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Szeged index of bipartite unicyclic graphs

HUI DONG AND BO ZHOU*

Department of Mathematics, South China Normal University

Guangzhou 510631, P. R. China

zhoubo@scnu.edu.cn

ABSTRACT. The Szeged index of a connected graph G is defined as the sum of products $n_1(e|G)n_2(e|G)$ over all edges $e = uv$ of G where $n_1(e|G)$ 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 In this paper, we determine the n-vertex bipartite unicyclic graphs with the first, the second, the third and the fourth smallest Szeged indices.

Keywords: Szeged index, unicyclic graphs, bipartite graphs, distance.

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1. INTRODUCTION

Topological indices are numerical graph invariants that quantitatively characterize molecular structure. The Wiener index is one of the oldest and the most thoroughly studied topological indices [1]. The Szeged index is another such topological index which coincides to the Wiener index on trees [2].

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$ For $e = uv \in E(G)$, 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 [2]

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

Gutman [2] determined the n-vertex unicyclic graphs with the smallest and the largest Szeged indices for $n\geq 3$. Zhou et al. [3] determined (in Proposition 3 there) the n-vertex unicyclic graphs with the second, the third and the fourth smallest Szeged indices as well as (in Proposition 5 there) the n-vertex unicyclic graphs with the first a few largest Szeged indices for $n\geq 6$.

The number of vertices of a graph G is denoted by $|G|$. Let P_n and C_n be respectively the n-vertex path and cycle. Note that a unicyclic graph is bipartite if and only if its unique cycle length is even. Let $C(n;T_1,T_2,\ldots,T_r)$ be the unicyclic graph with cycle $C_r=v_1v_2\ldots v_rv_1$, where the deletion of edges of the cycle results in vertex-disjoint trees $T_1,T_2,\ldots,T_r$ such that $\sum_{i=1}^{r}|T_i|=n$ and $v_i\in V(T_i)$ for $i=1,2,\ldots,r$. The trees $T_1,T_2,\ldots,T_r$ are called the branches of $C(n;T_1,T_2,\ldots,T_r)$.

For nonnegative integers a and b, let $P(r, s, a, b)$ 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_s of the cycle C_r where $s=1,2,\ldots,\left\lfloor \frac{r}{2}\right\rfloor+1$. Let $P_{n,r}=P\left(r,\frac{r}{2}+1,\left\lceil \frac{n-r}{2}\right\rceil,\left\lfloor \frac{n-r}{2}\right\rfloor\right)$ for even r, and $P_{n,r}=P(r,1,n-r,0)$ for odd r.

For odd $n\geq 7$, let H_n be the set of graphs $C(n;T_1,T_2,\ldots,T_r)$ with $|T_1|=|T_j|=|T_s|=2$, $|T_i|=1$ for $i\neq 1,j,s$, and either $1<j\leq\left\lfloor \frac{n+1}{4}\right\rfloor<\frac{n-1}{2}\leq s\leq\frac{n-5}{2}+j$ or $n-2-s\geq s-j\geq j-1\geq\left\lfloor \frac{n+1}{4}\right\rfloor$.

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 $l=1,2,\ldots,\frac{r}{2}+1$.

By inspection the bipartite graphs in Proposition 5 of [3], we have immediately the following.

Proposition 1. Among n-vertex bipartite unicyclic graphs 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, and $P\left(n-2, \frac{n}{2}-(s-3), 1, 1\right)$ for $s = 4, \ldots, \frac{n+4}{2}$ is the unique graph with the s-th largest Szeged index, which is equal to $\frac{1}{4}(n^3-2n^2+8n-8)-2(s-3)$;

(ii) if n is odd, then $P_{n,n-1}$, $P\left(n-3, \frac{n-1}{2}, 2, 1\right)$ and $P(n-3,1,3,0)$ are respectively the unique graphs with the first, the second and the third largest Szeged indices, which are equal to $\frac{1}{4}(n^3-n^2+3n-3)$, $\frac{1}{4}(n^3-3n^2+15n-21)$ and $\frac{1}{4}(n^3-3n^2+15n-29)$ respectively,

(a) for n = 7, $P\left(n-3, \frac{n-3}{2} 2, 1\right)$, $S\left(n-3, \frac{n-3}{2} 2, 1\right)$, and graphs in H_n 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 $S\left(n-3, \frac{n-3}{2} 2, 1\right)$, and graphs in H_n 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, $P\left(n-3, \frac{n-3}{2} 2, 1\right)$, is the unique graph with the fourth largest Szeged index, which is equal to $\frac{1}{4}(n^3-3n^2+15n-37)$, while $P\left(n-3, \frac{n-5}{2} 2, 1\right)$, $S\left(n-3, \frac{n-1}{2} 2, 1\right)$, and graphs in H_n are the unique graphs with the fifth largest Szeged index, which is equal to $\frac{1}{4}(n^3-3n^2+11n-9)$.

(b) for $n \geq 13$, $P\left(n-3, \frac{n-1}{2}-(s-4), 2, 1\right)$ for $s = 5, \ldots, \left\lceil \frac{n+9}{4} \right\rceil$ is the unique graph with the (s-1)-th largest Szeged index, which is equal to $\frac{1}{4}(n^3 - 3n^2 + 15n - 21) - 4(s-4)$, for $s = \frac{n+13}{4}$ with $n \equiv 3 \pmod 4$, $P\left(n-3, \frac{n-1}{2}-(s-4), 2, 1\right)$, $S\left(n-3, \frac{n-1}{2} 2, 1\right)$ and graphs in H_n are the unique graphs with the (s-1)-th largest Szeged index, which is equal to $\frac{1}{4}(n^3 - 3n^2 + 11n - 9)$. and for $s = \frac{n+15}{4}$ with $n \equiv 1 \pmod 4$, $S\left(n-3, \frac{n-1}{2} 2, 1\right)$ and graphs in H_n are the unique graphs with the (s-1)-th largest Szeged index, which is equal to $\frac{1}{4}(n^3 - 3n^2 + 11n - 9)$.

However, by similar inspection of Proposition 3 of [3], we find all the n-vertex unicyclic graphs with the first, the second, the third and the fourth smallest Szeged indices are not bipartite for $n \geq 6$. Therefore it is interesting to determine the n-vertex bipartite unicyclic graphs with the first a few smallest Szeged indices for $n \geq 6$.

2. Preliminaries

For $u, v \in V(G)$, let $d(u, v \mid G)$ be the distance between u and v in G, and let $D(u \mid G) = \sum_{v \in V(G)} d(u, v \mid G)$. Recall that Wiener index of the graph G is defined as $W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u, v \mid G) = \frac{1}{2} \sum_{u \in V(G)} D(u \mid G)$ and that if G is a tree then $W(G) = Sz(G)$. Let S_n be the n-vertex star.

Lemma 1. [4] Let $G = C(n; T_1, T_2, \ldots, T_r)$, where r is even. Then

$$Sz(G) = \sum_{i=1}^{r} W(T_i) + \sum_{i=1}^{r} (n - |T_i|) D(v_i | T_i) + \sum_{i=1}^{r} \sum_{j=1}^{r} |T_i| |T_j| d(v_i, v_j | C_r).$$

Lemma 2. [1] Let T be an n-vertex tree different from S_n. Then

$$W(T) > W(S_n) = (n-1)^2.$$

Lemma 3. [5] Let T be an n-vertex tree with $u \in V(T)$, where $n \geq 3$. Let x be the center of the star S_n. Then $D(u \mid T) \geq D(x \mid S_n) = n-1$ with equality if and only if $T = S_n$ and $u = x$.

Let $P_4 = v_1v_2v_3v_4$. Let $S_n^{'}$ be the tree obtained from P_4 by attaching $n-4$ pendent vertices to v_2 for $n \geq 5$, and $S_n^{''}$ the tree obtained from P_4 by attaching $n-5$ pendent vertices to v_2 and a pendent vertex to v_3 for $n \geq 6$.

Lemma 4. [5] 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.

Lemma 5. [5] Let T be an n-vertex tree with $n \geq 6$, $T \neq S_n$, $u \in V(T)$, 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 $D(u \mid T) \geq D(y \mid S_n^{''}) > D(x \mid S_n^{'}) = n$.

Let $S_{n,r}$ be the unicyclic graph obtained by attaching $n-r$ pendent verticies to a vertex of the cycle C_r, where $3 \leq r \leq n$.

Lemma 6. [3] Let G be an n-vertex unicyclic graph with cycle length r, where $4 \leq r \leq n$ and r is even. Then $Sz(G) \geq (n-1)(n-r) + \frac{r^2}{4}(2n-r)$ with equality if and only if $G = S_{n,r}$.

3. Results

Let Λ_n be the set of graphs $C(n;T_1,T_2,T_3,T_4)$ with three trivial branches. Let Γ_n be the set of graphs $C(n;T_1,T_2,T_3,T_4)$ in which there are exactly two trivial branches. Let Ψ_n be the set of graphs $C(n;T_1,T_2,T_3,T_4)$ in which there is exactly one trivial branch. Let Φ_n be the set of graphs $C(n;T_1,T_2,T_3,T_4)$ with no trivial branch. Suppose without loss of generality that $|T_1| \geq \max\{|T_2|,|T_3|,|T_4|\}$ in $C(n;T_1,T_2,T_3,T_4)$.

Lemma 7. $S_{n,4}$ is the unique n-vertex bipartite unicyclic graph with the smallest Szeged index, which is equal to $n^2 + 3n - 12$.

Proof. Let G be an n-vertex bipartite unicyclic graph with cycle length r, where r is even and $4 \le r \le n$. From Lemma 6, we have

$$Sz(G) \ge Sz(S_{n,r}) = (n-1)(n-r) + \frac{r^2}{4}(2n-r).$$

Let $f(x) = (n-1)(n-x) + \frac{x^2}{4}(2n-x)$, where $4 \le x \le n$. It is easily seen that

$$f'(x) = -\frac{3}{4}x^2 + nx - (n-1) \ge \min\{f'(4), f'(n)\} = \min\left\{3n-11, \frac{1}{4}(n-2)^2\right\} > 0.$$

Thus for fixed n, $Sz(S_{n,r}) = f(r)$ is increasing for $4 \le r \le n$. T he result follows easily.

Let $S_n(a,b,c,d)$ be the n-vertex unicyclic graph formed by attaching $a-1$, $b-1$, $c-1$ and $d-1$ pendent vertices to the four vertices of quadrangle consecutively, where $a,b,c,d \ge 1$, and $a+b+c+d = n$.

For $n \ge 6$, let $B_n^{'}$ be the n-vertex unicyclic graph formed by attaching $n-6$ pendent vertices and a path P_2 to one vertex of a quadrangle. For $n \ge 7$, let $B_n^{"}$ be the n-vertex unicyclic graph formed by attaching $n-7$ pendent vertices and the star S_3 at its center to one vertex of a quadrangle. Evidently, $B_n^{'}, B_n^{"} \in \Lambda_n$.

L emma 8 Among the graphs in Λ_n with $n \ge 7$, $B_n^{'}$ and $B_n^{"}$ are respectively the unique graphs with the second and the third smallest Szeged indices, which are equal to $n^2+4n-15$ and $n^2+5n-20$, respectively.

Proof. Let $G = C(n; T_1, T_2, T_3, T_4) \in \Lambda_n$. Note that $|T_1| = n-3$ and T_2, T_3, T_4 are all trivial. By Lemma 1, we have

$$Sz(G) = W(T_1) + 3D(v_1 | T_1) + 8(n-2)$$

which, together with Lemmas 4 and 5, implies that $B_n^{'}$ and $B_n^{"}$ are respectively the unique graphs in Λ_n with the second and the third smallest Szeged indices, where

$$Sz(B_n^{'}) = W(S_{n-3}^{'}) + 3(n-5+2) + 8(n-2) = n^2 + 4n - 15,$$

$$Sz(B_n^{"}) = W(S_{n-3}^{"}) + 3(n-6+4) + 8(n-2) = n^2 + 5n - 20.$$

This proves the result.

Lemma 9. Among the graphs in Γ_n with $n \geq 8$, $S_n(n-4,2,1,1)$ and $S_n(n-5,3,1,1)$ are respectively the unique graphs with the first and the second smallest Szeged indices, which are equal to $n^2+5n-22$ and $n^2+7n-36$, respectively.

Proof. Let $G = C(n;T_1,T_2,T_3,T_4) \in \Gamma_n$ with $|T_1| = a$, $|T_2| = b$, $|T_3| = c$, and $|T_4| = d$. It is easily seen that

$$Sz(S_n(a,b,c,d)) = n^2 - 5n + 4 + 2ab + 4ac + 2ad + 2bc + 4bd + 2cd.$$

Suppose that $G \neq S_n(n-4,2,1,1)$. Note that $a \geq b,c,d$. There are two cases.

Case 1. $c = d = 1$. Then $a+b = n-2$ and $(a,b) \neq (n-4,2)$. By Lemmas 1-3, $Sz(G) \geq Sz(S_n(a,b,1,1)) = n^2+n+2ab-6$. Obviously, for $n \geq 8$, $n^2+n+2ab-6$ is minimal if and only if $(a,b) = (n-5,3)$. Thus $Sz(G) \geq n^2+7n-36$ with equality if and only if $G = S_n(n-5,3,1,1)$. Note that $Sz(S_n(n-4,2,1,1)) = n^2+5n-22$. It follows that

$$\begin{aligned} Sz(G) &> Sz(S_n(n-5,3,1,1)) = n^2+7n-36 \\ &> Sz(S_n(n-4,2,1,1)) = n^2+5n-22 \end{aligned}$$

if $G \neq S_n(n-4,2,1,1)$, $S_n(n-5,3,1,1)$.

Case 2. $b = d = 1$. Then $a+c = n-2$. By Lemmas 1-3, we have

$$\begin{aligned} Sz(G) &\geq Sz(S_n(a,1,c,1)) = n^2-n+4ac \\ &\geq n^2-n+4(n-4)\cdot 2 \\ &= n^2+7n-32 \\ &> n^2+7n-36 \\ &= Sz(S_n(n-5,3,1,1)) \\ &> Sz(S_n(n-4,2,1,1)). \end{aligned}$$

By combining Cases 1 and 2, the result follows.

Lemma 10. Let $G \in \Psi_n$, where $n \geq 8$. Then

$$Sz(G) > Sz(S_n(n-5,3,1,1)) = n^2+7n-36.$$

Proof. Let $G = C(n; T_1, T_2, T_3, T_4) \in \Psi_n$ with $|T_1| = a$, $|T_2| = b$, $|T_3| = c$, and $|T_4| = d$. Note that $a \geq b, c, d$. Suppose without loss of generality that $b \geq d$. Then there are three cases.

Case 1. $d = 1$ and $a \geq b \geq c$. Then $a + b + c = n - 1$, $\frac{n-1-c}{2} \leq a \leq n - 1 - 2c$, and $2 \leq c \leq \frac{n-1}{3}$. Let $f(a,b,c) = 2ab + 4ac + 2bc + 2a + 4b + 2c$. It is easily seen that

$$Sz(S_n(a,b,c,1)) = n^2 - 5n + 4 + f(a,b,c).$$

Note that

$$\begin{aligned} f(a,b,c) &= 2a(n-1-c-a) + 4ac + 2(n-1-c-a)c \\ &\quad + 2a + 4(n-1-c-a) + 2c \\ &= -2a^2 + 2(n-2)a - 2c^2 + 2(n-2)c + 4(n-1) \\ &\geq \min\left\{ f\left(\frac{n-1-c}{2}, b, c\right), f(n-1-2c, b, c) \right\}. \end{aligned}$$

Thus $Sz(S_n(a,b,c,1)) \geq \min\left\{ Sz\left(S_n\left(\frac{n-1-c}{2}, b, c, 1\right)\right), Sz(S_n(n-1-2c, b, c, 1)) \right\}$. It is not difficult to check that

$$\begin{aligned} Sz\left(S_n\left(\frac{n-1-c}{2}, b, c, 1\right)\right) &= n^2 - 5n + 4 - 2\left(\frac{n-1-c}{2}\right)^2 \\ &\quad + 2(n-2)\left(\frac{n-1-c}{2}\right) - 2c^2 + 2(n-2)c + 4(n-1) \\ &= -\frac{5}{2}c^2 + (2n-3)c + \frac{3}{2}n^2 - 3n + \frac{3}{2} \\ &\geq -\frac{5}{2}\cdot 2^2 + (2n-3)\cdot 2 + \frac{3}{2}n^2 - 3n + \frac{3}{2} \\ &= \frac{3}{2}n^2 + n - \frac{29}{2} \\ &> n^2 + 7n - 36 = Sz(S_n(n-5,3,1,1)), \end{aligned}$$

and

$$\begin{aligned}Sz(S_n(n-1-2c,b,c,1)) &= n^2-5n+4-2(n-1-2c)^2\\ &\quad +2(n-2)(n-1-2c)-2c^2+2(n-2)c+4(n-1)\\ &= -10c^2+(6n-4)c+n^2-3n+2\\ &\geq -10\cdot 2^2+(6n-4)\cdot 2+n^2-3n+2\\ &= n^2+9n-46\\ &> n^2+7n-36 = Sz(S_n(n-5,3,1,1)).\end{aligned}$$

Thus by Lemmas 1-3, we have

$$Sz(G)\geq Sz(S_n(a,b,c,1)) > Sz(S_n(n-5,3,1,1)) = n^2+7n-36 \text{ for } n\geq 8.$$

Case 2. $d=1$ and $a\geq c>b$. Then $a+b+c=n-1$, $\frac{n-1-b}{2}\leq a<n-1-2b$, and $2\leq b<\frac{n-1}{3}$. Let

$$\begin{aligned}f(a,b,c) &= 2ab+4a(n-1-a-b)+2b(n-1-a-b)+2a+4b+2(n-1-a-b)\\ &= -4a^2+4(n-1-b)a-2b^2+2nb+2(n-1).\end{aligned}$$

Then

$$\begin{aligned}f(a,b,c) &> f(n-1-2b,b,c)\\ &= -10b^2+(6n-4)b+2(n-1)\\ &\geq -10\cdot 2^2+(6n-4)\cdot 2+2(n-1)\\ &= 14n-50.\end{aligned}$$

It follows that

$$\begin{aligned}Sz(S_n(a,b,c,1)) &= n^2-5n+4+f(a,b,c)\\ &> n^2-5n+4+14n-50\\ &= n^2+9n-46\\ &> n^2+7n-36 = Sz(S_n(n-5,3,1,1)).\end{aligned}$$

By Lemmas 1-3, we have $Sz(G)\geq Sz(S_n(a,b,c,1)) > Sz(S_n(n-5,3,1,1)) = n^2+7n-36$.

Case 3. $c=1$ and $a \ge b \ge d$. Then $a+b+d=n-1$, $\frac{n-1-d}{2} \le a \le n-1-2d$, $2 \le d \le \frac{n-1}{3}$. Thus by similar arguments as in Case 2, we have $Sz(G) \ge Sz(S_n(a,b,1,d)) > Sz(S_n(n-5,3,1,1)) = n^2+7n-36$. By combining Cases 1-3, the result follows.

Lemma 11. Let $G \in \Phi_n$, where $n \ge 8$. Then

$$Sz(G) > Sz(S_n(n-5,3,1,1)) = n^2+7n-36.$$

Proof. Let $G = C(n;T_1,T_2,T_3,T_4) \in \Phi_n$ with $|T_1|=a$, $|T_2|=b$, $|T_3|=c$, and $|T_4|=d$. Suppose without loss of generality that $b \ge d$. It is easily seen that

$$\begin{aligned} & Sz(S_n(a+1,b,c,d-1)) - Sz(S_n(a,b,c,d)) \\ &= 2(a+1)b + 4(a+1)c + 2(a+1)(d-1) + 4b(d-1) + 2c(d-1) \\ &\quad - (2ab + 4ac + 2ad + 4bd + 2cd) \\ &= 2(c+d-a-b-1) < 0, \end{aligned}$$

and then $Sz(S_n(a,b,c,d)) > Sz(S_n(a+1,b,c,d-1))$. If $G = S_n(a,b,c,d)$, then by Lemma 10, we have

$$\begin{aligned} Sz(G) = Sz(S_n(a,b,c,d)) &> Sz(S_n(a+1,b,c,d-1)) \\ &> \cdots > Sz(S_n(a+d-1,b,c,1)) \\ &> Sz(S_n(n-5,3,1,1)) = n^2+7n-36 \end{aligned}$$

and if $G \ne S_n(a,b,c,d)$, then by Lemmas 1-3, we have

$$Sz(G) > Sz(S_n(a,b,c,d)) > Sz(S_n(n-5,3,1,1)) = n^2+7n-36.$$

The proof is now completed.

Proposition 2. Among n-vertex bipartite unicyclic graphs with $n \ge 6$,

(i) for $n=6$, $S_6(2,2,1,1)$ and $B_6^{'}$ are respectively the unique bipartite unicyclic graphs with the second and the third smallest Szeged indices, which are equal to 44 and 45, respectively;

(ii) for $n=7$, $B_7^{'}$ and $S_7(3,2,1,1)$ are the unique bipartite unicyclic graphs with the second smallest Szeged index, which is equal to 62, while $B_7^{''}$ is the unique bipartite unicyclic graphs with the third smallest Szeged index, which is equal to 64;

(iii) for $n \geq 8$, $B_n^{'}$, $S_n(n-4,2,1,1)$ and $B_n^{''}$ are respectively the unique bipartite unicyclic graphs with the second, the third and the fourth smallest Szeged indices, which are $n^2+4n-15$, $n^2+5n-22$ and $n^2+5n-20$, respectively.

Proof. The cases $n=6,7$ may be checked easily. Suppose that $n \geq 8$.

B y Lemma 8,$B_n^{'}$ and $B_n^{''}$ are respectively the unique graphs in Λ_n with the second and the third smallest Szeged indices, which are equal to $n^2+4n-15$ and $n^2+5n-20$, respectively. By Lemma 9, $S_n(n-4,2,1,1)$ and $S_n(n-5,3,1,1)$ are respectively the unique graphs in Γ_n with the first and the second smallest Szeged indices, which are equal to $n^2+5n-22$ and $n^2+7n-36$. By Lemmas 10 and 11, if $G \in \Psi_n \cup \Phi_n$, then $Sz(G) > Sz(S_n(n-5,3,1,1)) = n^2+7n-36$. It follows that, among n-vertex bipartite unicyclic graphs with cycle length four, the graphs $B_n^{'}$, $S_n(n-4,2,1,1)$ and $B_n^{''}$ are respectively the unique graphs with the second, the third and the fourth smallest Szeged indices.

From the proof of Lemma 7, for any n-vertex bipartite unicyclic graph G with cycle length at least six, we have

$$Sz(G) \geq Sz(S_{n,6}) = n^2+11n-48 > n^2+7n-36 = Sz(S_n(n-5,3,1,1)).$$

The result follows easily.

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