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Author(s):

S. Li and J. Zhang

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LEXICOGRAPHICAL ORDERING BY SPECTRAL MOMENTS OF TREES WITH A GIVEN BIPARTITION

S. LI* AND J. ZHANG

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Abstract. Lexicographic ordering by spectral moments (S-order) among all trees is discussed in this paper. For two given positive integers p and q with $p \leqslant q$, we denote $\mathscr{T}_n^{p,q} = \{T : T$ is a tree of order n with a (p,q)-bipartition$\}$. Furthermore, the last four trees, in the S-order, among $\mathscr{T}_n^{p,q}$ $(4 \leqslant p \leqslant q)$ are characterized.
Keywords: Spectral moment; S-order, tree, bipartition.
MSC(2010): Primary: 05C50; Secondary: 15A18.

1. Introduction

Up to isomorphism, all graphs considered here are finite, simple and connected. Undefined terminology and notation may be referred to [1]. Let $G = (V_G, E_G)$ be a simple undirected graph with n vertices. By $G - v$ and $G - uv$ we denote the graph obtained from G by deleting vertex $v \in V_G$, or edge $uv \in E_G$, respectively (this notation is naturally extended if more than one vertex or edge is deleted). Similarly, $G + uv$ is obtained from G by adding edge $uv \notin E_G$. For $v \in V_G$, let $N_G(v)$ (or $N(v)$ for short) denote the set of all the adjacent vertices of v in G and $d(v) = |N_G(v)|$. A *leaf* of G is a vertex of degree one.

Let $A(G)$ be the adjacency matrix of a graph G, and let $\lambda_1(G), \lambda_2(G), \ldots, \lambda_n(G)$ be the eigenvalues of G in non-increasing order. The number $\sum_{i=1}^{n} \lambda_i^k(G)(k = 0, 1, \ldots, n-1)$ is called the kth *spectral moment* of G, denoted by $S_k(G)$. We know from [2] that $S_0 = n$, $S_1 = l$, $S_2 =$

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*Corresponding author.

$2m$, $S_3 = 6t$, where n, l, m, t denote the number of vertices, the number of loops, the number of edges and the number of triangles, respectively. Let $S(G) = (S_0(G), S_1(G), \ldots, S_{n-1}(G))$ be the sequence of spectral moments of G. For two graphs G_1 and G_2, we shall write $G_1 =_s G_2$ if $S_i(G_1) = S_i(G_2)$ for $i = 0, 1, \ldots, n-1$. Similarly, we have $G_1 \prec_s G_2$ (G_1 comes before G_2 in the S-order) if for some $k\,(1 \leqslant k \leqslant n-1)$, we have $S_i(G_1) = S_i(G_2)\,(i = 0, 1, \ldots, k-1)$ and $S_k(G_1) < S_k(G_2)$. We shall also write $G_1 \preceq_s G_2$ if $G_1 \prec_s G_2$ or $G_1 =_s G_2$. S-order was used in producing graph catalogs (see [6]). For a more general setting of spectral moments one may be referred to [5].

Investigation on S-order of graphs attracts more and more researchers' attention. Cvetković and Rowlinson [7] studied the S-order of trees and unicyclic graphs and characterized the first and the last graphs, in the S-order, of all trees and all unicyclic graphs with given girth, respectively. Wu and Liu [14, 16] determined the last $\lfloor \frac{d}{2} + 1 \rfloor$ and the last $\lfloor \frac{g}{2} + 2 \rfloor$ graphs, in the S-order, of all n-vertex trees with diameter $d\,(4 \leqslant d \leqslant n-3)$ and all n-vertex unicyclic graphs of girth g $(3 \leqslant g \leqslant n-3)$, respectively. Wu and Fan [15] determined the first and the last graphs in the S-order, of all unicyclic graphs and bicyclic graphs, respectively. Pan et al. [12] gave the first $\sum_{k=1}^{\lfloor \frac{n-1}{3} \rfloor} \left(\lfloor \frac{n-k-1}{2} \rfloor - k + 1 \right)$ graphs apart from a path, in the S-order, of all trees on n vertices, whereas Pan et al. [13] determined the last and the second last quasi-tree, in the S-order, among the set $\mathscr{L}(n, d_0) = \{G : G \text{ is a quasi-tree of order } n \text{ with } G - u_0 \text{ being a tree and } d_G(u_0) = d_0\}$, respectively.

Given a connected bipartite graph G with n vertices, its vertex set can be partitioned into two subsets V_1 and V_2, such that each edge joins a vertex in V_1 with a vertex in V_2. Suppose that V_1 has p vertices and V_2 has q vertices, where $p + q = n$ with $p \leqslant q$. Then we say that G has a (p, q)-*bipartition*. For convenience, let $\mathscr{T}_n^{p,q}$ be the set of all n-vertex trees, each of which has a (p, q)-bipartition.

In light of the information available on the spectral moments of graphs, it is natural to consider some other class of graphs. Trees with a (p, q)-bipartition are a reasonable starting point for such an investigation. The n-vertex trees with a (p, q)-bipartition have been considered in [8, 9, 10, 11, 16], whereas to the best of our knowledge, the spectral moments of trees in $\mathscr{T}_n^{p,q}\,(4 \leqslant p \leqslant q)$ were, so far, not considered. In this paper we characterize the last four trees, in the S-order, among $\mathscr{T}_n^{p,q}\,(4 \leqslant p \leqslant q)$. For more recent results on the spectral moments of graphs, one may be referred to [3, 4].

Throughout the text we denote by P_n, $K_{1,n-1}$ and C_n the path, star and cycle on n vertices, respectively. Let U_n be a graph obtained from C_{n-1} by attaching a leaf to one vertex of C_{n-1}, and let E_4 be a graph obtained by deleting an edge from a complete graph K_4. Also let E_5 be a graph obtained from two cycles C_3 and C_3' of length 3 by identifying one vertex of C_3 with one vertex of C_3'. The graphs U_4, U_5, E_4 and E_5 are depicted in Fig. 1. Let F be a graph. An *F-subgraph* of G is a subgraph

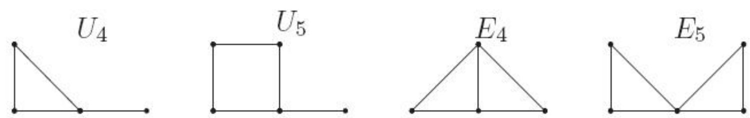

FIGURE 1. Four graphs U_4, U_5, E_4 and E_5.

of G which is isomorphic to the graph F. Let $\phi_G(F)$ (or $\phi(F)$) be the number of all F-subgraphs of G. For a tree T and two vertices v, u of T, the *distance* $\mathrm{dist}_T(u, v)$ between u and v is the number of edges on the unique path connecting them. Denote by $PV(T)$ the set of all pendant vertices of T.

Further on we need the following lemmas.

Lemma 1.1 ([7])**.** *The kth spectral moment of G is equal to the number of closed walks of length k.*

Lemma 1.2. *For every graph G, we have*

(i) $S_4(G) = 2\phi(P_2) + 4\phi(P_3) + 8\phi(C_4)$ (see [7]).
(ii) $S_5(G) = 30\phi(C_3) + 10\phi(U_4) + 10\phi(C_5)$ (see [14]).
(iii) $S_6(G) = 2\phi(P_2)+12\phi(P_3)+6\phi(P_4)+12\phi(K_{1,3})+12\phi(U_5)+36\phi(E_4)+24\phi(E_5) + 24\phi(C_3) + 48\phi(C_4) + 12\phi(C_6)$ (see [14]).

Given a connected graph G, its line graph is denoted by $L(G)$. It is easy to see that the size of $L(G)$ is equal to the number of P_3 of G. By [Exercise 1.5.10(a), 1], we have

Lemma 1.3. *If G is a simple connected graph, then* $\phi_G(P_3) = \sum_{v \in V_G} \binom{d(v)}{2}$.

Definition 1. *Assume that u, v, w are three distinct vertices of a tree T satisfying $uv \in E_T$, $d(u) = 1$, $d(w) \geqslant d(v)$ and $\mathrm{dist}_T(v, w) = 2$. Let $T[v \to w; 1]$ be the graph obtained from T by deleting the edge uv and adding the edge uw. In notation,*

$$T[v \to w; 1] = T - uv + uw,$$

and we say $T[v \to w; 1]$ is obtained from T by Operation I.

Remark 1. *If T is in $\mathscr{T}_n^{p,q}$, by Definition 1, it is easy to see that $T[v \to w; 1]$ is also in $\mathscr{T}_n^{p,q}$.*

Lemma 1.4. *Let T and $T[v \to w; 1]$ be the trees defined as above. Then*

$$T \prec_s T[v \to w; 1].$$

Proof. By Lemma 1.1, $S_i(T) = S_i(T[v \to w; 1])$ holds for $i = 0, 1, 2, 3$. In view of Lemma 1.2(i), $\phi_T(P_2) = \phi_{T[v\to w;1]}(P_2) = n - 1$, $\phi_T(C_4) = \phi_{T[v\to w;1]}(C_4) = 0$. By Lemma 1.3, we have

$$\begin{aligned}\phi_{T[v\to w;1]}(P_3) - \phi_T(P_3) =& \binom{d(w)+1}{2} + \binom{d(v)-1}{2} - \binom{d(w)}{2} - \binom{d(v)}{2} \\ =& d(w) - d(v) + 1 > 0.\end{aligned}$$

Hence, $S_4(T[v \to w; 1]) - S_4(T) = 4(\phi_{T[v\to w;1]}(P_3) - \phi_T(P_3)) > 0$, i.e., $T \prec_s T[v \to w; 1]$. □

Definition 2. *Let uw be an edge of a tree U with $d(w) \geqslant 2$. Let T be obtained from U and the star $K_{1,k+1}$ ($k \geqslant 2$) by identifying u with a pendant vertex of $K_{1,k+1}$ whose center is v. Let $T[v \to w; 2]$ be the graph obtained from T by deleting all edges vz and adding all edges wz, where $z \in W = N_T(v)\backslash\{u\}$. In notation,*

$$T[v \to w; 2] = T - \{vz : z \in W\} + \{wz : z \in W\}$$

and we say $T[v \to w; 2]$ is obtained from T by Operation II. Trees T and $T[v \to w; 2]$ are depicted in Fig. 2.

Remark 2. *If T is in $\mathscr{T}_n^{p,q}$, by Definition 2, it is easy to see that $T[v \to w; 2]$ is also in $\mathscr{T}_n^{p,q}$.*

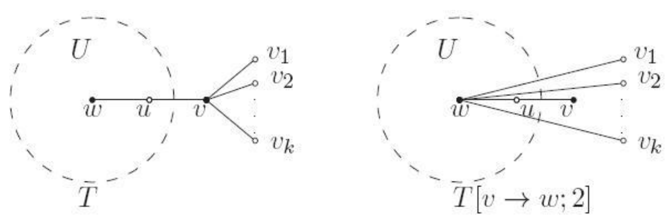

FIGURE 2. $T \Rightarrow T[v \to w; 2]$ by Operation II.

Lemma 1.5. *Let T and $T[v \to w; 2]$ be the trees described as above, then one has $T \prec_s T[v \to w; 2]$.*

Proof. By Lemma 1.1, $S_i(T) = S_i(T[v \to w; 2])$ holds for $i = 0, 1, 2, 3$. In view of Lemma 1.2(i), $\phi_T(P_2) = \phi_{T[v\to w;2]}(P_2) = n-1$ and $\phi_T(C_4) = \phi_{T[v\to w;2]}(C_4) = 0$. By Lemma 1.3,

$$\begin{aligned}\phi_{T[v\to w;2]}(P_3) - \phi_T(P_3) &= \binom{d(w)+k}{2} - \binom{d(w)}{2} - \binom{k+1}{2} \\ &= k(d(w)-1) > 0.\end{aligned}$$

Hence, we have $S_4(T[v \to w; 2]) - S_4(T) = 4(\phi_{T[v\to w;2]}(P_3) - \phi_T(P_3)) > 0$, i.e., $T \prec_s T[v \to w; 2]$. □

Lemma 1.6. *Let T be the tree as depicted in Fig. 2, and let T' be the tree obtained from T by deleting all edges $vv_i\,(i = 1, 2, \dots, k-1)$ and adding all edges $wv_i\,(i = 1, 2, \dots, k-1)$. Assume that w_1 is in $N_T(w) \setminus \{u\}$.*

(i) *If $d_T(w) \geqslant 2$ and $d_T(w_1) \geqslant 2$, one has $T \prec_s T'$.*

(ii) *If $d_T(w) = 2$ and $d_T(w_1) = 1$, one has $T =_s T'$.*

Proof. By Lemma 1.1, $S_i(T) = S_i(T')$ holds for $i = 0, 1, 2, 3$. In view of Lemma 1.2(i), $\phi_T(P_2) = \phi'_T(P_2) = n-1$ and $\phi_T(C_4) = \phi'_T(C_4) = 0$. By Lemma 1.3, we obtain that

$$\phi_T(P_3) = \phi'_T(P_3) = (k-1)(d_T(w) - 2).$$

If $d_T(w) > 2$, then it follows that $\phi_T(P_3) < \phi'_T(P_3)$. Hence, we have $S_4(T) < S_4(T')$, i.e., $T \prec_s T'$.

If $d_T(w) = 2$, then we get $\phi_T(P_3) = \phi'_T(P_3)$. In view of Lemma 1.2(iii), we see that

$$S_6(T') - S_6(T) = 6(k-1)(d_T(w_1) - 1).$$

If $d_T(w_1) \geq 2$, then we get $S_6(T) < S_6(T')$, i.e., $T \prec_s T'$. This completes the proof of (i).

If $d_T(w_1) = 1$, then we have $T \cong T'$, i.e., $T =_s T'$. This completes the proof of (ii). □

2. The last four trees in the S-order among $\mathscr{T}_n^{p,q}$

In this section, we determine the last four trees, in the S-order, among the set $\mathscr{T}_n^{p,q}\,(4 \leqslant p \leqslant q)$.

For convenience, let $B_{p,q}^{k,l}$, $D_{p,q}^{k,l}$ $(k,\, l \geqslant 0)$ be the trees as depicted in Fig. 3, where the degree of u is no less than that of v. In particular, $B_{p,q}^{0,0} \cong D_{p,q}^{0,0}$.

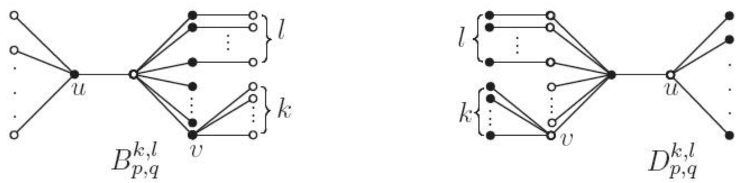

FIGURE 3. Trees $B_{p,q}^{k,l}$ and $D_{p,q}^{k,l}$ each of which contains p white points and q black points.

Theorem 2.1. *Let T be in $\mathscr{T}_n^{p,q}$, then one has $T \preceq_s B_{p,q}^{0,0}$ with equality if and only if $T \cong B_{p,q}^{0,0}$.*

Proof. Choose a tree T with a (p,q)-bipartition such that it is as large as possible with respect to the S-order. Let V_1, V_2 be the bipartition of the vertices of T with $V_1 = \{v_0, v_1, \ldots, v_{p-1}\}$, $V_2 = \{u_0, u_1, \ldots, u_{q-1}\}$. For convenience, let v_0 (respectively, u_0) be the vertex of maximal degree among V_1 (respectively, V_2) in T and let $A = N_T(v_0) \cap PV(T)$.

Hence, in order to complete the proof, it suffices to show the following claims.

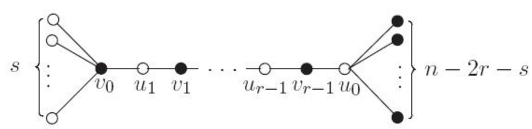

FIGURE 4. Tree $T(n, 2r, s)$ with some labelled vertices.

For convenience, let $T(n, k, a)$ be an n-vertex tree obtained by attaching a and $n-k-a$ pendant vertices to the two end-vertices of P_k, respectively. In particular, $D_{p,q}^{0,0} = T(n, 2, p-1)$.

Claim 1. $T \cong T(n, 2r, s)$ *(see Fig. 4) with $r \geq 1$ and $s \geq 0$.*

Proof of Claim 1. Assume otherwise. Then T must contain a pendant vertex $w \notin N_T(u_0) \cup N_T(v_0)$. Using Operations I and II, repeatedly, we can construct T_0 from T such that $T_0 \cong T(n, 2r, s)$ for some r and s. So by Lemmas 1.4 and 1.5 $T \prec_s T_0$, a contradiction to the choice of T.

This completes the proof of Claim 1. □

Claim 2. *In the tree described as above, u_0 is adjacent to v_0.*

Proof of Claim 2. If not, then $d(u_0, v_0) \geq 3$. Note that v_0 is the maximal degree vertex among V_1, hence $d_T(v_0) \neq 1$, which implies $A \neq \emptyset$. Using Operation Ⅱ, let

$$T_1 = T - \{v_0 z : z \in A\} + \{v_1 z : z \in A\}$$

then $T \prec_s T_1$ by Lemma 1.5, which contradicts the choice of T. This completes the proof of Claim 2. □

By Claims 1 and 2, we get that $T \cong B_{p,q}^{0,0}$. This completes the proof. □

Theorem 2.2. *For any $T \in \mathscr{T}_n^{p,q} \setminus \{B_{p,q}^{0,0}\}$ with $4 \leqslant p \leqslant q$, one has $T \preceq_s B_{p,q}^{0,1}$ with equality if and only if $T \cong B_{p,q}^{0,1}$.*

Proof. For any $T \in \mathscr{T}_n^{p,q} \setminus \{B_{p,q}^{0,0}\}$, from the proof of Theorem 2.1, it is easy to see that T can be transformed into $B_{p,q}^{0,0}$ by carrying the Operations I and Ⅱ repeatedly. Let $\mathscr{A}_1$ denote the set of all trees in $\mathscr{T}_n^{p,q}$ which can be transformed into $B_{p,q}^{0,0}$ by carrying Operation I once, and let $\mathscr{A}_2$ denote the set of all trees in $\mathscr{T}_n^{p,q}$ which can be transformed into $B_{p,q}^{0,0}$ by carrying Operation Ⅱ once. It follows from Lemmas 1.4 and 1.5 that the second last tree, in the S-order, among $\mathscr{T}_n^{p,q}$ must be in $\mathscr{A}_1 \cup \mathscr{A}_2$.

By definitions of $\mathscr{A}_1$ and $\mathscr{A}_2$, it is routine to check that $\mathscr{A}_1 = \{B_{p,q}^{0,1}, D_{p,q}^{0,1}\}$ (in particular, if $p = q$ then $B_{p,q}^{0,1} \cong D_{p,q}^{0,1}$; hence $\mathscr{A}_1 = \{B_{p,q}^{0,1}\}$ for $p = q$), $\mathscr{A}_2 = \{B_{p,q}^{k,0} : 2 \leqslant k \leqslant \lfloor \frac{p-1}{2} \rfloor\} \cup \{D_{p,q}^{k,0} : 2 \leqslant k \leqslant \lfloor \frac{q-1}{2} \rfloor\}$. Note that $B_{p,q}^{0,1}$ can be obtained from $B_{p,q}^{k,0}$ by using Operation I $(k-1)$ times. By Lemma 1.4, we have $B_{p,q}^{k,0} \prec_s B_{p,q}^{0,1}$ for $2 \leqslant k \leqslant \lfloor \frac{p-1}{2} \rfloor$. Similarly, we have $D_{p,q}^{k,0} \prec_s D_{p,q}^{0,1}$ with $2 \leqslant k \leqslant \lfloor \frac{q-1}{2} \rfloor$.

Hence, if $p = q$ then $B_{p,q}^{0,1}$ is just the second last tree, in the S-order, among $\mathscr{T}_n^{p,q}$ for $p \geqslant 4$. So in what follows we consider $p < q$.

In order to complete the proof, it suffices to compare $B_{p,q}^{0,1}$ with $D_{p,q}^{0,1}$. By Lemma 1.1, we have $S_i(B_{p,q}^{0,1}) = S_i(D_{p,q}^{0,1})$ for $i = 0, 1, 2, 3$. In view of Lemma 1.2(i), $\phi_{B_{p,q}^{0,1}}(P_2) = \phi_{D_{p,q}^{0,1}}(P_2) = n - 1$ and $\phi_{B_{p,q}^{0,1}}(C_4) =$

$\phi_{D^{0,1}_{p,q}}(C_4) = 0$. In view of Lemma 1.3, we have

$$\phi_{B^{0,1}_{p,q}}(P_3) - \phi_{D^{0,1}_{p,q}}(P_3) = \binom{p-1}{2} + \binom{q}{2} + 1 - \binom{p}{2} - \binom{q-1}{2} - 1 = q - p > 0.$$

Hence, $S_4(B^{0,1}_{p,q}) - S_4(D^{0,1}_{p,q}) = 4(\phi_{B_1}(P_3) - \phi_{D^{0,1}_{p,q}}(P_3)) > 0$, i.e., $D^{0,1}_{p,q} \prec_s B^{0,1}_{p,q}$.

This completes the proof. $\square$

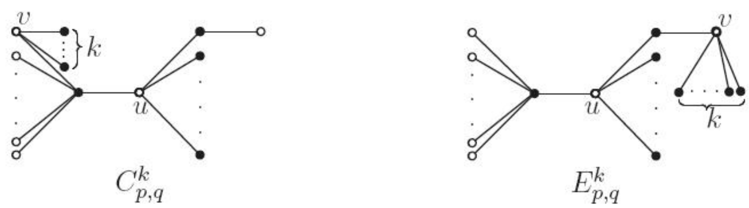

FIGURE 5. Trees $C^k_{p,q}$ and $E^k_{p,q}$ each of which contains p white points and q black points.

For convenience, let $C^k_{p,q}$, $E^k_{p,q}$ $(1 \leqslant k \leqslant q-2)$ be the trees as depicted in Fig. 5. It is easy to see that $C^k_{p,q}$, $E^k_{p,q} \in \mathscr{T}^{p,q}_n$.

Theorem 2.3. *Let p and q be positive integers with $4 \leqslant p \leqslant q$.*

(i) *For any $T \in \mathscr{T}^{p,q}_n \setminus \{B^{0,0}_{p,q}, B^{0,1}_{p,q}\}$ with $p = q$, we have $T \preceq_s B^{2,0}_{p,q}$ with equality if and only if $T \cong B^{2,0}_{p,q}$.*

(ii) *For any $T \in \mathscr{T}^{p,q}_n \setminus \{B^{0,0}_{p,q}, B^{0,1}_{p,q}\}$ with $p < q$, if $p > \frac{q+4}{2}$, then we have $T \preceq_s D^{0,1}_{p,q}$ with equality if and only if $T \cong D^{0,1}_{p,q}$; if $p \leqslant \frac{q+4}{2}$, then we have $T \preceq_s B^{2,0}_{p,q}$ with equality if and only if $T \cong B^{2,0}_{p,q}$.*

Proof. For any $T \in \mathscr{T}^{p,q}_n \setminus \{B^{0,0}_{p,q}, B^{0,1}_{p,q}\}$, by a similar discussion as in the proof of Theorem 2.2, T can be transformed into $B^{0,0}_{p,q}$ (respectively, $B^{0,1}_{p,q}$) by carrying Operations I and II repeatedly. Let $\mathscr{B}_1$ denote the set of all trees in $\mathscr{T}^{p,q}_n$ which can be transformed into $B^{0,1}_{p,q}$ by carrying Operation I once, and let $\mathscr{B}_2$ denote the set of all trees in $\mathscr{T}^{p,q}_n$ which can be transformed into $B^{0,1}_{p,q}$ by carrying Operation II once. It follows from Lemmas 1.4 and 1.5 that, if $p < q$ then the third last tree, in the S-order, among $\mathscr{T}^{p,q}_n$ must be in $\{D^{0,1}_{p,q}\} \cup \mathscr{A}_2 \cup \mathscr{B}_1 \cup \mathscr{B}_2$, where $\mathscr{A}_2$ is defined in the proof of Theorem 2.2. Note that if $p = q$, then $B^{0,1}_{p,q} \cong D^{0,1}_{p,q}$. Hence, the third last tree, in the S-order, among $\mathscr{T}_n^{p,q}$ with $p = q$ must be in $\mathscr{A}_2 \cup \mathscr{B}_1 \cup \mathscr{B}_2$.

By the definition of $\mathscr{B}_1$ and $\mathscr{B}_2$, it is routine to check that $\mathscr{B}_1 = \{B_{p,q}^{2,0}, B_{p,q}^{0,2}, C_{p,q}^1, E_{p,q}^1\}$ and $\mathscr{B}_2 = \{C_{p,q}^k : 2 \leqslant k \leqslant q-2\} \cup \{E_{p,q}^k : 2 \leqslant k \leqslant q-2\} \cup \{B_{p,q}^{k,1} : 2 \leqslant k \leqslant \lfloor \frac{p-2}{2} \rfloor\}$. We obtain (based on Lemma 1.4) that

$$B_{p,q}^{k,1} \prec_s B_{p,q}^{k-1,1} \prec_s \cdots \prec_s B_{p,q}^{1,1} \cong B_{p,q}^{0,2}.$$

We first show the following two facts.

Fact 1. *The last tree, in the S-order, among $\mathscr{A}_2$ is $B_{p,q}^{2,0}$.*

Proof of Fact 1. In graph $B_{p,q}^{k,0}$, we obtain (based on Lemma 1.4) that

$$B_{p,q}^{\lfloor \frac{p-1}{2} \rfloor,0} \prec_s B_{p,q}^{\lfloor \frac{p-1}{2} \rfloor-1,0} \prec_s \cdots \prec_s B_{p,q}^{k,0} \prec_s \cdots \prec_s B_{p,q}^{3,0} \prec_s B_{p,q}^{2,0}. \tag{2.1}$$

Similarly, we obtain

$$D_{p,q}^{\lfloor \frac{q-1}{2} \rfloor,0} \prec_s D_{p,q}^{\lfloor \frac{q-1}{2} \rfloor-1,0} \prec_s \cdots \prec_s D_{p,q}^{k,0} \prec_s \cdots \prec_s D_{p,q}^{3,0} \prec_s D_{p,q}^{2,0}. \tag{2.2}$$

Note that if $p = q$, it is easy to see that $B_{p,q}^{2,0} \cong D_{p,q}^{2,0}$, hence Fact 1 holds immediately. In what follows, we consider $p < q$.

In view of (2.1) and (2.2), it suffices to compare $B_{p,q}^{2,0}$ with that of $D_{p,q}^{2,0}$. In fact, by Lemma 1.1 one has $S_i(B_{p,q}^{2,0}) = S_i(D_{p,q}^{2,0})$ for $i = 0, 1, 2, 3$. In view of Lemma 1.2(i), $\phi_{B_{p,q}^{2,0}}(P_2) = \phi_{D_{p,q}^{2,0}}(P_2) = n-1$, $\phi_{B_{p,q}^{2,0}}(C_4) = \phi_{D_{p,q}^{2,0}}(C_4) = 0$ and by Lemma 1.3,

$$\phi_{B_{p,q}^{2,0}}(P_3) - \phi_{D_{p,q}^{2,0}}(P_3) = \binom{p-2}{2} + \binom{q}{2} - \binom{p}{2} - \binom{q-2}{2} = 2(q-p) > 0.$$

Hence, we have $S_4(B_{p,q}^{2,0}) - S_4(D_{p,q}^{2,0}) > 0$, i.e., $D_{p,q}^{2,0} \prec_s B_{p,q}^{2,0}$.

This completes the proof. □

Fact 2. *The last tree, in the S-order, among $\mathscr{B}_1 \cup \mathscr{B}_2$ is $B_{p,q}^{2,0}$.*

Proof of Fact 2. Note that by Lemma 1.6(i) we have $C_{p,q}^k \prec_s C_{p,q}^1$ for $k \geqslant 2$. Similarly, $E_{p,q}^k \prec_s E_{p,q}^1$ also holds for $k \geqslant 2$. So the last tree, in the S-order, among $\mathscr{B}_1 \cup \mathscr{B}_2$ must be in $\mathscr{B}_1$.

Note that $C_{p,q}^1$ and $E_{p,q}^1$ have the same degree sequence, hence by Lemma 1.3 we have

$$\phi_{E_{p,q}^1}(P_3) = \phi_{C_{p,q}^1}(P_3). \tag{2.3}$$

By Lemma 1.1, $S_i(B_{p,q}^{0,2}) = S_i(C_{p,q}^1) = S_i(E_{p,q}^1)$ holds for $i = 0, 1, 2, 3$. In view of Lemma 1.2(i), it is routine to check that $\phi_{C_{p,q}^1}(P_2) = \phi_{E_{p,q}^1}(P_2) =$

$\phi_{B^{0,2}_{p,q}}(P_2) = n-1$, $\phi_{C^1_{p,q}}(C_4) = \phi_{E^1_{p,q}}(C_4) = \phi_{B^{0,2}_{p,q}}(C_4) = 0$. By Lemma 1.3, one has

$$
\begin{aligned}
(2.4)\qquad \phi_{C^1_{p,q}}(P_3) - \phi_{B^{0,2}_{p,q}}(P_3) &= \left(\binom{p-1}{2} + \binom{q-1}{2} + 2\right) \\
&\quad - \left(\binom{p-2}{2} + \binom{q}{2} + 2\right) \\
&= -(q-p+1) < 0.
\end{aligned}
$$

In view of (2.4), $\phi_{C^1_{p,q}}(P_3) - \phi_{B^{0,2}_{p,q}}(P_3) < 0$. Hence, by Lemma 1.2(i), we have $S_4(C^1_{p,q}) < S_4(B^{0,2}_{p,q})$ and by (2.3) and (2.4), $S_4(E^1_{p,q}) < S_4(B^{0,2}_{p,q})$, i.e., $C^1_{p,q} \prec_s B^{0,2}_{p,q}$ and $E^1_{p,q} \prec_s B^{0,2}_{p,q}$.

On the other hand, $B^{0,2}_{p,q}$ can be transformed into $B^{2,0}_{p,q}$ by carrying Operation I once, and by Lemma 1.4 we have $B^{0,2}_{p,q} \prec_s B^{2,0}_{p,q}$. That is to say, $B^{2,0}_{p,q}$ is the last tree, in the S-order, among $\mathscr{B}_1 \cup \mathscr{B}_2$. $\square$

If $p = q$, by Facts 1 and 2, we obtain that $B^{2,0}_{p,q}$ is just the last tree, in the S-order, among $\mathscr{T}^{p,q}_n \setminus \{B^{0,0}_{p,q}, B^{0,1}_{p,q}\}$. This completes the proof of (i).

Now in what follows we consider $p < q$. According to Facts 1 and 2, it suffices to compare $B^{2,0}_{p,q}$ with $D^{0,1}_{p,q}$ in this case.

By Lemma 1.1, $S_i(D^{0,1}_{p,q}) = S_i(B^{2,0}_{p,q})$ holds for $i = 0, 1, 2, 3$. In view of Lemma 1.2(i), it is routine to check that $\phi_{D^{0,1}_{p,q}}(P_2) = \phi_{B^{2,0}_{p,q}}(P_2) = n-1$, $\phi_{D^{0,1}_{p,q}}(C_4) = \phi_{B^{2,0}_{p,q}}(C_4) = 0$. Furthermore, by Lemma 1.3, we have

$$
\begin{aligned}
(2.5)\qquad \phi_{D^{0,1}_{p,q}}(P_3) - \phi_{B^{2,0}_{p,q}}(P_3) &= \left(\binom{p}{2} + \binom{q-1}{2} + 1\right) \\
&\quad - \left(\binom{p-2}{2} + \binom{q}{2} + 3\right) \\
&= 2p - 4 - q.
\end{aligned}
$$

If $p > \frac{q+4}{2}$, then in view of (2.5) we have $\phi_{D^{0,1}_{p,q}}(P_3) > \phi_{B^{2,0}_{p,q}}(P_3)$. By Lemma 1.2(i), $S_4(D^{0,1}_{p,q}) > S_4(B^{2,0}_{p,q})$ holds. So we have $B^{2,0}_{p,q} \prec_s D^{0,1}_{p,q}$. So in this case $D^{0,1}_{p,q}$ is the third last tree, in the S-order, among $\mathscr{T}^{p,q}_n$.

If $p = \frac{q+4}{2}$, then in view of (2.5) we have $\phi_{D^{0,1}_{p,q}}(P_3) = \phi_{B^{2,0}_{p,q}}(P_3)$. Hence, $S_4(D^{0,1}_{p,q}) = S_4(B^{2,0}_{p,q})$ holds by Lemma 1.2(i). In view of Lemma

1.2(ii), $S_5(D^{0,1}_{p,q}) = S_5(B^{2,0}_{p,q})$ holds. By direct computing, we have

$$\begin{aligned}\phi_{D^{0,1}_{p,q}}(P_4) - \phi_{B^{2,0}_{p,q}}(P_4) =& [(p-1)\times 1 + (q-2)(p-1)] \\ & - [(p-3)(q-1) + 2\times(q-1)] = 0,\\ \phi_{D^{0,1}_{p,q}}(K_{1,3}) - \phi_{B^{2,0}_{p,q}}(K_{1,3}) =& \left(\binom{p}{3} + \binom{q-1}{3}\right) \\ & - \left(\binom{p-2}{3} + \binom{q}{3} + 1\right) \\ =& \frac{-(q-3)^2+1}{4} < 0.\end{aligned}$$

The last inequality follows by $q > p \geqslant 4$. In view of Lemma 1.2(iii), we have $S_6(D^{0,1}_{p,q}) - S_6(B^{2,0}_{p,q}) = 3[-(q-3)^2+1] < 0$, i.e., $D^{0,1}_{p,q} \prec_s B^{2,0}_{p,q}$. That is to say, $B^{2,0}_{p,q}$ is the third last tree, in the S-order, among $\mathscr{T}_n^{p,q}$ for $p = \frac{q+4}{2}$.

If $p < \frac{q+4}{2}$, then in view of (2.5) we have $\phi_{D^{0,1}_{p,q}}(P_3) < \phi_{B^{2,0}_{p,q}}(P_3)$. By Lemma 1.2(i), $S_4(D^{0,1}_{p,q}) < S_4(B^{2,0}_{p,q})$ holds. So we have $D^{0,1}_{p,q} \prec_s B^{2,0}_{p,q}$. Hence, $B^{2,0}_{p,q}$ is the third last tree, in the S-order, among $\mathscr{T}_n^{p,q}$ for $p < \frac{q+4}{2}$.

This completes the proof of (ii). $\square$

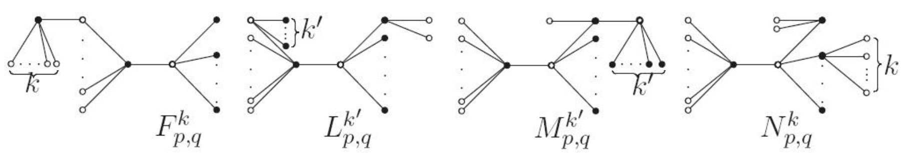

FIGURE 6. Trees $F^k_{p,q}, L^{k'}_{p,q}, M^{k'}_{p,q}$ and $N^k_{p,q}$ each of which contains p white points and q black points.

For convenience, let $F^k_{p,q}$, $L^{k'}_{p,q}$, $M^{k'}_{p,q}$ and $N^k_{p,q}$ $(1 \leqslant k \leqslant p-2, 1 \leqslant k' \leqslant q-2)$ be the trees as depicted in Fig. 6, it is easy to see that $F^k_{p,q}$, $L^{k'}_{p,q}$, $M^{k'}_{p,q}$, $N^k_{p,q}$ are in $\mathscr{T}_n^{p,q}$.

Theorem 2.4. *Given positive integers p and q with $4 \leqslant p < q$ and $p+q=n$.*

(i) *If $p > \frac{q+4}{2}$, then for any $T \in \mathscr{T}_n^{p,q} \setminus \{B^{0,0}_{p,q}, B^{0,1}_{p,q}, D^{0,1}_{p,q}\}$, we have $T \preceq_s B^{2,0}_{p,q}$ with equality if and only if $T \cong B^{2,0}_{p,q}$.*
(ii) *If $p = \frac{q+4}{2}$, then for any $T \in \mathscr{T}_n^{p,q} \setminus \{B^{0,0}_{p,q}, B^{0,1}_{p,q}, B^{2,0}_{p,q}\}$, we have $T \preceq_s D^{0,1}_{p,q}$ with equality if and only if $T \cong D^{0,1}_{p,q}$.*

(iii) *If* $p < \frac{q+4}{2}$, *then for any* $T \in \mathscr{T}_n^{p,q} \setminus \{B_{p,q}^{0,0}, B_{p,q}^{0,1}, B_{p,q}^{2,0}\}$, *we have* $T \preceq_s B_{p,q}^{0,2}$ *with equality if and only if* $T \cong B_{p,q}^{0,2}$.

Proof. For any $T \in \mathscr{T}_n^{p,q}$ such that $T \ncong B_{p,q}^{0,0}, B_{p,q}^{0,1}, D_{p,q}^{0,1}, B_{p,q}^{2,0}$, by a similar discussion as in the proof of Theorem 2.2, T can be transformed into $B_{p,q}^{0,0}$ (respectively, $B_{p,q}^{0,1}, D_{p,q}^{0,1}, B_{p,q}^{2,0}$) by carrying Operations I and II repeatedly. Let $\mathscr{C}_1$ (respectively, $\mathscr{D}_1$) denote the set of all trees in $\mathscr{T}_n^{p,q}$ which can be transformed into $D_{p,q}^{0,1}$ (respectively, $B_{p,q}^{2,0}$) by carrying Operation I once, and let $\mathscr{C}_2$ (respectively, $\mathscr{D}_2$) denote the set of all trees in $\mathscr{T}_n^{p,q}$ which can be transformed into $D_{p,q}^{0,1}$ (respectively, $B_{p,q}^{2,0}$) by carrying Operation II once.

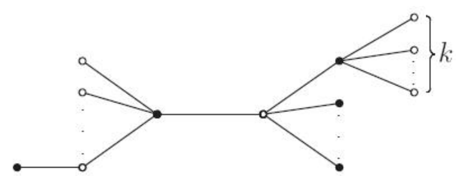

FIGURE 7. $Q_{p,q}^k$ which contains p white and q black points.

(i) $p > \frac{q+4}{2}$. The last tree, in the S-order, among $\mathscr{T}_n^{p,q} \setminus \{B_{p,q}^{0,0}, B_{p,q}^{0,1}, D_{p,q}^{0,1}\}$ must be in $\mathscr{A}_2 \cup \mathscr{B}_1 \cup \mathscr{B}_2 \cup \mathscr{C}_1 \cup \mathscr{C}_2$, where $\mathscr{A}_2$ is defined in the proof of Theorem 2.2, $\mathscr{B}_1$, $\mathscr{B}_2$ are defined in the proof of Theorem 2.3, while $\mathscr{C}_1 = \{D_{p,q}^{2,0}, D_{p,q}^{0,2}, C_{p,q}^1, F_{p,q}^1\}$, $\mathscr{C}_2 = \{F_{p,q}^k : 2 \leqslant k \leqslant q-2\} \cup \{Q_{p,q}^k : 2 \leqslant k \leqslant p-2\} \cup \{D_{p,q}^{k,1} : 2 \leqslant k \leqslant \lfloor \frac{q-2}{2} \rfloor\}$, where $Q_{p,q}^k$ is depicted in Fig. 7. We obtain (based on Lemmas 1.6(i)) that, for $k = 2, 3, \ldots, p-2$,

$$Q_{p,q}^k \prec_s Q_{p,q}^1.$$

Furthermore, we have

$$Q_{p,q}^1 \prec_s D_{p,q}^{2,0}.$$

In fact, by Lemma 1.1, $S_i(Q_{p,q}^1) = S_i(D_{p,q}^{2,0})$ holds for $i = 0, 1, 2, 3$. Note that $\phi_{Q_{p,q}^1}(P_2) = \phi_{D_{p,q}^{2,0}}(P_2) = n-1$, $\phi_{Q_{p,q}^1}(C_4) = \phi_{D_{p,q}^{2,0}}(C_4) = 0$. By Lemma 1.3, we have $\phi_{Q_{p,q}^1}(P_3) = \phi_{D_{p,q}^{2,0}}(P_3)$. Hence, we get $S_4(Q_{p,q}^1) = S_4(D_{p,q}^{2,0})$. In view of Lemma 1.2(iii), we obtain that

$$\begin{aligned} S_6(D_{p,q}^{2,0}) - S_6(Q_{p,q}^1) &= 6[(q-1)(q-2) - (p-2)(p-3)] + 6 \\ &> 6[(p-1)(p-2) - (p-2)(p-3)] + 6 \\ &= 12(p-2) + 6 > 0. \end{aligned}$$

Hence, we get $S_6(Q^1_{p,q}) < S_6(D^{2,0}_{p,q})$, i.e., $Q^1_{p,q} \prec_s D^{2,0}_{p,q}$.

In view of the proof of Facts 1 and 2 in the proof of Theorem 2.3, we know that the last tree, in the S-order, among $\mathscr{A}_2 \cup \mathscr{B}_1 \cup \mathscr{C}_1$ is $B^{2,0}_{p,q}$. In what follows we show that for any T in $\mathscr{C}_1 \cup \mathscr{B}_2$, we have $T \prec_s B^{2,0}_{p,q}$.

In fact, by Lemma 1.6(i), we have $C^k_{p,q} \prec_s C^1_{p,q}$ and $F^k_{p,q} \prec_s F^1_{p,q}$ for $k \geqslant 2$. By the proof of Theorem 2.3, we know that $C^1_{p,q} \prec_s B^{2,0}_{p,q}$ and $D^{0,2}_{p,q} \prec_s D^{2,0}_{p,q} \prec_s B^{2,0}_{p,q}$. By Lemma 1.1, we have $S_i(B^{2,0}_{p,q}) = S_i(F^1_{p,q})$ for $i = 0, 1, 2, 3$. In view of Lemma 1.2(i), it is routine to check that $\phi_{B^{2,0}_{p,q}}(P_2) = \phi_{F^1_{p,q}}(P_2) = n - 1$, $\phi_{B^{2,0}_{p,q}}(C_4) = \phi_{F^1_{p,q}}(C_4) = 0$. By Lemma 1.3,

$$\begin{aligned}
\phi_{B^{2,0}_{p,q}}(P_3) - \phi_{F^1_{p,q}}(P_3) &= \binom{p-2}{2} + \binom{q}{2} + \binom{3}{2} \\
&\quad - \left(\binom{p-1}{2} + \binom{q-1}{2} + 2\right) \\
&= q - p + 2 > 0.
\end{aligned}$$

Hence, $S_4(B^{2,0}_{p,q}) - S_4(F^1_{p,q}) = 4(q-p+2) > 0$, i.e., $F^1_{p,q} \prec_s B^{2,0}_{p,q}$. This completes the proof of (i).

In what follows, we consider $p \leqslant \frac{q+4}{2}$. By Lemmas 1.4, 1.5 and Theorem 2.3(ii), the last tree, in the S-order, among $\mathscr{T}^{p,q}_n \setminus \{B^{0,0}_{p,q}, B^{0,1}_{p,q}, B^{2,0}_{p,q}\}$ must be in $\mathscr{A}_1 \cup \mathscr{A}_2 \cup \mathscr{B}_1 \cup \mathscr{B}_2 \cup \mathscr{D}_1 \cup \mathscr{D}_2 \setminus \{B^{0,1}_{p,q}, B^{2,0}_{p,q}\}$, where $\mathscr{A}_1$, $\mathscr{A}_2$ are defined in the proof of Theorem 2.2, $\mathscr{B}_1$, $\mathscr{B}_2$ are defined in the proof of Theorem 2.3, while $\mathscr{D}_2 = \{L^k_{p,q} : 2 \leqslant k \leqslant q-2\} \cup \{M^k_{p,q} : 2 \leqslant k \leqslant q-2\} \cup \{N^k_{p,q} : 2 \leqslant k \leqslant p-4\}$, $\mathscr{D}_1 = \{B^{2,1}_{p,q}, B^{0,2}_{p,q}, L^1_{p,q}, M^1_{p,q}\}$ if $4 \leqslant p < 7$ and $\mathscr{D}_1 = \{B^{3,0}_{p,q}, B^{2,1}_{p,q}, B^{0,2}_{p,q}, L^1_{p,q}, M^1_{p,q}\}$ if $p \geqslant 7$.

(ii) $p = \frac{q+4}{2}$. In this case, we consider the following two cases according to $\mathscr{D}_1$.

Case 1. $\mathscr{D}_1 = \{B^{2,1}_{p,q}, B^{0,2}_{p,q}, L^1_{p,q}, M^1_{p,q}\}$ with $4 \leqslant p < 7$.

First we determine the last tree, in the S-order, among $\mathscr{D}_1 \cup \mathscr{D}_2$. It is easy to see (based on Lemma 1.4), we have $B^{2,1}_{p,q} \prec_s B^{0,2}_{p,q}$. Note that, for $k \geqslant 2$, by Lemma 1.6 we have $L^k_{p,q} \prec_s L^1_{p,q}$, $M^k_{p,q} \prec_s M^1_{p,q}$ and $N^k_{p,q} \preceq_s B^{2,1}_{p,q}$.

By Lemma 1.1, $S_i(L^1_{p,q}) = S_i(M^1_{p,q}) = S_i(B^{0,2}_{p,q})$ holds for $i = 0, 1, 2, 3$. By Lemma 1.2(i), we have $\phi_{L^1_{p,q}}(P_2) = \phi_{M^1_{p,q}}(P_2) = \phi_{B^{0,2}_{p,q}}(P_2) = n - 1$, $\phi_{L^1_{p,q}}(C_4) = \phi_{M^1_{p,q}}(C_4) = \phi_{B^{0,2}_{p,q}}(C_4) = 0$. Note that $L^1_{p,q}$ and $M^1_{p,q}$ have the same degree sequence, thus by Lemma 1.3 $\phi_{L^1_{p,q}}(P_3) = \phi_{M^1_{p,q}}(P_3)$. Hence,

$$\begin{aligned}\phi_{L^1_{p,q}}(P_3) - \phi_{B^{0,2}_{p,q}}(P_3) &= \phi_{M^1_{p,q}}(P_3) - \phi_{B^{0,2}_{p,q}}(P_3)\\ &= \left(\binom{p-2}{2} + \binom{q-1}{2} + 3 + 1\right)\\ &\quad - \left(\binom{p-2}{2} + \binom{q}{2} + 2\right)\\ &= 3 - q < 0.\end{aligned}$$

The last inequality follows by $q > p \geqslant 4$. By Lemma 1.2(i), we have $S_4(L^1_{p,q}) - S_4(B^{0,2}_{p,q}) = S_4(M^1_{p,q}) - S_4(B^{0,2}_{p,q}) = 4(\phi_{M^1_{p,q}}(P_3) - \phi_{B^{0,2}_{p,q}}(P_3)) < 0$, i.e., $L^1_{p,q} \prec_s B^{0,2}_{p,q}$ and $M^1_{p,q} \prec_s B^{0,2}_{p,q}$. Hence, $B^{0,2}_{p,q}$ is the last tree, in the S-order, among $\mathscr{D}_1 \cup \mathscr{D}_2$.

By the proof of Fact 2 in Theorem 2.3, we obtain that $B^{0,2}_{p,q}$ is the last graph, in the S-order, among $(\mathscr{B}_1 \cup \mathscr{B}_2) \setminus \{B^{2,0}_{p,q}\}$.

Note that for $p < 7$, it is routine to check that $(\mathscr{A}_1 \cup \mathscr{A}_2) \setminus \{B^{0,1}_{p,q}, B^{2,0}_{p,q}\} = \{D^{2,0}_{p,q}, D^{0,1}_{p,q}\}$. By Lemma 1.4, we have $D^{2,0}_{p,q} \prec_s D^{0,1}_{p,q}$. In order to complete the proof, it suffices to compare $B^{0,2}_{p,q}$ with $D^{0,1}_{p,q}$.

By Lemma 1.1, $S_i(D^{0,1}_{p,q}) = S_i(B^{0,2}_{p,q})$ holds for $i = 0, 1, 2, 3$. It is routine to check that $\phi_{D^{0,1}_{p,q}}(P_2) = \phi_{B^{0,2}_{p,q}}(P_2) = n - 1$ and $\phi_{D^{0,1}_{p,q}}(C_4) = \phi_{B^{0,2}_{p,q}}(C_4) = 0$. By Lemma 1.3,

$$\begin{aligned}\phi_{D^{0,1}_{p,q}}(P_3) - \phi_{B^{0,2}_{p,q}}(P_3) &= \left(\binom{p}{2} + \binom{q-1}{2} + 1\right) - \left(\binom{q}{2} + \binom{p-2}{2} + 2\right)\\ &= 2p - q - 3 = 1.\end{aligned}$$

In view of Lemma 1.2(i), we have $S_4(B^{0,2}_{p,q}) < S_4(D^{0,1}_{p,q})$, i.e.,

$$B^{0,2}_{p,q} \prec_s D^{0,1}_{p,q}. \tag{2.6}$$

That is to say, our result holds in this case.

Case 2. $\mathscr{D}_1 = \{B^{3,0}_{p,q}, B^{2,1}_{p,q}, B^{0,2}_{p,q}, L^1_{p,q}, M^1_{p,q}\}$ with $p \geqslant 7$.

First we determine the last tree, in the S-order, among $\mathscr{D}_1 \cup \mathscr{D}_2$. In fact, by a similar discussion as in Case 1 of determining the last graph, in the S-order, among $\mathscr{D}_1 \cup \mathscr{D}_2$, we can obtain that in this case, the last graph, in the S-order, among $(\mathscr{D}_1 \setminus \{B^{3,0}_{p,q}\}) \cup \mathscr{D}_2$ is just $B^{0,2}_{p,q}$. Hence, it suffices to compare $B^{3,0}_{p,q}$ with $B^{0,2}_{p,q}$.

In fact, by Lemma 1.1 $S_i(B^{0,2}_{p,q}) = S_i(B^{3,0}_{p,q})$ holds for $i = 0, 1, 2, 3$. It is routine to check that $\phi_{B^{3,0}_{p,q}}(P_2) = \phi_{B^{0,2}_{p,q}}(P_2) = n-1$ and $\phi_{B^{3,0}_{p,q}}(C_4) = \phi_{B^{0,2}_{p,q}}(C_4) = 0$. By Lemma 1.3 we have

$$\begin{aligned}\phi_{B^{0,2}_{p,q}}(P_3) - \phi_{B^{3,0}_{p,q}}(P_3) &= \left(\binom{p-2}{2} + \binom{q}{2} + 2\right) \\ &\quad - \left(\binom{p-3}{2} + \binom{q}{2} + \binom{4}{2}\right) \\ &= p - 7 \geqslant 0.\end{aligned}$$

If $p > 7$, by Lemma 1.2(i) $S_4(B^{0,2}_{p,q}) > S_4(B^{3,0}_{p,q})$, i.e., $B^{3,0}_{p,q} \prec_s B^{0,2}_{p,q}$.

If $p = 7$, we have $\phi_{B^{0,2}_{p,q}}(P_3) = \phi_{B^{3,0}_{p,q}}(P_3)$. By direct computing, we have $\phi_{B^{0,2}_{p,q}}(P_4) = \phi_{B^{3,0}_{p,q}}(P_4) = (p-1)(q-1)$ and

$$\begin{aligned}\phi_{B^{0,2}_{p,q}}(K_{1,3}) - \phi_{B^{3,0}_{p,q}}(K_{1,3}) &= \binom{p-2}{3} + \binom{q}{3} - \binom{p-3}{3} - \binom{q}{3} \\ &= \frac{1}{2}(p-3)(p-4) > 0.\end{aligned}$$

By Lemma 1.2(iii), we have $S_6(B^{0,2}_{p,q}) - S_6(B^{3,0}_{p,q}) = 6(p-3)(p-4) > 0$, i.e.,

$$B^{3,0}_{p,q} \prec_s B^{0,2}_{p,q}. \tag{2.7}$$

Hence, $B^{0,2}_{p,q}$ is the last graph, in the S-order, among $\mathscr{D}_1 \cup \mathscr{D}_2$ in this case.

By the proof of Fact 2 in Theorem 2.3, we obtain that $B^{0,2}_{p,q}$ is the last graph, in the S-order, among $(\mathscr{B}_1 \cup \mathscr{B}_2) \setminus \{B^{2,0}_{p,q}\}$.

Note that if $p \geqslant 7$, it is routine to check that

$$\begin{aligned}(\mathscr{A}_1 \cup \mathscr{A}_2) \setminus \{B^{0,1}_{p,q}, B^{2,0}_{p,q}\} =& \{D^{0,1}_{p,q}\} \cup \left\{B^{k,0}_{p,q} : 3 \leqslant k \leqslant \left\lfloor \frac{p-1}{2} \right\rfloor\right\} \\ & \cup \left\{D^{k,0}_{p,q} : 2 \leqslant k \leqslant \left\lfloor \frac{q-1}{2} \right\rfloor\right\}.\end{aligned} \tag{2.8}$$

By Lemma 1.4, we have $D^{2,0}_{p,q} \prec_s D^{0,1}_{p,q}$. In view of (2.1), (2.2) and (2.8), it suffices to compare $B^{3,0}_{p,q}$ with $D^{0,1}_{p,q}$.

In view of (2.7), we obtain that $B^{3,0}_{p,q} \prec_s B^{0,2}_{p,q}$. If $p \geqslant 7$, by a similar discussion as in the proof of (2.6), we can also show that $B^{0,2}_{p,q} \prec_s D^{0,1}_{p,q}$. Hence, $B^{3,0}_{p,q} \prec_s D^{0,1}_{p,q}$.

Combining with the proof as above, we obtain that $D^{0,1}_{p,q}$ is the fourth last tree, in the S-order, among $\mathscr{T}^{p,q}_n$. This completes the proof of (ii).

(iii) Let $p < \frac{q+4}{2}$. We proceed by considering the following two possible cases with respect to $\mathscr{D}_1$.

Case 1. $\mathscr{D}_1 = \{B^{2,1}_{p,q},\, B^{0,2}_{p,q},\, L^1_{p,q},\, M^1_{p,q}\}$ with $4 \leqslant p < 7$.

By a similar discussion as in the proof of Case 1 in (ii), we know that $B^{0,2}_{p,q}$ is the last tree, in the S-order, among $(\mathscr{A}_2 \cup \mathscr{B}_1 \cup \mathscr{B}_2 \cup \mathscr{D}_1 \cup \mathscr{D}_2) \setminus \{B^{2,0}_{p,q}\}$. Note that $p < 7$, it is routine to check that $\mathscr{A}_1 \setminus \{B^{0,1}_{p,q}\} = \{D^{0,1}_{p,q}\}$. In order to complete the proof, it suffices to compare $B^{0,2}_{p,q}$ with $D^{0,1}_{p,q}$.

By Lemma 1.1, $S_i(D^{0,1}_{p,q}) = S_i(B^{0,2}_{p,q})$ holds for $i = 0, 1, 2, 3$. It is routine to check that $\phi_{D^{0,1}_{p,q}}(P_2) = \phi_{B^{0,2}_{p,q}}(P_2) = n - 1$ and $\phi_{D^{0,1}_{p,q}}(C_4) = \phi_{B^{0,2}_{p,q}}(C_4) = 0$. By Lemma 1.3,

$$\begin{aligned}\phi_{D^{0,1}_{p,q}}(P_3) - \phi_{B^{0,2}_{p,q}}(P_3) &= \left(\binom{p}{2} + \binom{q-1}{2} + 1\right) - \left(\binom{q}{2} + \binom{p-2}{2} + 2\right)\\ &= 2p - q - 3.\end{aligned}$$

If $p < \frac{q+3}{2}$, by Lemma 1.2(i), we have $S_4(D^{0,1}_{p,q}) < S_4(B^{0,2}_{p,q})$, i.e., $D^{0,1}_{p,q} \prec_s B^{0,2}_{p,q}$.

If $p = \frac{q+3}{2}$, we have $S_4(D^{0,1}_{p,q}) = S_4(B^{0,2}_{p,q})$. By Lemma 1.2(ii), $S_5(D^{0,1}_{p,q}) = S_5(B^{0,2}_{p,q})$. By direct computing, we have $\phi_{D^{0,1}_{p,q}}(P_4) = \phi_{B^{0,2}_{p,q}}(P_4) = (p-1)(q-1)$ and

$$\begin{aligned}\phi_{D^{0,1}_{p,q}}(K_{1,3}) - \phi_{B^{0,2}_{p,q}}(K_{1,3}) &= \binom{p}{3} + \binom{q-1}{3} - \binom{p-2}{3} - \binom{q}{3}\\ &= \frac{-(q-2)^2 + 1}{4} < 0.\end{aligned}$$

Hence, by Lemma 1.2(iii), we have $S_6(D^{0,1}_{p,q}) - S_6(B^{0,2}_{p,q}) = 3[-(q-2)^2 + 1] < 0$, i.e., $D^{0,1}_{p,q} \prec_s B^{0,2}_{p,q}$. So in this case, $B^{0,2}_{p,q}$ is the fourth last tree, in the S-order, among $\mathscr{T}^{p,q}_n$.

Case 2. $\mathscr{D}_1 = \{B^{3,0}_{p,q},\, B^{2,1}_{p,q},\, B^{0,2}_{p,q},\, L^1_{p,q},\, M^1_{p,q}\}$ with $p \geqslant 7$.

By a similar discussion as in the proof of Case 2 in (ii), we know that $B^{0,2}_{p,q}$ is the last tree, in the S-order, among $(\mathscr{A}_2 \cup \mathscr{B}_1 \cup \mathscr{B}_2 \cup \mathscr{D}_1 \cup \mathscr{D}_2) \setminus \{B^{2,0}_{p,q}\}$. It is routine to check that $\mathscr{A}_1 \setminus \{B^{0,1}_{p,q}\} = \{D^{0,1}_{p,q}\}$. In order to complete the proof, it suffices to compare $B^{0,2}_{p,q}$ with $D^{0,1}_{p,q}$. By a similar discussion as in the proof of Case 1 in (iii), we have $D^{0,1}_{p,q} \prec_s B^{0,2}_{p,q}$. Hence, in this case $B^{0,2}_{p,q}$ is the fourth last tree in the S-order, among $\mathscr{T}^{p,q}_n$. This completes the proof of (iii). $\square$

Theorem 2.5. *If $4 \leqslant p = q$, then for any $T \in \mathscr{T}_n^{p,q} \setminus \{B_{p,q}^{0,0}, B_{p,q}^{0,1}, B_{p,q}^{2,0}\}$, we have $T \preceq_s B_{p,q}^{0,2}$ with equality if and only if $T \cong B_{p,q}^{0,2}$.*

Proof. Up to isomorphism, for any $T \in \mathscr{T}_n^{p,q} \setminus \{B_{p,q}^{0,0}, B_{p,q}^{0,1}, B_{p,q}^{2,0}\}$, by a similar discussion as above, T can be transformed into $B_{p,q}^{0,0}$ (respectively, $B_{p,q}^{0,1}$, $B_{p,q}^{2,0}$) by carrying the Operations I and II repeatedly. By Lemmas 1.4 and 1.5, the last tree, in the S-order, among $\mathscr{T}_n^{p,q} \setminus \{B_{p,q}^{0,0}, B_{p,q}^{0,1}, B_{p,q}^{2,0}\}$ must be in $\mathscr{A}_1 \cup \mathscr{A}_2 \cup \mathscr{B}_1 \cup \mathscr{B}_2 \cup \mathscr{D}_1 \cup \mathscr{D}_2 \setminus \{B_{p,q}^{0,1}, B_{p,q}^{2,0}\}$, where $\mathscr{A}_1$, $\mathscr{A}_2$ (respectively, $\mathscr{B}_1$, $\mathscr{B}_2$) are defined in the proof of Theorem 2.2 (respectively, Theorem 2.3), and $\mathscr{D}_1$, $\mathscr{D}_2$ are defined in the proof of Theorem 2.4. We proceed by considering the following two possible cases.

Case 1. $\mathscr{D}_1 = \{B_{p,q}^{2,1}, B_{p,q}^{0,2}, L_{p,q}^1, M_{p,q}^1\}$ with $4 \leqslant p < 7$.

By a similar discussion as the proof of Case 1 in Theorem 2.4(ii), we obtain that $B_{p,q}^{0,2}$ is the last tree, in the S-order, among $\mathscr{D}_1 \cup \mathscr{D}_2$. By the proof of Fact 2 in Theorem 2.3, we obtain that $B_{p,q}^{0,2}$ is the last graph, in the S-order, among $(\mathscr{B}_1 \cup \mathscr{B}_2) \setminus \{B_{p,q}^{2,0}\}$. It is routine to check that in this case $(\mathscr{A}_1 \cup \mathscr{A}_2) \setminus \{B_{p,q}^{0,1}, B_{p,q}^{2,0}\} = \emptyset$. Hence, $B_{p,q}^{0,2}$ is the last tree, in the S-order, among $\mathscr{T}_n^{p,q} \setminus \{B_{p,q}^{0,0}, B_{p,q}^{0,1}, B_{p,q}^{2,0}\}$.

Case 2. $\mathscr{D}_1 = \{B_{p,q}^{3,0}, B_{p,q}^{2,1}, B_{p,q}^{0,2}, L_{p,q}^1, M_{p,q}^1\}$ with $p \geqslant 7$.

By a similar discussion as the proof of Case 2 in Theorem 2.4(ii), we obtain that $B_{p,q}^{0,2}$ is the last tree, in the S-order, among $(\mathscr{D}_1 \cup \mathscr{D}_2 \cup \mathscr{A}_1 \cup \mathscr{A}_2) \setminus \{B_{p,q}^{0,1}, B_{p,q}^{2,0}\}$. By the proof of Fact 2 in Theorem 2.3, we obtain that $B_{p,q}^{0,2}$ is the last graph, in the S-order, among $(\mathscr{B}_1 \cup \mathscr{B}_2) \setminus \{B_{p,q}^{2,0}\}$. Hence, $B_{p,q}^{0,2}$ is the last tree, in the S-order, among $\mathscr{T}_n^{p,q} \setminus \{B_{p,q}^{0,0}, B_{p,q}^{0,1}, B_{p,q}^{2,0}\}$.

This completes the proof. □

3. Conclusion and remarks

Summarizing the results in Section 2, we can obtain the last four graphs in the S-order of the set of n-vertex trees with a (p, q)-bipartition.

Combining with Theorems 2.1, 2.2, 2.3(ii) and 2.4, we have

Theorem 3.1. *Given positive integers p, q with $4 \leqslant p < q$ and $p+q = n$.*

(i) *If $p > \frac{q+4}{2}$, the last four trees, in the S-order, among $\mathscr{T}_n^{p,q}$ are as follows: $B_{p,q}^{2,0}, D_{p,q}^{0,1}, B_{p,q}^{0,1}, B_{p,q}^{0,0}$.*

(ii) *If $p = \frac{q+4}{2}$, the last four trees, in the S-order, among $\mathscr{T}_n^{p,q}$ are as follows: $D_{p,q}^{0,1}, B_{p,q}^{2,0}, B_{p,q}^{0,1}, B_{p,q}^{0,0}$.*

(iii) *If* $p < \frac{q+4}{2}$, *the last four trees, in the* S*-order, among* $\mathscr{T}_n^{p,q}$ *are as follows:* $B_{p,q}^{0,2}, B_{p,q}^{2,0}, B_{p,q}^{0,1}, B_{p,q}^{0,0}$.

Combining with Theorems 2.1, 2.2, 2.3(i) and 2.5, we have

Theorem 3.2. *If* $4 \leqslant p = q$, *the last four trees, in the* S*-order, among the set* $\mathscr{T}_n^{p,q}$ *are as follows:* $B_{p,q}^{0,2}$, $B_{p,q}^{2,0}$, $B_{p,q}^{0,1}$, $B_{p,q}^{0,0}$.

In this paper, we determine the last four graphs, in the S-order, of the set of n-vertex trees with a (p, q)-bipartition. It is natural to consider the following research problem: How can we determine the first k graphs, in the S-order, of the set of n-vertex trees with a (p, q)-bipartition? It seems difficult but interesting.

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(Shuchao Li) Faculty of Mathematics and Statistics, Central China Normal University, 430079, Wuhan, P. R. China
E-mail address: `lscmath@mail.ccnu.edu.cn`

(Jiajia Zhang) Faculty of Mathematics and Statistics, Central China Normal University, 430079, Wuhan, P. R. China
E-mail address: `jjzhang08@foxmail.com`