r-1)n-r^3+r & \text{if } r \text{ is even} \end{cases}$$

with equality if and only if $G = S_{n,r}$.

Proof. By the definition of the Szeged index, if r is odd, then

$$\begin{aligned} Sz(S_{n,r}) &= 1\cdot(n-1)\cdot(n-r)+(r-1)\cdot(r-1) \\ &\quad +(r-1)\cdot(n-r+1-2)\cdot(r-1) \\ &= n^2+(r^2-3r)n-r^3+2r^2, \end{aligned}$$

and if r is even, then

$$\begin{aligned} Sz(S_{n,r}) &= 1\cdot(n-1)\cdot(n-r)+r\cdot(n-r)\cdot r \\ &= n^2+(r^2-r-1)n-r^3+r. \end{aligned}$$

Let $G = C_r(T_1, T_2, \dots, T_r)$ be a graph with the smallest Szeged index among graphs in $\mathbb{U}_{n,r}$. We need only to show that $G = S_{n,r}$.

By Lemmas 1, 2 and 6, T_i is a star with center v_i for $i = 1, 2, \dots, r$. Suppose that $t_k, t_l \geq 3$ with $k \neq l$. Let $w \in V(T_l)$ with $w \neq v_l$. Suppose without loss of generality that $N_k + \frac{1}{2}t_k \leq N_l + \frac{1}{2}t_l$ if r is odd and that $N_k \leq N_l$ if r is even. By Lemma 5, $Sz(G - \{v_l w\} + \{v_k w\}) < Sz(G)$, a contradiction. Thus there can not be two trees of $T_1, T_2, \dots, T_r$ with at least three vertices in G, i.e., $G = S_{n,r}$. □

Let Γ_n be the set of graphs $C_3(T_1, T_2, T_3)$ in $\mathbb{U}_n$ with $|T_1| = |T_2| = 2$. Let Ψ_n be the set of graphs $C_3(T_1, T_2, T_3)$ in $\mathbb{U}_n$ with $|T_3| \geq |T_2| \geq \max\{|T_1|, 3\}$. Let Φ_n be the set of graphs in $\mathbb{U}_n$ with cycle length at least four. Then $\mathbb{U}_n = \Gamma_n \cup \Psi_n \cup \Phi_n$.

For $n \geq 7$, let B'_n be the graph in Γ_n formed by attaching a path P_2 and $n-7$ pendent vertices to the vertex of degree two in $C_3(P_2, P_2, P_1)$.

Lemma 7. *Among the graphs in Γ_n with $n \geq 7$, B'_n is the unique graph with the second smallest Szeged index, which is equal to n^2+n-12.*

Proof. The case $n = 7$ is trivial. Let $G = C_3(T_1, T_2, T_3) \in \Gamma_n$ with $n \geq 8$. Note that $|T_1| = |T_2| = 2$. By Lemma 6, we have

$$\begin{aligned} Sz(G) &= 1+1+W(T_3)+n-2+n-2+4W_{v_3}(T_3) \\ &\quad +2[2\cdot 2+2\cdot(n-4)+2\cdot(n-4)] \\ &\quad -[2\cdot 2+2\cdot(n-4)+2\cdot(n-4)] \\ &= 6n-14+W(T_3)+4W_{v_3}(T_3), \end{aligned}$$

which, together with Lemmas 3 and 4, implies that B'_n is the unique graph in Γ_n with the second smallest Szeged index, which is equal to n^2+n-12. □

Let $S_n(a,b,c) = C_3(T_1,T_2,T_3)$ with $|T_1| = a$, $|T_2| = b$, $|T_3| = c$, $a+b+c = n$, and $a,b,c \geq 2$, where T_1 (T_2, T_3, respectively) is a star with center v_1 (v_2, v_3, respectively). Let G'_n for $n \geq 8$ be the graph obtained from $S_{n-1}(2,3,n-6)$ by attaching a pendent vertex to a pendent vertex at v_3, and G''_n for $n \geq 9$ the graph obtained from $S_{n-1}(2,2,n-5)$ by attaching a pendent vertex to the pendent vertex at v_2.

Lemma 8. *Among the graphs in Ψ_n, $S_n(2,3,n-5)$ for $n \geq 8$ is the unique graph with the smallest Szeged index, which is equal to n^2+n-16; 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 Szeged index, which is equal to 61 for $n = 8$, 75 for $n = 9$, and $n^2+2n-25$ for $n \geq 10$.*

Proof. For $n \geq 8$, let $G = C_3(T_1,T_2,T_3) \in \Psi_n$ with $c \geq b \geq \max\{a,3\}$, where $|T_1| = a$, $|T_2| = b$, $|T_3| = c$ and $a+b+c = n$.

If in G, $T_1 = P_2$ and $T_2 = S_3$ with v_2 its center, then by Lemma 6, $Sz(G) = 8n - 22 + W(T_3) + 5W_{v_3}(T_3)$, which, together with Lemmas 1–4, implies that, among the graphs $C_3(T_1,T_2,T_3) \in \Psi_n$ with $T_1 = P_2$ and $T_2 = S_3$ with v_2 its center, $S_n(2,3,n-5)$ and G'_n are the unique graphs with the smallest Szeged index n^2+n-16 and the second smallest Szeged index $n^2+2n-19$, respectively.

For $n = 8$, the graphs in Ψ_8 are $S_8(2,3,3)$, G'_8 and $C_3(P_2,P_3,P_3)$ with v_2 being a terminal vertex of one P_3 and v_3 a terminal vertex of the other P_3, where $Sz(S_8(2,3,3)) = 56 < Sz(G'_8) = 61 < Sz(C_3(P_2,P_3,P_3)) = 66$. Thus $S_8(2,3,3)$ and G'_8 are the unique graphs in Ψ_8 respectively with the smallest and the second smallest Szeged indices, which are equal to 56 and 61, respectively.

For $n = 9$, by Lemmas 1, 2 and 6, the graphs in Ψ_9 with the smallest Szeged index are just the graphs $S_9(2,3,4)$ and $S_9(3,3,3)$ with smaller Szeged index, which is equal to $\min\{74,75\} = 74$. Thus $S_9(2,3,4)$ is the unique graph in Ψ_9 with the smallest Szeged index, which is equal to 74. By the proof at the beginning, the graphs in Ψ_9 with the second smallest Szeged index are just the graphs in G'_9, G''_9 and $S_9(3,3,3)$ with the smallest Szeged index, which is equal to $\min\{80,80,75\} = 75$. Thus $S_9(3,3,3)$ is the unique graph in Ψ_9 with the second smallest Szeged index, which is equal to 75.

For $n \geq 10$, suppose first that $G = S_n(a,b,c)$ and $G \neq S_n(2,3,n-5), S_n(2,4,n-6)$. Since $N_1 = \sum_{i\neq 1} t_i d_{i1} = b+c$, $N_2 = \sum_{i\neq 2} t_i d_{i2} = a+c$ and $N_3 = \sum_{i\neq 3} t_i d_{i3} = a+b$, it is easily seen that $N_3 + \frac{1}{2}c \leq N_2 + \frac{1}{2}b \leq N_1 + \frac{1}{2}a$. By Lemmas 5 and 6, if $a = 2$, then

$$\begin{aligned} Sz(S_n(2,b,c)) &> Sz(S_n(2,4,n-6)) = n^2+2n-25 \\ &> Sz(S_n(2,3,n-5)) = n^2+n-16, \end{aligned}$$

and if $a \geq 3$, then

$$Sz(S_n(a,b,c)) \geq Sz(S_n(3,3,n-6)) = n^2+2n-24 > n^2+2n-25.$$

If $G \neq S_n(a,b,c)$, then by the proof at the beginning and applying Lemmas 1, 2 and 6, we have either $Sz(G) \geq Sz(G_n') = Sz(G_n'') = n^2+2n-19 > n^2-2n-25$ for $a=2$, or $Sz(G) > Sz(S_n(a,b,c)) \geq Sz(S_n(3,3,n-6)) > n^2+2n-25$ for $a \geq 3$. Thus, for $n \geq 10$, $S_n(2,3,n-5)$ and $S_n(2,4,n-6)$ are the unique graphs with the smallest and the second smallest Szeged indices, which are equal to n^2+n-16 and $n^2+2n-25$, respectively. The result follows. □

Theorem 1. *Among the graphs in* $\mathbb{U}_n$,
(i) $S_{n,3}$ *for* $n \geq 6$ *is the unique graph with the smallest Szeged index, which is equal to* n^2-9;
(ii) B_7' *for* $n=7$, *and* $S_n(2,3,n-5)$ *for* $n \geq 8$ *are the unique graphs with the second smallest Szeged index, which is equal to* 44 *for* $n=7$, *and* n^2+n-16 *for* $n \geq 8$;
(iii) B_8' *for* $n=8$, $S_9(3,3,3)$ *for* $n=9$, $S_n(2,4,n-6)$ *for* $10 \leq n \leq 12$, $S_{13}(2,4,7)$ *and* B_{13}' *for* $n=13$, *and* B_n' *for* $n \geq 14$ *are the unique graphs with the third smallest Szeged index, which is equal to* 60 *for* $n=8$, 75 *for* $n=9$, $n^2+2n-25$ *for* $10 \leq n \leq 12$, 170 *for* $n=13$, *and* n^2+n-12 *for* $n \geq 14$.

Proof. By Proposition 1, if r is odd, then

$$\begin{aligned} Sz(S_{n,r+1}) - Sz(S_{n,r}) &= (4r-1)n - 5r^2 - 2r \\ &\geq (4r-1)\cdot 2(r+1) - 5r^2 - 2r \\ &= 3r^2+4r-2 > 0 \end{aligned}$$

for $3 \leq r \leq \lfloor \frac{n}{2} \rfloor - 1$, implying that $Sz(S_{n,r+1}) > Sz(S_{n,r})$, and

$$\begin{aligned} Sz(S_{n,r+2}) - Sz(S_{n,r}) &= (4r-2)n - 6r^2 - 4r \\ &\geq (4r-2)\cdot 2(r+2) - 6r^2 - 4r \\ &= 2r^2+8r-8 > 0 \end{aligned}$$

for $3 \leq r \leq \lfloor \frac{n}{2} \rfloor - 2$, implying that $Sz(S_{n,r+2}) > Sz(S_{n,r})$. If r is even, then

$$Sz(S_{n,r+1}) - Sz(S_{n,r}) = -n - r^2 + 1 < 0$$

for $4 \leq r \leq \lfloor \frac{n}{2} \rfloor - 1$, implying that $Sz(S_{n,r+1}) < Sz(S_{n,r})$, and

$$\begin{aligned} Sz(S_{n,r+2}) - Sz(S_{n,r}) &= (4r+2)n - 6r^2 - 12r - 6 \\ &\geq (4r+2)\cdot 2(r+2) - 6r^2 - 12r - 6 \\ &= 2r^2+8r+2 > 0 \end{aligned}$$

for $4 \leq r \leq \lfloor \frac{n}{2} \rfloor - 2$, implying that $Sz(S_{n,r+2}) > Sz(S_{n,r})$. It follows that $Sz(S_{n,r+1}) > Sz(S_{n,r})$ for odd r with $3 \leq r \leq \lfloor \frac{n}{2} \rfloor - 1$, $Sz(S_{n,r+1}) < Sz(S_{n,r})$ for even r with $4 \leq r \leq \lfloor \frac{n}{2} \rfloor - 1$, and $Sz(S_{n,r})$ is increasing with respect to odd

$r \in \{3,5,\dots,\lfloor \frac{n}{2} \rfloor\}$ and even $r \in \{4,6,\dots,\lfloor \frac{n}{2} \rfloor\}$. Then by Proposition 1, $S_{n,3}$ for $n \geq 6$ is the unique graph with the smallest Szeged index, which is equal to n^2-9, proving (i). Moreover, $S_{n,4}$ for $n=8,9$ and $S_{n,5}$ for $n \geq 10$ are the unique graphs in Φ_n with the smallest Szeged index, which are equal to $n^2+11n-60$ and $n^2+10n-75$, respectively.

Now we prove (ii). The case $n=7$ is trivial. For $n \geq 8$, the graphs in $\mathbb{U}_n$ with the second smallest Szeged index are just the graphs in $\mathbb{U}_n \setminus \{S_{n,3}\} = (\Gamma_n \setminus \{S_{n,3}\}) \cup \Psi_n \cup \Phi_n$ with the smallest Szeged index, which, by Lemmas 7 and 8, is equal to

$$\begin{aligned}&\min\{Sz(B_n'), Sz(S_n(2,3,n-5)), Sz(S_{n,4})\}\\ &= \min\{n^2+n-12, n^2+n-16, n^2+11n-60\} = n^2+n-16\end{aligned}$$

for $n=8,9$, and

$$\begin{aligned}&\min\{Sz(B_n'), Sz(S_n(2,3,n-5)), Sz(S_{n,5})\}\\ &= \min\{n^2+n-12, n^2+n-16, n^2+10n-75\} = n^2+n-16\end{aligned}$$

for $n \geq 10$. Then (ii) follows.

From (i) and (ii) and by Lemmas 7 and 8, we find that the graphs in $\mathbb{U}_n$ for $n \geq 8$ with the third smallest Szeged index are just the graphs in

$$\mathbb{U}_n \setminus \{S_{n,3}, S_n(2,3,n-5)\} = (\Gamma_n \setminus \{S_{n,3}\}) \cup (\Psi_n \setminus \{S_n(2,3,n-5)\} \cup \Phi_n$$

for $n \geq 8$, which is equal to

$$\min\{Sz(B_8'), Sz(G_8'), Sz(S_{8,4})\} = \min\{60, 61, 92\} = 60$$

for $n=8$,

$$\min\{Se(B_9'), Sz(S_9(3,3,3)), Sz(S_{9,4})\} = \min\{78, 75, 120\} = 75$$

for $n=9$, and

$$\begin{aligned}&\min\{Sz(B_n'), Sz(S_n(2,4,n-6)), Sz(S_{n,5})\}\\ &= \min\{n^2+n-12, n^2+2n-25, n^2+10n-75\}\end{aligned}$$

i.e., $n^2+2n-25$ for $10 \leq n \leq 12$, $n^2+2n-25 = n^2+n-12 = 170$ for $n=13$, and n^2+n-12 for $n \geq 14$. Now (iii) follows easily. $\square$

4. Fully loaded unicyclic graphs with large Szeged indices

For $3 \leq r \leq \lfloor \frac{n}{2} \rfloor$, let $P_{n,r} = C_r(T_1, T_2, \dots, T_r)$ with $T_1 = \cdots = T_{r-1} = P_2$ and $T_r = P_{n-2(r-1)}$ with a terminal vertex v_r.

Proposition 2. *Let $G \in \mathbb{U}_{n,r}$ with $3 \leq r \leq \lfloor \frac{n}{2} \rfloor$. Then*

$$Sz(G) \leq \begin{cases} \frac{1}{6}[n^3+(-6r^2+12r-7)n+10r^3-24r^2+14r] & \text{if } r \text{ is odd} \\ \frac{1}{6}[n^3+(-6r^2+24r-13)n+10r^3-36r^2+20r] & \text{if } r \text{ is even} \end{cases}$$

with equality if and only if $G = P_{n,r}$.

Proof. By the definition of the Szeged index, if r is odd, then

$$\begin{aligned} Sz(P_{n,r}) &= 1\cdot(n-1)\cdot r + 2\cdot(n-2)+\cdots+(n-2r+1)\cdot(2r-1)\\ &\quad +(r-1)\cdot(r-1)+(r-1)\cdot(n-r+1-2)\cdot(r-1)\\ &= \frac{1}{6}[n^3+(-6r^2+12r-7)n+10r^3-24r^2+14r], \end{aligned}$$

and if r is even, then

$$\begin{aligned} Sz(P_{n,r}) &= 1\cdot(n-1)\cdot r+2\cdot(n-2)+\cdots+(n-2r+1)\cdot(2r-1)+r\cdot(n-r)\cdot r\\ &= \frac{1}{6}[n^3+(-6r^2+24r-13)n+10r^3-36r^2+20r]. \end{aligned}$$

Let $G = C_r(T_1, T_2, \ldots, T_r)$ be a graph with the largest Szeged index among graphs in $\mathbb{U}_{n,r}$. We need only to show that $G = P_{n,r}$.

By Lemmas 1, 2 and 6, T_i is a path with a terminal vertex v_i for each $i = 1, 2, \ldots, r$. Then by Lemma 6, we have

$$\begin{aligned} Sz(G) &= \sum_{i=1}^{r}\frac{1}{6}(t_i^3-t_i)+\sum_{i=1}^{r}\frac{1}{2}(n-t_i)t_i(t_i-1)+\sum_{i=1}^{r}\sum_{j=1}^{r}t_it_jd_{ij}-\varepsilon_r\sum_{i<j}t_it_j\\ &= -\frac{1}{3}\sum_{i=1}^{r}t_i^3+\frac{1}{2}(n+1)\sum_{i=1}^{r}t_i^2-\frac{1}{2}n^2-\frac{1}{6}n+\sum_{i=1}^{r}\sum_{j=1}^{r}t_it_jd_{ij}-\varepsilon_r\sum_{i<j}t_it_j. \end{aligned}$$

Suppose that there exist distinct k, l, m with $1 \le k, l, m \le r$, such that $t_k, t_l, t_m \ge 3$ and $t_m \ge \max\{t_k, t_l\}$.

Case 1. 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, $G' \in \mathbb{U}_{n,r}$. Note that $2t_l + 2d_{kl} < t_l + t_m + r \le n < n+2$. Then

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

and thus $Sz(G) < Sz(G')$, which is a contradiction. Thus $r-2$ of $t_1, t_2, \ldots, t_r$ are equal to 2, say $t_i = 2$ for $i \ne k, l$. Let $t_k = a$ and $t_l = b$. We write $G = G_{a,b}$, where $a, b \ge 2$ and $a + b = n - 2(r-2)$. Note that $N_k = 2W_{v_k}(C_r) + (b-2)d_{kl}$ and $N_l = 2W_{v_l}(C_r) + (a-2)d_{kl}$. If $a \ge b \ge 3$, then since that $a+b+2d_{kl} < a+b+r \le n+1$ and $2b + 2d_{kl} < a+b+r < n+2$, we have

$$\begin{aligned} &Sz(G_{a,b})-Sz(G_{a+1,b-1})\\ &= [a^2+(n+1)b+4W_{v_l}(C_r)+2(a-2)d_{kl}]\\ &-[b^2+(n+1)a+4W_{v_k}(C_r)+2(b-2)d_{kl}]+2b+2d_{kl}-(n+2) \end{aligned}$$

$$= (a-b)[a+b+2d_{kl}-(n+1)]+2b+2d_{kl}-(n+2) < 0,$$

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

Case 2. 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, $G' \in \mathbb{U}_{n,r}$. Note that $2t_l+2d_{kl} \leq t_l+t_m+r \leq n < n+1$. Then

$$Sz(G)-Sz(G') = (t_k^2+nt_l+2N_l)-(t_l^2+nt_k+2N_k)+2t_l+2d_{kl}-(n+1) < 0,$$

and thus $Sz(G) < Sz(G')$, which is a contradiction. Thus $r-2$ of $t_1, t_2, \ldots, t_r$ are equal to 2, say $t_i = 2$ for $i \neq k, l$. Let $t_k = a$ and $t_l = b$. We write $G = G_{a,b}$, where $a, b \geq 2$ and $a+b = n-2(r-2)$. Note that $N_k = 2W_{v_k}(C_r)+(b-2)d_{kl}$ and $N_l = 2W_{v_l}(C_r)+(a-2)d_{kl}$. If $a \geq b \geq 3$, then since that $a+b+2d_{kl} \leq a+b+r \leq n$ and $2b+2d_{kl} \leq a+b+r < n+1$, we have

$$\begin{aligned}
Sz(G_{a,b})-Sz(G_{a+1,b-1}) &= [a^2+nb+4W_{v_l}(C_r)+2(a-2)d_{kl}]\\
&\quad -[b^2+na+4W_{v_k}(C_r)+2(b-2)d_{kl}]+2b+2d_{kl}-(n+1)\\
&= (a-b)(a+b+2d_{kl}-n)+2b+2d_{kl}-(n+1) < 0,
\end{aligned}$$

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

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

Let $P_n(a,b,c,d) = C_4(T_1,T_2,T_3,T_4)$ with $|T_1| = a$, $|T_2| = b$, $|T_3| = c$, $|T_4| = d$, $a+b+c+d = n$, and $a,b,c,d \geq 2$, where T_1 (T_2, T_3, T_4, respectively) is a path with a terminal vertex v_1 (v_2, v_3, v_4, respectively). Let $P'_{n,4}$ be the graph formed by attaching a pendent vertex to the neighbor of the pendent vertex of T_4 in $P_{n-1,4}$.

Lemma 9. *Among the graphs in $\mathbb{U}_{n,4}$ with $n \geq 9$, $S_{9,4}$ for $n = 9$ and $P_n(2,3,2,n-7)$ for $n \geq 10$ are the unique graphs with the second largest Szeged index, which is equal to 120 for $n = 9$, and $\frac{1}{6}(n^3-19n+198)$ for $n \geq 10$; $P_n(2,2,3,n-7)$ for $n = 10, 11$, $P_n(2,4,2,n-8)$ for $12 \leq n \leq 16$, $P_{17}(2,4,2,9) = P'_{17,4}$ for $n = 17$, and $P'_{n,4}$ for $n \geq 18$ are the unique graphs with the third largest Szeged index, which is equal to $\frac{1}{6}(n^3-31n+306)$ for $n = 10, 11$, $\frac{1}{6}(n^3-25n+264)$ for $12 \leq n \leq 16$, 792 for $n = 17$ and $\frac{1}{6}(n^3-19n+162)$ for $n \geq 18$.*

Proof. The case $n = 9$ is trivial. Let $G = C_4(T_1,T_2,T_3,T_4) \in \mathbb{U}_{n,4}$ with $n \geq 10$.

Suppose first that there is exactly one tree, say T_4 with more than two vertices. Note that $t_1 = t_2 = t_3 = 2$. By Lemma 6, we have $Sz(G) = 19n-67+W(T_4)+6W_{v_4}(T_4)$. In this case, by Lemmas 3 and 4, we know that $P'_{n,4}$ is the unique graph with the second largest Szeged index, which is equal to $\frac{1}{6}(n^3-19n+162)$.

Suppose that there are two trees (T_3 and T_4, or T_2 and T_4) with more than two vertices. By the proof of Proposition 2, we have

$$Sz(G) \le Sz(P_n(2,2,t_3,t_4)) \le Sz(P_n(2,2,3,n-7)) = \frac{1}{6}(n^3-31n+306)$$

or

$$Sz(G) \le Sz(P_n(2,t_2,2,t_4)) \le Sz(P_n(2,3,2,n-7)) = \frac{1}{6}(n^3-19n+198).$$

If there are three or four trees with more than two vertices, then by the proof of Proposition 2, we have

$$Sz(G) \le Sz(P_n(t_1,t_2,t_3,t_4)) \le \max\{Sz(P_n(2,2,3,n-7)), Sz(P_n(2,3,2,n-7))\}.$$

It follows that the graphs in $\mathbb{U}_{n,4}$ with the second largest Szeged index are just the graphs in $\mathbb{U}_{n,4} \setminus \{P_{n,4}\}$ with the largest Szeged index, which is equal to

$$\begin{aligned}
&\max\{Sz(P'_{n,4}), Sz(P_n(2,2,3,n-7)), Sz(P_n(2,3,2,n-7))\}\\
&= \max\left\{\frac{1}{6}(n^3-19n+162), \frac{1}{6}(n^3-31n+306), \frac{1}{6}(n^3-19n+198)\right\}\\
&= \frac{1}{6}(n^3-19n+198).
\end{aligned}$$

Thus $P_n(2,3,2,n-7)$ is the unique graph in $\mathbb{U}_{n,4}$ for $n \ge 10$ with the second largest Szeged index, which is equal to $\frac{1}{6}(n^3-19n+198)$.

Suppose that T_2 and T_4 have more than two vertices. If $t_2 = 3$ and $G \ne P_n(2,3,2,n-7)$, then

$$\begin{aligned}
Sz(G) &\le \max\{Sz(C_4(P_2,S_3,P_2,P_{n-7})), Sz(C_4(P_2,P_3,P_2,P'_{n-7}))\}\\
&= \max\left\{\frac{1}{6}(n^3-25n+216), \frac{1}{6}(n^3-25n+216)\right\}\\
&= \frac{1}{6}(n^3-25n+216),
\end{aligned}$$

where v_2 is the center of S_3 and v_4 is a terminal vertex of P_{n-7} in $C_4(P_2,S_3,P_2,P_{n-7})$, and v_2 is a terminal vertex of P_3 and v_4 is a terminal vertex of P'_{n-7} for $n = 11$ and a terminal vertex of P'_{n-7} whose neighbor has degree two for $n \ge 12$ in $C_4(P_2,P_3,P_2,P'_{n-7})$. And if $t_2 \ge 4$, then we have

$$Sz(G) \le Sz(P_n(2,t_2,2,t_4)) \le Sz(P_n(2,4,2,n-8)) = \frac{1}{6}(n^3-25n+264).$$

Thus the graphs in $\mathbb{U}_{n,4}$ with the third largest Szeged index are just the graphs in $\mathbb{U}_{n,4} \setminus \{P_{n,4}, P_n(2,3,2,n-7)\}$ with the largest Szeged index, which is equal to

$$\max\{Sz(P'_{n,4}), Sz(P_n(2,2,3,n-7)), Sz(C_4(P_2,S_3,P_2,P_{n-7})),$$
$$Sz(C_4(P_2,P_3,P_2,P'_{n-7})), Sz(P_n(2,4,2,n-8))\}$$

$$= \max\left\{\frac{1}{6}(n^3-19n+162), \frac{1}{6}(n^3-31n+306), \frac{1}{6}(n^3-25n+216), \frac{1}{6}(n^3-25n+264)\right\}$$

i.e., $\frac{1}{6}(n^3-31n+306)$ for $n = 10, 11$, $\frac{1}{6}(n^3-25n+264)$ for $12 \le n \le 16$, $\frac{1}{6}(n^3-25n+264) = \frac{1}{6}(n^3-19n+162) = 792$ for $n = 17$, and $\frac{1}{6}(n^3-19n+162)$ for $n \ge 18$. Thus $P_n(2,2,3,n-7)$ for $n = 10, 11$, $P_n(2,4,2,n-8)$ for $12 \le n \le 16$, $P_{17}(2,4,2,9) = P'_{17,4}$ for $n = 17$, and $P'_{n,4}$ for $n \ge 18$ are the unique graphs with the third largest Szeged index, which is equal to $\frac{1}{6}(n^3-31n+306)$ for $n = 10, 11$, $\frac{1}{6}(n^3-25n+264)$ for $12 \le n \le 16$, 792 for $n = 17$ and $\frac{1}{6}(n^3-19n+162)$ for $n \ge 18$. The result follows. □

Theorem 2. *Among the graphs in* $\mathbb{U}_n$,
(i) $P_{n,3}$ *for* $n = 6, 7$ *and* $P_{n,4}$ *for* $n \ge 8$ *are the unique graphs with the largest Szeged index, which is equal to* $\frac{1}{6}(n^3-25n+96)$ *for* $n = 6, 7$, *and* $\frac{1}{6}(n^3-13n+144)$ *for* $n \ge 8$;
(ii) $S_{7,3}$ *for* $n = 7$, $P_{8,3}$ *for* $n = 8$, $S_{9,4}$ *for* $n = 9$, *and* $P_n(2,3,2,n-7)$ *for* $n \ge 10$ *are the unique graphs with the second largest Szeged index, which is equal to* 40 *for* $n = 7$, 68 *for* $n = 8$, 120 *for* $n = 9$, *and* $\frac{1}{6}(n^3-19n+198)$ *for* $n \ge 10$;
(iii) $C_3(P_2, P_3, P_3)$ *with* v_2 *a terminal vertex of* P_3 *and* v_3 *a terminal vertex of* P_3 *for* $n = 8$, $P_{9,3}$ *for* $n = 9$, $P_n(2,2,3,n-7)$ *for* $n = 10, 11$, $P_n(2,4,2,n-8)$ *for* $12 \le n \le 16$, $P_{17}(2,4,2,9) = P'_{17,4}$ *for* $n = 17$, *and* $P'_{n,4}$ *for* $n \ge 18$ *are the unique graphs with the third largest Szeged index, which is equal to* 66 *for* $n = 8$, 100 *for* $n = 9$, $\frac{1}{6}(n^3-31n+306)$ *for* $n = 10, 11$, $\frac{1}{6}(n^3-25n+264)$ *for* $12 \le n \le 16$, 792 *for* $n = 17$, *and* $\frac{1}{6}(n^3-19n+162)$ *for* $n \ge 18$.

Proof. The cases $n = 6, 7$ are obvious. Suppose that $n \ge 8$. Let $f_1(r) = Sz(P_{n,r})$ if r is odd, and $f_2(r) = Sz(P_{n,r})$ if r is even. If r is odd with $3 \le r \le \lfloor \frac{n}{2} \rfloor - 1$, then by Proposition 2,

$$\begin{aligned} f_2(r+1) - f_1(r) &= 2n + 3r^2 - 6r - 1 \ge 2 \cdot 2(r+1) + 3r^2 - 6r - 1 \\ &= 3r^2 - 2r + 3 > 0, \end{aligned}$$

implying that $f_2(r+1) > f_1(r)$. If r is even with $4 \le r \le \lfloor \frac{n}{2} \rfloor - 1$, then by Proposition 2,

$$\begin{aligned} f_1(r+1) - f_2(r) &= (-4r+2)n + 7r^2 - 4r \\ &\le (-4r+2) \cdot 2(r+1) + 7r^2 - 4r \\ &= -r^2 - 8r + 4 < 0, \end{aligned}$$

implying that $f_1(r+1) < f_2(r)$.

For fixed n, taking the derivatives for $f_i(r)$ where $i = 1, 2$, whose expressions are given in Proposition 2, we have

$$f_1'(r) = \frac{1}{3}[15r^2 - (6n+24)r + 6n + 7],$$

$$f_2'(r) = \frac{1}{3}[15r^2 - (6n+36)r + 12n + 10].$$

The two roots of $f_1'(r) = 0$ are r_1 and r_2, where

$$r_1 = \frac{3n+12-\sqrt{9(n-1)^2+30}}{15} < \frac{3n+12-3(n-1)}{15} = 1 < 3,$$

$$r_2 = \frac{3n+12+\sqrt{9(n-1)^2+30}}{15} > \frac{3n+12+3(n-1))}{15} = \frac{2}{5}n + \frac{3}{5} > 3,$$

and $r_2 < \lfloor \frac{n}{2} \rfloor$. Hence, for fixed $n \geq 8$, $f_1'(r) < 0$ for $3 \leq r < r_2$ and $f_1'(r) \geq 0$ for $r_2 \leq r \leq \lfloor \frac{n}{2} \rfloor$. Then, for fixed $n \geq 8$, $f_1(r)$ is decreasing for $3 \leq r < r_2$ and increasing for $r_2 \leq r \leq \lfloor \frac{n}{2} \rfloor$. The two roots of $f_2'(r) = 0$ are r_3 and r_4, where

$$r_3 = \frac{3n+18-\sqrt{9(n-4)^2+30}}{15} < \frac{3n+18-3(n-4)}{15} = 2 < 4,$$

$$r_4 = \frac{3n+18+\sqrt{9(n-4)^2+30}}{15} > \frac{3n+18+3(n-4)}{15} = \frac{2}{5}n + \frac{2}{5} \geq 4$$

for $n \geq 9$, and $r_4 < \lfloor \frac{n}{2} \rfloor$ for $n \geq 8$. Hence, for fixed $n \geq 9$, $f_2'(r) < 0$ for $4 \leq r < r_4$ and $f_2'(r) \geq 0$ for $r_4 \leq r \leq \lfloor \frac{n}{2} \rfloor$. Then, for fixed $n \geq 9$, $f_2(r)$ is decreasing for $4 \leq r < r_4$ and increasing for $r_4 \leq r \leq \lfloor \frac{n}{2} \rfloor$. Note that $\frac{2}{5}n < r_4 < r_2 < \frac{2}{5}n + 1$ for $n \geq 8$. Let $G \in \mathbb{U}_n$.

By Proposition 2 and the properties of $f_1(r)$ and $f_2(r)$, we have

$$\begin{aligned} Sz(G) \leq Sz(P_{n,r}) &\leq \max\left\{f_2(4), f_2\left(\frac{n}{2}\right)\right\} \\ &= \max\left\{\frac{1}{6}(n^3 - 13n + 144), \frac{1}{8}(n^3 + 4n^2 - 4n)\right\} \\ &= \frac{1}{6}(n^3 - 13n + 144) \end{aligned}$$

if $n \geq 8$ and $n \equiv 0 \pmod 4$,

$$\begin{aligned} Sz(G) \leq Sz(P_{n,r}) &\leq \max\left\{f_2(4), f_2\left(\frac{n-1}{2}\right)\right\} \\ &= \max\left\{\frac{1}{6}(n^3 - 13n + 144), \frac{1}{8}(n^3 + 3n^2 + 7n - 27)\right\} \\ &= \frac{1}{6}(n^3 - 13n + 144) \end{aligned}$$

if $n \geq 9$ and $n \equiv 1 \pmod 4$,

$$\begin{aligned} Sz(G) \leq Sz(P_{n,r}) &\leq \max\left\{f_2(4), f_2\left(\frac{n-2}{2}\right)\right\} \\ &= \max\left\{\frac{1}{6}(n^3 - 13n + 144), \frac{1}{8}(n^3 + 2n^2 + 24n - 88)\right\} \end{aligned}$$

$$= \frac{1}{6}(n^3 - 13n + 144)$$

if $n \geq 10$ and $n \equiv 2 \pmod 4$, and

$$Sz(G) \leq Sz(P_{n,r}) \leq \max\left\{ f_2(4), f_2\left(\frac{n-3}{2}\right)\right\}$$
$$= \max\left\{ \frac{1}{6}(n^3 - 13n + 144), \frac{1}{8}(n^3 + n^2 + 47n - 193)\right\}$$
$$= \frac{1}{6}(n^3 - 13n + 144)$$

if $n \geq 11$ and $n \equiv 3 \pmod 4$. Thus $P_{n,4}$ is the unique graph in $\mathbb{U}_n$ with the largest Szeged index, and then the graphs in $\mathbb{U}_n$ with the second largest Szeged index are just the graphs in $\mathbb{U}_n \setminus \{P_{n,4}\}$ with the largest Szeged index.

Case 1. $n \geq 8$ and $n \equiv 0 \pmod 4$. The largest Szeged index of graphs in $\mathbb{U}_n \setminus \{P_{n,4}\}$ is equal to $f_1(3) = 68$ for $n = 8$ and

$$\max\left\{Sz(P_n(2,3,2,n-7)), f_1(3), f_2(6), f_2\left(\frac{n}{2}\right)\right\}$$
$$= \max\left\{ \frac{1}{6}(n^3 - 19n + 198), \frac{1}{6}(n^3 - 25n + 96), \frac{1}{6}(n^3 - 85n + 984), \frac{1}{8}(n^3 + 4n^2 - 4n)\right\}$$
$$= \frac{1}{6}(n^3 - 19n + 198)$$

for $n \geq 12$. Thus $P_{8,3}$ for $n = 8$ and $P_n(2,3,2,n-7)$ for $n \geq 12$ are the unique graphs in $\mathbb{U}_n$ with the second largest Szeged index. It follows that the graphs in $\mathbb{U}_n$ with the third largest Szeged index are just the graphs in $\mathbb{U}_8 \setminus \{P_{8,4}, P_{8,3}\}$ for $n = 8$ and $\mathbb{U}_n \setminus \{P_{n,4}, P_n(2,3,2,n-7)\}$ for $n \geq 12$ with the largest Szeged index, which is equal to $Sz(C_3(P_2, P_3, P_3)) = 66$ for $n = 8$, where one P_3 has a terminal vertex v_2 and the other P_3 has a terminal vertex v_3 in $C_3(P_2, P_3, P_3)$,

$$\max\left\{Sz(P_n(2,4,2,n-8)), f_1(3), f_2(6), f_2\left(\frac{n}{2}\right)\right\}$$
$$= \max\left\{ \frac{1}{6}(n^3 - 25n + 264), \frac{1}{6}(n^3 - 25n + 96), \frac{1}{6}(n^3 - 85n + 984), \frac{1}{8}(n^3 + 4n^2 - 4n)\right\}$$
$$= \frac{1}{6}(n^3 - 25n + 264)$$

for $n = 12, 16$, and

$$\max\left\{Sz(P'_{n,4}), f_1(3), f_2(6), f_2\left(\frac{n}{2}\right)\right\}$$
$$= \max\left\{ \frac{1}{6}(n^3 - 19n + 162), \frac{1}{6}(n^3 - 25n + 96), \frac{1}{6}(n^3 - 85n + 984), \frac{1}{8}(n^3 + 3n^2 + 7n - 27)\right\}$$
$$= \frac{1}{6}(n^3 - 19n + 162)$$

for $n \geq 20$. Thus $C_3(P_2, P_3, P_3)$ with v_2 being a terminal vertex of P_3 and v_3 being a terminal vertex of P_3 for $n = 8$, $P_n(2,4,2,n-8)$ for $n = 12, 16$, and $P'_{n,4}$ for $n \geq 20$ are the unique graphs in $\mathbb{U}_n$ with the third largest Szeged index.

Case 2. $n \geq 9$ and $n \equiv 1 \pmod 4$. The largest Szeged index of graphs in $\mathbb{U}_n \setminus \{P_{n,4}\}$ is equal to $\max\{Sz(S_{9,4}), f_1(3)\} = \max\{120, 100\} = 120$ for $n = 9$ and

$$\max\left\{Sz(P_n(2,3,2,n-7)), f_1(3), f_2(6), f_2\left(\frac{n-1}{2}\right)\right\}$$
$$= \max\left\{\frac{1}{6}(n^3 - 19n + 198), \frac{1}{6}(n^3 - 25n + 96), \frac{1}{6}(n^3 - 85n + 984), \frac{1}{8}(n^3 + 3n^2 + 7n - 27)\right\}$$
$$= \frac{1}{6}(n^3 - 19n + 198)$$

for $n \geq 13$. Thus $S_{9,4}$ for $n = 9$ and $P_n(2,3,2,n-7)$ for $n \geq 13$ are the unique graphs in $\mathbb{U}_n$ with the second largest Szeged index. Then the graphs in $\mathbb{U}_n$ with the third largest Szeged index are just the graphs in $\mathbb{U}_9 \setminus \{P_{9,4}, S_{9,4}\}$ for $n = 9$ and $\mathbb{U}_n \setminus \{P_{n,4}, P_n(2,3,2,n-7)\}$ for $n \geq 13$ with the largest Szeged index, which is equal to $Sz(P_{9,3}) = 100$ for $n = 9$,

$$\max\{Sz(P_{13}(2,4,2,5)), f_1(3), f_2(6)\} = \max\{356, 328, 346\} = 356$$

for $n = 13$,

$$\max\{Sz(P_{17}(2,4,2,9)), Sz(P'_{17,4}), f_1(3), f_2(6), f_2(8)\}$$
$$= \max\{792, 792, 764, 742, 734\} = 792$$

for $n = 17$, and

$$\max\left\{Sz(P'_{n,4}), f_1(3), f_2(6), f_2\left(\frac{n-1}{2}\right)\right\}$$
$$= \max\left\{\frac{1}{6}(n^3 - 19n + 162), \frac{1}{6}(n^3 - 25n + 96), \frac{1}{6}(n^3 - 85n + 984), \frac{1}{8}(n^3 + 3n^2 + 7n - 27)\right\}$$
$$= \frac{1}{6}(n^3 - 19n + 162)$$

for $n \geq 21$. Thus $P_{9,3}$ for $n = 9$, $P_{13}(2,4,2,5)$ for $n = 13$, $P_{17}(2,4,2,9)$ and $P'_{17,4}$ for $n = 17$, and $P'_{n,4}$ for $n \geq 21$ are the unique graphs in $\mathbb{U}_n$ with the third largest Szeged index.

Case 3. $n \geq 10$ and $n \equiv 2 \pmod 4$. The largest Szeged index of graphs in $\mathbb{U}_n \setminus \{P_{n,4}\}$ is equal to $\max\{Sz(P_{10}(2,3,2,3)), f_1(3), f_1(5)\} = \max\{168, 141, 125\} = 168$ for $n = 10$, and

$$\max\left\{Sz(P_n(2,3,2,n-7)), f_1(3), f_2(6), f_2\left(\frac{n-2}{2}\right)\right\}$$
$$= \max\left\{\frac{1}{6}(n^3 - 19n + 198), \frac{1}{6}(n^3 - 25n + 96), \frac{1}{6}(n^3 - 85n + 984), \frac{1}{8}(n^3 + 2n^2 + 24n - 88)\right\}$$
$$= \frac{1}{6}(n^3 - 19n + 198)$$

for $n \geq 14$. Thus for $n \geq 10$, $P_n(2,3,2,n-7)$ is the unique graph in $\mathbb{U}_n$ with the second largest Szeged index. Then the graphs in $\mathbb{U}_n$ with the third largest Szeged index are just the graphs in $\mathbb{U}_n \setminus \{P_{n,4}, P_n(2,3,2,n-7)\}$ with the largest Szeged index, which is equal to $\max\{Sz(P_{10}(2,2,3,3)), f_1(3), f_1(5)\} = \max\{166, 141, 125\} = 166$ for $n = 10$, $\max\{Sz(P_{14}(2,4,2,6)), f_1(3), f_2(6)\} = \max\{443, 415, 423\} = 443$ for $n = 14$, and

$$\begin{aligned} &\max\left\{Sz(P'_{n,4}), f_1(3), f_2(6), f_2\left(\frac{n-2}{2}\right)\right\} \\ &= \max\left\{\frac{1}{6}(n^3-19n+162), \frac{1}{6}(n^3-25n+96), \frac{1}{6}(n^3-85n+984), \frac{1}{8}(n^3+2n^2+24n-88)\right\} \\ &= \frac{1}{6}(n^3-19n+162) \end{aligned}$$

for $n \geq 18$. Thus $P_{10}(2,2,3,3)$ for $n = 10$, $P_{14}(2,4,2,6)$ for $n = 14$, and $P'_{n,4}$ for $n \geq 18$ are the unique graphs in $\mathbb{U}_n$ with the third largest Szeged index.

Case 4. $n \geq 11$ and $n \equiv 3 \pmod 4$. The largest Szeged index of graphs in $\mathbb{U}_n \setminus \{P_{n,4}\}$ is equal to

$$\max\{Sz(P_{11}(2,3,2,4)), f_1(3), f_1(5)\} = \max\{220, 214, 164\} = 220$$

for $n = 11$, and

$$\begin{aligned} &\max\left\{Sz(P_n(2,3,2,n-7)), f_1(3), f_2(6), f_2\left(\frac{n-3}{2}\right)\right\} \\ &= \max\left\{\frac{1}{6}(n^3-19n+198), \frac{1}{6}(n^3-25n+96), \frac{1}{6}(n^3-85n+984), \frac{1}{8}(n^3+n^2+47n-193)\right\} \\ &= \frac{1}{6}(n^3-19n+198) \end{aligned}$$

for $n \geq 15$. Thus $P_n(2,3,2,n-7)$ for $n \geq 11$ is the unique graph in $\mathbb{U}_n$ with the second largest Szeged index. Then the graphs in $\mathbb{U}_n$ for $n \geq 11$ with the third largest Szeged index are just the graphs in $\mathbb{U}_n \setminus \{P_{n,4}, P_n(2,3,2,n-7)\}$ with the largest Szeged index, which is equal to

$$\max\{Sz(P_{11}(2,2,3,4)), f_1(3), f_1(5)\} = \max\{216, 214, 164\} = 216$$

for $n = 11$, $\max\{Sz(P_{15}(2,4,2,7)), f_1(3), f_2(6)\} = \max\{544, 516, 514\} = 544$ for $n = 15$, and

$$\begin{aligned} &\max\left\{Sz(P'_{n,4}), f_1(3), f_2(6), f_2\left(\frac{n-3}{2}\right)\right\} \\ &= \max\left\{\frac{1}{6}(n^3-19n+162), \frac{1}{6}(n^3-25n+96), \frac{1}{6}(n^3-85n+984), \frac{1}{8}(n^3+n^2+47n-193)\right\} \\ &= \frac{1}{6}(n^3-19n+162) \end{aligned}$$

for $n \geq 19$. Thus $P_{11}(2,2,3,4)$ for $n = 11$, $P_{15}(2,4,2,7)$ for $n = 15$, and $P'_{n,4}$ for $n \geq 19$ are the unique graphs in $\mathbb{U}_n$ with the third largest Szeged index.

By combining Cases 1–4, the result follows easily. □

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Author's address

Xuli Qi
School of Mathematics and Statistics, Central China Normal University, Wuhan 430079, P. R. China
E-mail address: qixuli-1212@163.com