TAIWANESE JOURNAL OF MATHEMATICS
Vol. 27, No. 4, pp. 647–683, August 2023
DOI: 10.11650/tjm/230204

On the Maximal Number of Maximum Dissociation Sets in Forests with Fixed Order and Dissociation Number

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Abstract. Given a graph G with $S \subseteq V_G$, we call S a maximum dissociation set if the induced subgraph $G[S]$ contains no path of order 3, and subject to this condition, the subset S has the maximum cardinality. The dissociation number of G is the cardinality of a maximum dissociation set. Inspired by the results of [26, 27] on the maximal number of maximum dissociation sets, in this contribution we investigate the maximal number of maximum dissociation sets in forests with fixed order and dissociation number. Firstly, a lower bound on the dissociation number of a forest with fixed order is established, and all extremal graphs are determined. Secondly, all trees (resp. forests) having the largest and the second largest number of maximum dissociation sets among trees (resp. forests) with given order and dissociation number are completely characterized. Finally, we show that the results in [26, 27] can be deduced by our results.

1. Introduction

We start by introducing the background information which will lead to our main results. Our main results will also be given in this section.

1.1. Background and definitions

In this paper, we consider only simple, undirected and finite graphs. Let $G = (V_G, E_G)$ be a graph, where V_G is its vertex set and E_G is its edge set. The *order* of G is the number $n = |V_G|$ of its vertices and its *size* is the number $|E_G|$ of its edges. Denote by P_n and $K_{1,n-1}$ the path and the star on n vertices, respectively. For two graphs G and H we define $G \cup H$ to be their disjoint union. In addition, we use kG to denote the disjoint union of k copies of G. Unless otherwise stated, we follow the traditional notation and terminology (see also [28]).

For a graph G with a vertex subset $S \subseteq V_G$, denote by $G[S]$ the subgraph of G induced by S. For a vertex $v \in V_G$, let $N_G(v)$ be the neighborhood of v in G, and

Received June 25, 2022; Accepted February 22, 2023.
Communicated by Daphne Der-Fen Liu.
2020 *Mathematics Subject Classification.* 05C69, 05C35, 05C75.
Key words and phrases. dissociation set, dissociation number, tree, forest.
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$N_G[v] := N_G(v) \cup \{v\}$ be the closed neighborhood of v in G. Denote by $d_G(v) := |N_G(v)|$ the *degree* of v in G. Here, as elsewhere, we drop the index referring to the underlying graph if the reference is clear. A vertex v is called a *pendant vertex* (or a *leaf*) of G if $d_G(v) = 1$. A vertex is called *quasi-pendant* if it is adjacent to some pendant vertex.

A subset S of V_G is a *dissociation set* if the induced subgraph $G[S]$ contains no path of order 3. A *maximum dissociation set* of G is a dissociation set with the maximum cardinality. The *dissociation number* of G, denoted by $\psi(G)$, is the cardinality of a maximum dissociation set in G. The problem of computing $\psi(G)$ has been proposed by Yannakakis [30] and was shown to be NP-complete for the class of bipartite graphs. It is also known that the problem is NP-complete for planar graphs with a maximum vertex degree of 4; see [24]. On the other hand, Cameron and Hell [7] showed that the problem is polynomially solvable for chordal graphs, weakly chordal graphs, asteroidal triple-free graphs, and interval-filament graphs. For more advances along this line, we refer the reader to see [1, 5, 22]. Note that a vertex subset S of G is a dissociation set if and only if its complement $V_G \setminus S$ is a 3-*path vertex cover*, i.e., a set of vertices intersecting every path of order 3 in G. The 3-path vertex cover problem is to find a minimum 3-path vertex cover in a given graph, which was extensively studied; see [4, 6, 14, 29].

An *independent set* in a graph is a set of pairwise non-adjacent vertices. The *independence number* of a graph G, denoted by $\alpha(G)$, is the maximum cardinality of an independent set. A *maximal independent set* is an independent set that is not a proper subset of any other independent sets. An independent set in G is *maximum* if it has cardinality $\alpha(G)$.

Around 1960, Erdős and Moser raised the following well-known problems: What is the maximum number of cliques in a graph with order n, and which graphs attaining this value? Both questions were solved by Moon and Moser [21], and this classical result initiates the study of the graphs with given order that have the maximum number of (maximal, or maximum) independent sets.

Characterizing graphs with the extremal number of maximal independent sets (resp. maximum independent sets) was extensively studied. Liu [18] and Li et al. [17] characterized the n-vertex bipartite graphs with the maximal number of maximal independent sets. Ying et al. [31] determined the n-vertex graphs with at most r cycles having the largest number of maximal independent sets. Jin et al. [10, 11] identified the trees (resp. general graphs) having the second and third largest number of maximal independent sets. Zito [32] determined the trees with the greatest number of maximum independent sets for n-vertex trees. Jou and Chang [12] obtained the maximum number of maximum independent sets of some families of graphs, such as trees, forests and triangle-free graphs. Alvarado et al. [2] proved that every tree with independence number α has at most $2^{\alpha-1}+1$ maximum independent sets.

In particular, the problem of identifying graphs of given order and independence number having maximal number of (maximal, or maximum) independent sets attracts much attention. Mohr and Rautenbach [19] determined the maximum number of maximum independent sets of trees with given order and independence number. In 2017, Lehner and Wagner [15] investigated connected graphs with fixed order and independence number which maximize the number of independent sets of any fixed cardinality. Mohr and Rautenbach [20] characterized all connected graphs with fixed order and independence number which maximize the number of maximum independent sets. For more advances on the number of maximal (resp. maximum) independent sets, we refer the readers to [3, 9, 13, 16, 23, 25] and the references cited therein.

Note that the dissociation set is a natural generalization of the independent set. Hence it is interesting and challenging to consider the problems on the number of dissociation sets as those of independent sets of graphs. Very recently, Tu, Zhang and Shi [27] characterized all trees having the maximum number of maximum dissociation sets among the set of trees with given order. Tu, Zhang and Du [26] determined all trees with the maximum number of maximum dissociation sets among trees with fixed dissociation number.

Motivated directly by the results of [19,20] and those of [26,27], in this contribution we consider the analogous problem of finding the maximal number of maximum dissociation sets and the extremal graphs for trees (resp. forests) with fixed order and dissociation number.

1.2. Basic notations and main results

In this subsection, we give some basic notation and then describe our main results. For a graph G, denote by $MD(G)$ the set of all maximum dissociation sets of G. Put $\Phi(G) := |MD(G)|$.

Our first main result establishes a lower bound on the dissociation number of a forest with fixed order, and all the corresponding extremal forests are characterized. For each positive integer i, we construct a sequence of trees R_i with order $3i$ as follows:

(i) $R_1 \cong P_3$;

(ii) if $i \geq 2$, then R_i is obtained by adding an edge to connect a vertex of R_{i-1} and a vertex of P_3.

Theorem 1.1. *Let F be a forest with order n. Then $\psi(F) \geq 2n/3$ with equality if and only if each component, say T, of F satisfies $|V_T| \equiv 0 \pmod 3$ and $T \cong R_{|V_T|/3}$.*

For $n \leq 2k+1$, denote by $T^*_{n,k}$ the graph obtained from the star $K_{1,k}$ by attaching a pendant edge to each of certain $n-k-1$ non-central vertices of $K_{1,k}$. Let $T_1, \ldots, T_r$

be r nontrivial trees. For $1 \leq i \leq r$, choose a pendant vertex v_i of T_i such that the degree of the unique neighbor of v_i is maximal. Define $O_{T_1,\dots,T_r}$ to be the tree obtained from $T_1,\dots,T_r$, by identifying $v_1,\dots,v_r$. We say the resulted vertex a *major vertex* of $O_{T_1,\dots,T_r}$. If $T_1\cup\cdots\cup T_r = a_1T_{i_1}\cup\cdots\cup a_tT_{i_t}$ with $a_1+\cdots+a_t = r$, then $O_{T_1,\dots,T_r}$ is denoted $O_{a_1T_{i_1},\dots,a_tT_{i_t}}$. Let $O^T_{a_1T_{i_1},\dots,a_tT_{i_t}}$ be the tree obtained by adding an edge to connect the major vertex of $O_{a_1T_{i_1},\dots,a_tT_{i_t}}$ and an arbitrary vertex of the tree T. Let $\mathfrak{T}(n,\psi)$ denote the set of trees with fixed order n and dissociation number ψ.

Our second result characterizes all trees with order n and dissociation number $\psi \in \{n, n-1, n-2\}$ having the largest and the second largest number of maximum dissociation sets.

Theorem 1.2. *Let T be in $\mathfrak{T}(n,\psi)$ with $\psi \in \{n, n-1, n-2\}$.*

(i) *If $\psi = n$, then $T \in \{P_1, P_2\}$ and $\Phi(T) = 1$.*

(ii) *If $\psi = n-1$, then $n \geq 3$ and*

$$\Phi(T) \leq \begin{cases} 3 & \text{if } n = 3, \\ 2 & \text{if } n = 4, \\ 1 & \text{if } n \geq 5. \end{cases}$$

Equality holds if and only if $T \in \mathcal{T}_1(n,n-1)$, where

$$\mathcal{T}_1(n,n-1) = \begin{cases} \{P_3\} & \text{if } n = 3, \\ \{P_4\} & \text{if } n = 4, \\ \{T^*_{n,k} : (n-1)/2 \leq k \leq n-1\} & \text{if } n \geq 5. \end{cases}$$

Furthermore, if $T \notin \mathcal{T}_1(n,n-1)$, then $T \cong K_{1,3}$ and $\Phi(T) = 1$.

(iii) *If $\psi = n-2$, then $n \geq 6$ and*

$$\Phi(T) \leq \begin{cases} 6 & \text{if } n = 6, \\ 4 & \text{if } n = 7, \\ 3 & \text{if } n \geq 8. \end{cases}$$

Equality holds if and only if $T \in \mathcal{T}_1(n,n-2)$, where

$$\mathcal{T}_1(n,n-2) = \begin{cases} \{P_6\} & \text{if } n = 6, \\ \{O_{P_2,P_3,P_4}, O_{P_2,P_3,K_{1,3}}\} & \text{if } n = 7, \\ \{O_{T_1,xP_2,yP_3} : T_1 \in \{P_4, K_{1,3}\} \text{ and } x + 2y = n-4\} & \\ \quad \cup\{O_{P_2,P_3,T^*_{5,3}}\} & \text{if } n \geq 8. \end{cases}$$

Furthermore, if $T \notin \mathcal{T}_1(n, n-2)$, then $\Phi(T) \le f(2)$, where

$$f(2) = \begin{cases} 5 & \text{if } n = 6, \\ 3 & \text{if } n = 7, \\ 2 & \text{if } n \ge 8. \end{cases}$$

Equality holds if and only if $T \in \mathcal{T}_2(n, n-2)$, where

$$\mathcal{T}_2(n, n-2) = \begin{cases} \{O_{2P_2,P_4}, O_{2P_2,K_{1,3}}\} & \text{if } n = 6, \\ \{P_7, O_{3P_2,P_4}, O_{3P_2,K_{1,3}}\} & \text{if } n = 7, \\ \{O_{T_1,xP_2,yP_3} : T_1 \in \{P_5, T^*_{5,3}\} \text{ and } x + 2y = n - 5\} & \\ \quad \setminus \{O_{P_2,P_3,T^*_{5,3}}\} & \text{if } n \ge 8. \end{cases}$$

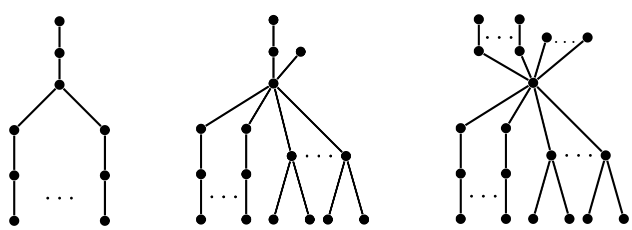
The next result characterizes all trees with fixed order n and dissociation number ψ ($\le n-3$) having the largest and the second largest number of maximum dissociation sets.

Theorem 1.3. *Let T be a tree in $\mathfrak{T}(n, \psi)$ with $n \ge 9$ and $n - \psi \ge 3$. Put $t := n - \psi$. Then*

$$\Phi(T) \le \begin{cases} 3^{t-1} + t + 1 & \text{if } n = 3t, \\ 3^{t-1} + 1 & \text{if } n = 3t + 1, \\ 3^{t-1} & \text{if } n \ge 3t + 2. \end{cases} \tag{1.1}$$

Equality holds if and only if $T \in \mathcal{T}_1(n, \psi)$ (see Figure 1.1), where

$$\mathcal{T}_1(n, \psi) = \begin{cases} \{O_{P_3,(t-1)P_4}\} & \text{if } n = 3t, \\ \{O_{P_2,P_3,t'P_4,(t-t'-1)K_{1,3}} : 0 \le t' \le t-1\} & \text{if } n = 3t + 1, \\ \{O_{xP_2,yP_3,t'P_4,(t-t'-1)K_{1,3}} : x + 2y = n - 3t + 2 & \\ \quad \text{and } 0 \le t' \le t - 1\} & \text{if } n \ge 3t + 2. \end{cases}$$



(a) $n = 3t$ (b) $n = 3t + 1$ (c) $n \ge 3t + 2$

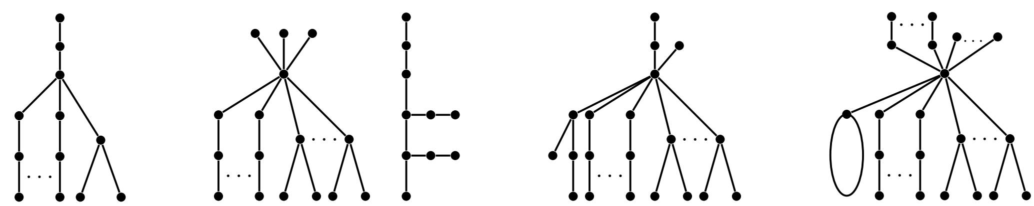
Figure 1.1: Trees in $\mathcal{T}_1(n, \psi)$.

Furthermore, if $T \notin \mathcal{T}_1(n,\psi)$, then $\Phi(T) \le f(t)$, where

$$f(t) = \begin{cases} 3^{t-1}+t & \text{if } n = 3t, \\ 3^{t-1} & \text{if } n = 3t+1, \\ 2\cdot 3^{t-2}+1 & \text{if } n = 3t+2, \\ 2\cdot 3^{t-2} & \text{if } n \ge 3t+3. \end{cases} \tag{1.2}$$

Equality holds if and only if $T \in \mathcal{T}_2(n,\psi)$ (see Figure 1.2), where

$$\mathcal{T}_2(n,\psi) = \begin{cases} \{O_{P_3,(t-2)P_4,K_{1,3}}\} & \text{if } n = 3t, \\ \{O_{3P_2,t'P_4,(t-t'-1)K_{1,3}} : 0 \le t' \le t-1\} \cup \{O_{P_3,P_4,T^*_{5,3}}\} & \text{if } n = 3t+1, \\ \{O_{P_2,P_3,T^*_{5,3},t'P_4,(t-t'-2)K_{1,3}} : 0 \le t' \le t-2\} & \text{if } n = 3t+2, \\ \{O^{P_{2l}}_{xP_2,yP_3,t'P_4,(t-t'-l)K_{1,3}} : x+2y = n-3t+l-1, & \\ \quad 0 \le t' \le t-l \text{ and } l \in \{2,3\}\} & \text{if } n \ge 3t+3. \end{cases}$$



(a) $n = 3t$ (b) $n = 3t+1$ (c) $n = 3t+2$ (d) $n \ge 3t+3$

Figure 1.2: Trees in $\mathcal{T}_2(n,\psi)$, and the ellipse in the last graph stands for P_{2l} with $l \in \{2,3\}$.

Denote by $\mathfrak{F}(n,\psi)$ the set of forests with order n and dissociation number ψ, and each of which does not contain P_1 or P_2 as a component (i.e., the order of each component is at least 3).

Our last main result characterizes all the forests with the largest and second largest number of maximum dissociation sets among $\mathfrak{F}(n,\psi)$.

Theorem 1.4. *Let F be a forest in $\mathfrak{F}(n,\psi)$ with at least two components and let $t := n-\psi$. Then $n \ge 6$ and*

$$\Phi(F) \le \begin{cases} 3^{t} & \text{if } n = 3t, \\ 2\cdot 3^{t-1} & \text{if } n = 3t+1, \\ 4\cdot 3^{t-2} & \text{if } n = 3t+2, \\ 3^{t-1} & \text{if } n \ge 3t+3. \end{cases} \tag{1.3}$$

Equality holds if and only if $F \in \mathcal{F}_1(n,\psi)$, *where*

$$\mathcal{F}_1(n,\psi) = \begin{cases} \{tP_3\} & \text{if } n = 3t, \\ \{P_4 \cup (t-1)P_3\} & \text{if } n = 3t+1, \\ \{2P_4 \cup (t-2)P_3\} & \text{if } n = 3t+2, \\ \{T \cup lP_3 : T \in \mathcal{T}_1(n-3l, \psi-2l) \text{ and } 0 < l < t\} & \text{if } n \geq 3t+3. \end{cases}$$

Furthermore, if $F \in \mathfrak{F}(n,\psi) \setminus \mathcal{F}_1(n,\psi)$, *then* $n \geq 7$, $t \geq 2$ *and the following hold:*

(i) *If* $t = 2$, *then* $\Phi(F) \leq h(2)$, *where*

$$h(2) = \begin{cases} 3 & \text{if } n \in \{7,8\}, \\ 2 & \text{if } n \geq 9. \end{cases} \tag{1.4}$$

Equality holds if and only if $F \in \mathcal{F}_2(n, n-2)$, *where*

$$\mathcal{F}_2(n,n-2) = \begin{cases} \{K_{1,3} \cup P_3\} & \text{if } n = 7, \\ \{T \cup P_3 : T \in \mathcal{T}_1(5,4)\} & \text{if } n = 8, \\ \{T \cup P_4 : T \in \mathcal{T}_1(n-4, n-5)\} & \text{if } n \geq 9. \end{cases}$$

(ii) *If* $t \geq 3$, *then* $\Phi(F) \leq h(t)$, *where*

$$h(t) = \begin{cases} 2 \cdot 3^{t-1} & \text{if } n = 3t, \\ 4 \cdot 3^{t-2} & \text{if } n = 3t+1, \\ 3^{t-1} & \text{if } n = 3t+2, \\ 8 \cdot 3^{t-3} & \text{if } n = 3t+3, \\ 2 \cdot 3^{t-2} & \text{if } n \geq 3t+4. \end{cases} \tag{1.5}$$

Equality holds if and only if $F \in \mathcal{F}_2(n,\psi)$, *where*

$$\begin{aligned} &\mathcal{F}_2(n,\psi) \\ &= \begin{cases} \{P_6 \cup (t-2)P_3\} & \text{if } n = 3t, \\ \{T \cup (t-2)P_3 : T \in \mathcal{T}_1(7,5)\} \cup \{P_6 \cup P_4 \cup (t-3)P_3\} & \text{if } n = 3t+1, \\ \{T \cup lP_3 : T \in \mathcal{T}_1(n-3l, \psi-2l) \text{ with } 0 < l < t\} & \text{if } n = 3t+2, \\ \{3P_4 \cup (t-3)P_3\} & \text{if } n = 3t+3, \\ \{T \cup P_{2s} \cup lP_3 : s \in \{2,3\}, T \in \mathcal{T}_1(n-2s-3l, \psi-s-2l-1) & \\ \quad \text{and } l+s \leq t\} & \\ \quad \cup \{T \cup lP_3 : T \in \mathcal{T}_2(n-3l, \psi-2l) \text{ and } 0 < l < t-1\} & \text{if } n \geq 3t+4. \end{cases} \end{aligned}$$

The remainder of this paper is organized as follows: In Section 2 we give the proof of Theorem 1.1. In Section 3 we present the proofs of Theorems 1.2 and 1.3. In Section 4 we give the proof of Theorem 1.4. In the last section, we give some brief comments on our findings and show that all main results in [26, 27] can be deduced by the results obtained in this paper.

2. Proof of Theorem 1.1

In this section, we give the proof of Theorem 1.1, which establishes a lower bound on the dissociation number of a forest with fixed order, and all the corresponding extremal graphs are characterized.

In a rooted tree with root r, the *level* of a vertex v, denoted by $l(v)$, is the length of the unique path rTv from the root r to the vertex v. Each vertex on the path rTv, not including the vertex v itself, is called an *ancestor* of v, and each vertex with v as its ancestor is a *descendant* of v. The immediate ancestor of v is its *parent*, and the vertices whose parent is v are its *children*.

Proof of Theorem 1.1. In order to complete the proof, it suffices to show $\psi(T) \geq 2|V_T|/3$ for each tree T. We prove this result by induction on the order n of a tree T.

If $1 \leq n \leq 6$, then it is straightforward to check that $\psi(T) \geq 2n/3$ and the equality holds if and only if $T \cong R_1$ if $n = 3$ and $T \cong R_2$ if $n = 6$, as desired. Next, we assume that the result is true for each tree with order less than n.

Now, let T be a tree with order n (≥ 7). Change the tree T into a rooted tree by choosing any vertex as the root. Assume u is a vertex such that all of its children are leaves, and subject to this condition, the level of u is as large as possible. If $l(u) = 0$, then $T \cong K_{1,n-1}$ and so $\psi(T) = n - 1 > 2n/3$, as desired. So, in what follows, we assume that $l(u) \geq 1$.

If $d_T(u) \geq 3$, i.e., u has at least two children, then let T' be a tree obtained from T by deleting u and all of its children. It is routine to check that $|V_{T'}| = n - d_T(u) < n$ and $\psi(T') = \psi(T) - d_T(u) + 1$. By applying induction on T', one has

$$\psi(T') \geq \frac{2|V_{T'}|}{3}. \tag{2.1}$$

The equality in (2.1) holds if and only if $|V_{T'}| \equiv 0 \pmod 3$ and $T' \cong R_{|V_{T'}|/3}$. Therefore,

$$\psi(T) \geq \frac{2n + d_T(u) - 3}{3} \geq \frac{2n}{3},$$

and $\psi(T) = 2n/3$ holds if and only if $|V_{T'}| \equiv 0 \pmod 3$, $T' \cong R_{|V_{T'}|/3}$ and $d_T(u) = 3$, which is equivalent to $n \equiv 0 \pmod 3$ and $T \cong R_{n/3}$, as desired.

We consider the rest case, i.e., $d_T(u) = 2$. Let w be the parent of u. In view of the proof as above, it is sufficient to consider that each children of w is either a pendant vertex or a quasi-pendant vertex with degree two in T. Let $T'' = T - T_w$, where T_w is a subtree of T rooted at w. Put $a_i := \{v : v \in N_{T_w}(w) \text{ and } d_{T_w}(v) = i\}$ for $i \in \{1, 2\}$. It is straightforward to check that $|V_{T''}| = n - a_1 - 2a_2 - 1 < n$ and $\psi(T'') = \psi(T) - a_1 - 2a_2$. Applying induction on T'' yields

$$\psi(T'') \geq \frac{2|V_{T''}|}{3}. \tag{2.2}$$

The equality in (2.2) holds if and only if $|V_{T''}| \equiv 0 \pmod 3$ and $T'' \cong R_{|V_{T''}|/3}$. It follows that

$$\psi(T) \geq \frac{2n + a_1 + 2a_2 - 2}{3} \geq \frac{2n}{3},$$

the last inequality follows by $a_1 + 2a_2 \geq 2a_2 \geq 2$. In addition, $\psi(T) = 2n/3$ holds if and only if $|V_{T''}| \equiv 0 \pmod 3$, $T'' \cong R_{|V_{T''}|/3}$ and $a_1 + 2a_2 = 2$, that is to say, $n \equiv 0 \pmod 3$ and $T \cong R_{n/3}$, as desired.

This completes the proof. □

3. Proofs of Theorems 1.2 and 1.3

In this section, we give the proofs of Theorems 1.2 and 1.3, which characterize trees with the maximal number of maximum dissociation sets among $\mathfrak{T}(n, \psi)$. All trees with order at most 10 are listed in Appendix of [8]. Hence, we can use it to check the result of Theorem 1.2(ii)–(iii) for trees with smaller orders.

Proof of Theorem 1.2. (i) Let $t := n - \psi$. If $t = 0$, then each maximum dissociation set contains all vertices of T. Hence T does not contain any path of order 3. It follows that $n \in \{1, 2\}$. Then the assertion follows immediately.

(ii) In view of Theorem 1.1, one has $n \geq 3t = 3$. Let S be a maximum dissociation set of T and let v be the unique vertex not in S. Hence $G[S] \cong aP_1 \cup bP_2$ for some nonnegative integers a, b with $a + 2b = n - 1$. Therefore, $T \cong T^*_{n,a+b}$.

If $n = 3$, then $T \cong P_3$ and $\Phi(T) = 3$. If $n = 4$, then $T \in \{P_4, K_{1,3}\}$. Clearly, $\Phi(T) = 2$ if $T \cong P_4$ and $\Phi(T) = 1$ if $T \cong K_{1,3}$. If $n \geq 5$, then either $b = 2$ or $a + b \geq 3$ holds. Hence all maximum dissociation sets do not contain v. Therefore, $V_T \setminus \{v\}$ is the unique maximum dissociation set of T and so $\Phi(T) = 1$.

(iii) Based on Theorem 1.1, one has $n \geq 3t = 6$. If $T \in \mathfrak{T}(6, 4)$, then $T \in \{P_6, O_{2P_2,P_4},$

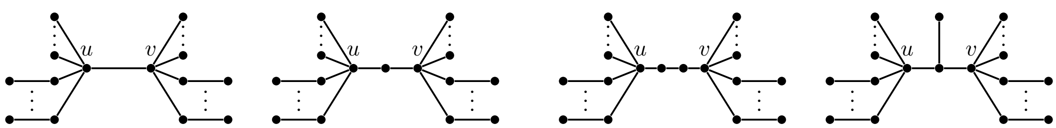
$O_{2P_2,K_{1,3}}\}$. Clearly, $\Phi(O_{2P_2,P_4}) = \Phi(O_{2P_2,K_{1,3}}) = 5 < 6 = \Phi(P_6)$. If $T \in \mathfrak{T}(7,5)$, then

$$\Phi(T) = \begin{cases} 4 & \text{if } T \in \{O_{P_2,P_3,P_4}, O_{P_2,P_3,K_{1,3}}\}, \\ 3 & \text{if } T \in \{P_7, O_{3P_2,P_4}, O_{3P_2,K_{1,3}}\}, \\ 2 & \text{if } T \in \{O_{2P_2,P_5}\}, \\ 1 & \text{otherwise.} \end{cases}$$

If $T \in \mathfrak{T}(8,6)$, then

$$\Phi(T) = \begin{cases} 3 & \text{if } T \in \{O_{T_1,xP_2,yP_3} : T_1 \in \{P_4, K_{1,3}\} \text{ and } x+2y=4\} \cup \{O_{P_2,P_3,T^*_{5,3}}\}, \\ 2 & \text{if } T \in \{O_{T_1,xP_2,yP_3} : T_1 \in \{P_5, T^*_{5,3}\} \text{ and } x+2y=3\} \setminus \{O_{P_2,P_3,T^*_{5,3}}\}, \\ 1 & \text{otherwise.} \end{cases}$$

Next, we consider $n \geq 9$. Let S be a maximum dissociation set of T and assume that $\{u,v\} = V_T \setminus S$. Then $|S| = n-2$ and $G[S] \cong aP_1 \cup bP_2$ for some nonnegative integers a, b with $a + 2b = n-2$. It is routine to check that T must be one of the following graphs depicted in Figure 3.1. Assume, without loss of generality, that $N_{T_i}(u) \setminus \{v\}$ (resp. $N_{T_i}(v) \setminus \{u\}$) contains a_{i1} (resp. a_{i2}) pendant vertices and b_{i1} (resp. b_{i2}) quasi-pendant vertices with $a_{i1} + 2b_{i1} \geq a_{i2} + 2b_{i2}$, here $i \in \{1,2,3,4\}$.



(a) T_1 (b) T_2 (c) T_3 (d) T_4

Figure 3.1: All possible structures of T if $n - \psi = 2$.

Assume that $T \cong T_i$ for some $i \in \{1,2,3,4\}$. If $a_{i1} + 2b_{i1} \geq 4$ or $a_{i1} = 3$ and $b_{i1} = 0$, then each maximum dissociation set of T does not contain u. Put $T' := T - T_u$. Therefore, $\Phi(T) = \Phi(T')$. Note that $|V_{T'}| - \psi(T') = 1$. Together with (ii), one has $\Phi(T') \leq 3$ and the equality holds if and only if $T' \cong P_3$. Hence $\Phi(T) \leq 3$ and the equality holds if and only if $T \in \mathcal{T}_1(n, n-2)$. On the other hand, if $T' \ncong P_3$, then $\Phi(T') \leq 2$ and the equality holds if and only if $T' \cong P_4$. It follows that if $T \notin \mathcal{T}_1(n, n-2)$, then $\Phi(T) \leq 2$ and the equality holds if and only if $T \in \mathcal{T}_2(n, n-2)$, as desired.

Note that $n \geq 9$. So, in what follows, it suffices to consider that $a_{i1} = 1$ and $b_{i1} = 1$. Clearly, T can not be the first graph T_1 in Figure 3.1. If $T \cong T_2$, then $a_{22} + 2b_{22} = 3$. Therefore, $a_{22} = 3$ and $b_{22} = 0$, or $a_{22} = 1$ and $b_{22} = 1$. It is routine to check that $\Phi(T) = 1$.

If $T \cong T_3$, then $2 \leq a_{32} + 2b_{32} \leq 3$. If $a_{32} + 2b_{32} = 2$, then $a_{32} = 2$ and $b_{32} = 0$, or $a_{32} = 0$ and $b_{32} = 1$. If $a_{32} + 2b_{32} = 3$, then either $a_{32} = 3$ and $b_{32} = 0$, or $a_{32} = 1$ and $b_{32} = 1$ holds. It is routine to check that, in all cases, $\Phi(T) = 1$.

If $T \cong T_4$, then by a similar discussion as above, we obtain $\Phi(T) = 1$.

Consequently, we infer that for $n \geq 9$, $\Phi(T) \leq 3$ and the equality holds if and only if $T \in \mathcal{T}_1(n, n-2)$, and $\Phi(T) \leq 2$ if $T \notin \mathcal{T}_1(n, n-2)$ and the equality holds if and only if $T \in \mathcal{T}_2(n, n-2)$.

This completes the proof. $\square$

Next, we give the proof of Theorem 1.3, which concentrates on trees with order $n \geq 9$ and dissociation number $\psi \leq n-3$. In the following discussion, we call a tree *special* if it is isomorphic to a tree in the family $\mathcal{T}_2(n, \psi)$ for $\psi \leq n-2$. For a graph G, denote by $t(G) := |V_G| - \psi(G)$. For a vertex $v \in V_G$, let

$$\begin{aligned}
\Phi_v(G) &= |\{S \in MD(G) : v \in S\}|, \\
\Phi_{\overline{v}}(G) &= |\{S \in MD(G) : v \notin S\}|, \\
\Phi_v^0(G) &= |\{S \in MD(G) : v \in S \text{ and } d_{G[S]}(v) = 0\}|, \\
\Phi_v^1(G) &= |\{S \in MD(G) : v \in S \text{ and } d_{G[S]}(v) = 1\}|.
\end{aligned}$$

Proof of Theorem 1.3. It is straightforward to check that for a tree $T \in \mathcal{T}_1(n, \psi)$, $\Phi(T)$ attains the upper bound in (1.1). By a direct calculation, we obtain that the upper bound in (1.1) is larger than $f(t)$ given in (1.2) for $t \geq 3$. Hence, in order to prove the theorem, it suffices to show that if $T \in \mathfrak{T}(n, \psi) \setminus \mathcal{T}_1(n, \psi)$, then $\Phi(T) \leq f(t)$ and the equality holds if and only if $T \in \mathcal{T}_2(n, \psi)$.

Suppose, to the contrary, that the result is false. Among all the counterexamples, choose $T_0 \in \mathfrak{T}(n, \psi) \setminus \mathcal{T}_1(n, \psi)$ such that its order is as small as possible. Put $n_0 := |V_{T_0}|$, $\psi_0 := |\psi(T_0)|$ and $t_0 := n_0 - \psi_0$. Note that $n_0 \geq 9$ and $t_0 \geq 3$. Since T_0 is a counterexample, T_0 satisfies

(i) either $\Phi(T_0) > f(t_0)$;

(ii) or $\Phi(T_0) = f(t_0)$ but T_0 is not special.

To prove this theorem, we first develop several lemmas. In particular, for a path $P_k = v_1 v_2 \ldots v_k$, we define $v_{\lceil k/2 \rceil}$ to be the major vertex of P_k. The subsequent result can be checked directly, and we omit the detailed proof here.

Lemma 3.1. *Let T be a tree in $\mathcal{T}_1(|V_T|, \psi(T))$ with $t(T) \geq 1$ and v be a vertex of T. Then $\Phi_{\overline{v}}(T) \leq 2$ if $T \cong O_{P_2, P_3, T^*_{5,3}}$, and $\Phi_{\overline{v}}(T) \leq 3^{t(T)-1}$ otherwise. The equality holds if and* *only if v is the major vertex of T or any vertex of P_3. In addition, if v is not the major vertex of T, then*

$$\Phi_{\overline{v}}(T) \leq \begin{cases} 3^{t(T)-2} + t(T) & \text{if } |V_T| = 3t(T), \\ 3^{t(T)-2} + 1 & \text{if } |V_T| = 3t(T) + 1, \\ 3^{t(T)-2} & \text{if } |V_T| \geq 3t(T) + 2. \end{cases}$$

Lemma 3.2. *Let T be a tree not in $\mathcal{T}_1(|V_T|, \psi(T))$ with $|V_T| < |V_{T_0}| - 1$. Assume that $t(T) \geq 1$ and v is a vertex of T. Then*

$$\Phi_{\overline{v}}(T) \leq \begin{cases} 3^{t(T)-1} & \text{if } |V_T| = 3t(T) \text{ or } 3t(T)+1, \\ 2 \cdot 3^{t(T)-2} & \text{if } |V_T| \geq 3t(T) + 2. \end{cases} \tag{3.1}$$

In particular, if $T \cong P_7$, then $\Phi_{\overline{v}}(T) \leq 2$ and the equality holds if and only if v is adjacent to the major vertex of T; if $T \cong O_{P_3,P_4,T^*_{5,3}}$, then $\Phi_{\overline{v}}(T) \leq 6$ and the equality holds if and only if v is a vertex with maximum degree in T.

Proof. Let v be a vertex of T. If $t(T) = 1$, then $T \cong K_{1,3}$ and $\Phi_{\overline{v}}(T) \leq 1$, as desired. Next, we consider the case $t(T) \geq 2$. By the choice of T_0, we know that $\Phi(T) \leq f(t(T))$ with equality if and only if T is special. Hence (3.1) holds for $|V_T| = 8$, or $|V_T| = 3t(T)+1$, or $|V_T| \geq 3t(T) + 3$. Next, we consider $|V_T| = 3t(T) + 2$ and $|V_T| \neq 8$. If T is not special, then the result holds immediately. If T is special, it is routine to check that each vertex is contained in some maximum dissociation set of T. Hence $\Phi_{\overline{v}}(T) \leq \Phi(T) - 1 = 2 \cdot 3^{t(T)-2}$, as desired.

Now, we consider the case $|V_T| = 3t(T)$. If $\Phi_{\overline{v}}(T) = 0$, then we are done. If $\Phi_{\overline{v}}(T) \neq 0$, then let T' be a tree obtained from T by attaching a pendant vertex u to v. Then $\Phi_{\overline{v}}(T) \leq \Phi(T')$. In addition,

$$|V_{T'}| = |V_T| + 1 \leq n_0 - 1 \quad \text{and} \quad \psi(T') = \psi(T) + 1,$$

where $n_0 = |V_{T_0}|$. Hence $t(T') = t(T)$ and $|V_{T'}| = 3t(T') + 1$. If $T' \in \mathcal{T}_1(|V_{T'}|, \psi(T'))$, then v is a quasi-pendant vertex of $O_{P_2,P_3,t'P_4,(t(T)-t'-1)K_{1,3}}$ for some integer t' with $0 \leq t' \leq t(T) - 1$. That is to say, T is a graph obtained from $O_{P_2,P_3,t'P_4,(t(T)-t'-1)K_{1,3}}$ by deleting the pendant vertex which is adjacent to v. It is straightforward to check that $\Phi_{\overline{v}}(T) \leq 3^{t(T)-1}$, as desired. If $T' \notin \mathcal{T}_1(|V_{T'}|, \psi(T'))$, then by the choice of T_0, one has $\Phi_{\overline{v}}(T) \leq \Phi(T') \leq f(t(T')) = 3^{t(T)-1}$, as desired.

If $T \in \{P_7, O_{P_3,P_4,T^*_{5,3}}\}$, the results can be checked easily. This completes the proof. □

Lemma 3.3. *Let u be a quasi-pendant vertex of T_0. Then u has exactly one child.*

Proof. Suppose that u has a children, where $a \geq 2$. Let w be the parent of u, and let $T' = T_0 - (N[u] \setminus \{w\})$. Hence $|V_{T'}| = n_0 - a - 1 < n_0$. Put $t' := t(T')$. We proceed by distinguishing two possible cases.

Case 1*:* $a = 2$. In this case, $|V_{T'}| = n_0 - 3$ and $\psi(T') = \psi_0 - 2$. Hence $t' = t_0 - 1 \geq 2$. Note that a maximum dissociation set of T' containing w can be extended in a unique way to a maximum dissociation set of T_0, and a maximum dissociation set of T' not containing w can be extended in exactly three ways to a maximum dissociation set of T_0. Note that each maximum dissociation set in T_0 must be the form as above. Thus,

$$\Phi(T_0) = \Phi_w(T') + 3\Phi_{\overline{w}}(T') = \Phi(T') + 2\Phi_{\overline{w}}(T').$$

If $T' \notin \mathcal{T}_1(|V_{T'}|, \psi(T'))$, then by the choice of T_0, we know that $\Phi(T') \leq f(t')$ with equality if and only if T' is special. Together with Theorem 1.2(iii) and Lemma 3.2, one has

$$\Phi(T_0) = \Phi(T') + 2\Phi_{\overline{w}}(T') \leq \begin{cases} 3^{t_0-2} + t_0 - 1 + 2 \cdot 3^{t_0-2} & \text{if } n_0 = 3t_0, \\ 3^{t_0-2} + 2 \cdot 3^{t_0-2} & \text{if } n_0 = 3t_0 + 1, \\ 2 \cdot 3^{t_0-3} + 1 + 4 \cdot 3^{t_0-3} & \text{if } n_0 = 3t_0 + 2, \\ 2 \cdot 3^{t_0-3} + 4 \cdot 3^{t_0-3} & \text{if } n_0 \geq 3t_0 + 3. \end{cases}$$

Hence, if $n_0 = 3t_0$, then $\Phi(T_0) < 3^{t_0-1} + t_0$, a contradiction. If $n_0 = 3t_0 + 1$, then $\Phi(T_0) \leq 3^{t_0-1}$ and the equality holds if and only if T' is special and $\Phi_{\overline{w}}(T') = 3^{t_0-2}$. It follows that w is the major vertex of T' and $T' \notin \{P_7, O_{P_3,P_4,T^*_{5,3}}\}$. Therefore, T_0 is special, a contradiction. If $n_0 \geq 3t_0 + 2$, then $\Phi(T_0) \leq f(t_0)$ and the equality holds if and only if T' is special with $n' \neq 8$ and $\Phi_{\overline{w}}(T') = 2 \cdot 3^{t_0-3}$. Thus, w is the major vertex of T'. That is to say, $\Phi(T_0) = f(t_0)$ holds if and only if T_0 is special, a contradiction.

Next, we assume that $T' \in \mathcal{T}_1(|V_{T'}|, \psi(T'))$. If $n_0 = 3t_0$, then in view of (1.1) and Lemma 3.1, one has

$$\Phi(T_0) = \Phi(T') + 2\Phi_{\overline{w}}(T') \leq 3^{t_0-2} + t_0 + 2 \cdot 3^{t_0-2} = 3^{t_0-1} + t_0$$

and the equality holds if and only if $\Phi_{\overline{w}}(T') = 3^{t_0-2}$, i.e., w is the major vertex of T'. It follows that T_0 is special, a contradiction. If $n_0 \geq 3t_0 + 1$ and $T' \ncong O_{P_2,P_3,T^*_{5,3}}$, then together with $T_0 \notin \mathcal{T}_1(n_0, \psi_0)$, we obtain that w is not the major vertex of T'. In view of (1.1) and Lemma 3.1, one has

$$\Phi(T_0) = \Phi(T') + 2\Phi_{\overline{w}}(T') \leq \begin{cases} 3^{t_0-2} + 1 + 2 \cdot 3^{t_0-3} + 2 & \text{if } n_0 = 3t_0 + 1, \\ 3^{t_0-2} + 2 \cdot 3^{t_0-3} & \text{if } n_0 \geq 3t_0 + 2. \end{cases}$$

Clearly, $\Phi(T_0) < f(t_0)$ if $n_0 \geq 3t_0+1$, which contradicts the choice of T_0. If $T' \cong O_{P_2,P_3,T^*_{5,3}}$, then by Lemma 3.1, one has $\Phi(T_0) = \Phi(T') + 2\Phi_{\overline{w}}(T') \leq 7$ and the equality holds if and only if w is the major vertex of T', which implies that T_0 is special, a contradiction.

Case 2: $a \geq 3$. In this case, each maximum dissociation set of T_0 contains all children of u and hence does not contain u. Therefore, S is a maximum dissociation set of T' if and only if $S \cup (N(u) \setminus \{w\})$ is a maximum dissociation set of T_0. That is, $\Phi(T_0) = \Phi(T')$. Furthermore, $\psi(T') = \psi_0 - a$ and $t' = t_0 - 1 \geq 2$.

If $T' \notin \mathcal{T}_1(|V_{T'}|, \psi(T'))$, then by the choice of T_0 and Theorem 1.2(iii), one has

$$\Phi(T_0) = \Phi(T') \leq 3^{t'-1} + t' = 3^{t_0-2} + t_0 - 1 < 2 \cdot 3^{t_0-2} \leq f(t_0),$$

a contradiction.

If $T' \in \mathcal{T}_1(|V_{T'}|, \psi(T'))$, then by (1.1) we obtain

$$\Phi(T_0) = \Phi(T') \leq 3^{t'-1} + t' + 1 = 3^{t_0-2} + t_0 \leq 2 \cdot 3^{t_0-2} \leq f(t_0),$$

and all equalities throughout hold if and only if $n_0 \geq 3t_0 + 3$, $t_0 = 3$ and $|V_{T'}| = 3t'$, that is, $T' \cong P_6$ and $n_0 \geq 12$. This implies that $\Phi(T_0) = f(t_0)$ holds if and only if T_0 is a tree obtained by adding an edge to connect a vertex of P_6 and the center vertex of K_{1,n_0-7} with $n_0 \geq 12$, i.e., T_0 is special, a contradiction.

This completes the proof. □

It is easy to see that the diameter of T_0 is at least 4. We root T_0 at an end vertex of a longest path in T_0. Let v be a leaf of maximum depth in T_0 and $vuwhs$ be a subpath of the path from v to the root of T_0. In order to complete the proof, we need to characterize the local structure of T_0 by the following claims. The first one can be deduced by Lemma 3.3 immediately.

Claim 3.4. u has exactly one child in T_0.

Assume that w has q children each of which is a leaf and p children each of which is a quasi-pendant vertex. Let $Q = \{w' : w' \in N_T(w) \text{ with } d_T(w') = 1\}$ and $P = V_{T_w} \setminus (Q \cup \{w\})$. By Lemma 3.3, each neighbor of w in P has exactly one child, in particular, $|P| = 2p$.

Claim 3.5. $p = 1$.

Proof. Suppose, to the contrary, that $p \geq 2$. Then all vertices in $P \cup Q$ belong to all maximum dissociation sets of T_0, and hence w is not in any maximum dissociation set of T_0. Let $T' = T - (P \cup Q \cup \{w\})$. Then $n' := |V_{T'}| = n_0 - 2p - q - 1$ and $\psi' := \psi(T') = \psi_0 - 2p - q$. Thus, $t' := t(T') = t_0 - 1 \geq 2$. Note that S is a maximum dissociation set of T' if and only if $S \cup P \cup Q$ is a maximum dissociation set of T_0. It follows that $\Phi(T_0) = \Phi(T')$.

If $T' \notin \mathcal{T}_1(n', \psi')$, then by the choice of T_0 and Theorem 1.2(iii), one has

$$\Phi(T_0) = \Phi(T') \le 3^{t_0-2} + t_0 - 1 < 2 \cdot 3^{t_0-2} \le f(t_0),$$

a contradiction.

If $T' \in \mathcal{T}_1(n', \psi')$, then by (1.1) we obtain

$$\Phi(T_0) = \Phi(T') \le \begin{cases} 3^{t_0-2} + t_0 & \text{if } n' = 3t', \\ 3^{t_0-2} + 1 & \text{if } n' = 3t' + 1, \\ 3^{t_0-2} & \text{if } n' \ge 3t' + 2. \end{cases}$$

Hence $\Phi(T_0) \le 2 \cdot 3^{t_0-2} \le f(t_0)$, and all the equalities throughout hold if and only if $n' = 3t'$, $t_0 = 3$ and $n_0 \ge 3t_0 + 3$. That is, $T' \cong P_6$ and $n_0 \ge 12$. Hence T_0 is special, a contradiction.

This completes the proof of Claim 3.5. □

Claim 3.6. $q = 0$.

Proof. Suppose that $q \ge 1$. Let $T' = T - (P \cup Q \cup \{w\})$. We proceed by considering the following two possible cases.

Case 1*:* $q = 1$. In this case, $n' := |V_{T'}| = n_0 - 4$ and $\psi' := \psi(T') = \psi_0 - 3$. Hence $t' := t(T') = t_0 - 1 \ge 2$. In view of Theorem 1.1, we have

$$\psi_0 - 3 = \psi' \ge \frac{2n'}{3} = \frac{2(n_0 - 4)}{3}.$$

That is, $n_0 \ge 3t_0 + 1$. Notice that a maximum dissociation set of T' containing h can be extended in a unique way to a maximum dissociation set of T_0, and a maximum dissociation set of T' not containing h can be extended in two ways to a maximum dissociation set of T_0. In addition, all maximum dissociation sets of T_0 are of those forms. Thus,

$$\Phi(T_0) = \Phi_h(T') + 2\Phi_{\overline{h}}(T') = \Phi(T') + \Phi_{\overline{h}}(T').$$

If $T' \notin \mathcal{T}_1(n', \psi')$, then by the choice of T_0, Theorem 1.2(iii) and Lemma 3.2, one obtains

$$\Phi(T_0) = \Phi(T') + \Phi_{\overline{h}}(T') \le \begin{cases} 3^{t_0-2} + t_0 - 1 + 3^{t_0-2} & \text{if } n_0 = 3t_0 + 1, \\ 3^{t_0-2} + 3^{t_0-2} & \text{if } n_0 = 3t_0 + 2, \\ 2 \cdot 3^{t_0-3} + 1 + 2 \cdot 3^{t_0-3} & \text{if } n_0 \ge 3t_0 + 3. \end{cases}$$

Hence $\Phi(T_0) < f(t_0)$, a contradiction.

If $T' \in \mathcal{T}_1(n', \psi')$, then by (1.1) and Lemma 3.1, we get

$$\Phi(T_0) = \Phi(T') + \Phi_{\overline{h}}(T') \leq \begin{cases} 3^{t_0-2} + t_0 + 3^{t_0-2} & \text{if } n_0 = 3t_0 + 1, \\ 3^{t_0-2} + 1 + 3^{t_0-2} & \text{if } n_0 = 3t_0 + 2, \\ 3^{t_0-2} + 3^{t_0-2} & \text{if } n_0 \geq 3t_0 + 3. \end{cases}$$

Therefore, if $n_0 = 3t_0 + 1$, then $\Phi(T_0) \leq 2 \cdot 3^{t_0-2} + t_0 \leq 3^{t_0-1}$, and all the equalities throughout hold if and only if $\Phi_{\overline{h}}(T') = 3^{t_0-2}$ and $t_0 = 3$, which is equivalent to $T' \cong P_6$ and h is the major vertex of T'. It follows that $T_0 \cong O_{P_3,P_4,T^*_{5,3}}$, i.e., T_0 is special, a contradiction. If $n_0 \geq 3t_0 + 2$, then $\Phi(T_0) \leq f(t_0)$, and the equality holds if and only if $\Phi_{\overline{h}}(T') = 3^{t_0-2}$, which implies that h is the major vertex of T' and $T' \ncong O_{P_2,P_3,T^*_{5,3}}$. Hence T_0 is special, a contradiction.

Case 2: $q \geq 2$. In this case, all vertices in $P \cup Q$ belong to all maximum dissociation sets of T_0, and no maximum dissociation set of T_0 contains w. By a similar discussion as that of Claim 3.5, we can get a contradiction.

This completes the proof of Claim 3.6. □

Now, by Claims 3.5 and 3.6 and Lemma 3.3, we obtain that each descendant of h has degree at most 2. Assume, without loss of generality, that h contains x children each of which has exactly two descendants, y children each of which has exactly one descendant, and z children each of which is a leaf. Let X, Y and Z be the set of the x, y and z children of h and all descendants of them, respectively. In particular, $|X| = 3x$, $|Y| = 2y$ and $|Z| = z$.

Claim 3.7. $z = 0$.

Proof. Suppose, to the contrary, that $z \geq 1$. Let $T' = T_0 - X$. Then $n' := |V_{T'}| = n_0 - 3x$ and $\psi' := \psi(T') = \psi_0 - 2x$. Hence $t' := t(T') = t_0 - x$. Note that $\mathrm{diam}(T') \geq 2$. Therefore, $t' \geq 1$ and $x \leq t_0 - 1$. Bear in mind that $z \geq 1$. If S is a maximum dissociation set containing h in T', then $d_{T'[S]}(h) = 1$. Thus, a maximum dissociation set of T' containing h can be extended in a unique way to a maximum dissociation set of T_0; a maximum dissociation set of T' not containing h can be extended in 3^x ways to a maximum dissociation set of T_0. In addition, each maximum dissociation set of T_0 is of such a form. So,

$$\Phi(T_0) = \Phi_h(T') + 3^x \Phi_{\overline{h}}(T') = \Phi(T') + (3^x - 1)\Phi_{\overline{h}}(T').$$

Firstly, we assume that $T' \notin \mathcal{T}_1(n', \psi')$. If $x = t_0 - 1$, then by Theorem 1.2(ii), we know $T' \cong K_{1,3}$. Therefore, $n_0 = 3t_0 + 1$ and T_0 is special, a contradiction. Hence $x \leq t_0 - 2$.

By the choice of T_0, we obtain that $\Phi(T') \leq f(t')$ and the equality holds if and only if T' is special. Combining with Theorem 1.2(iii) and Lemma 3.2, one has

$$\begin{aligned}\Phi(T_0) &= \Phi(T') + (3^x - 1)\Phi_{\overline{h}}(T') \\ &\leq \begin{cases} 3^{t_0-x-1} + t_0 - x + (3^x-1)3^{t_0-x-1} & \text{if } n' = 3t', \\ 3^{t_0-x-1} + (3^x-1)3^{t_0-x-1} & \text{if } n' = 3t'+1, \\ 2\cdot 3^{t_0-x-2} + 1 + (3^x-1)\cdot 2\cdot 3^{t_0-x-2} & \text{if } n' = 3t'+2, \\ 2\cdot 3^{t_0-x-2} + (3^x-1)\cdot 2\cdot 3^{t_0-x-2} & \text{if } n' \geq 3t'+3. \end{cases}\end{aligned}$$

Hence, if $n' = 3t'$, i.e., $n_0 = 3t_0$, then $\Phi(T_0) \leq 3^{t_0-1} + t_0 - x < 3^{t_0-1} + t_0 = f(t_0)$, a contradiction. If $n' = 3t'+1$, i.e., $n_0 = 3t_0+1$, then $\Phi(T_0) \leq 3^{t_0-1} = f(t_0)$, and the equality holds if and only if T' is special and $\Phi_{\overline{h}}(T') = 3^{t_0-x-1}$. Therefore, $T' \notin \{P_7, O_{P_3,P_4,T^*_{5,3}}\}$ and h is the major vertex of T'. Hence T_0 is special, a contradiction. If $n' = 3t'+2$, i.e., $n_0 = 3t_0+2$, then $\Phi(T_0) \leq 2\cdot 3^{t_0-2} + 1$, and the equality holds if and only if T' is special with $n' \neq 8$ and $\Phi_{\overline{h}}(T') = 2\cdot 3^{t_0-x-2}$. Thus, h is the major vertex of T' and so T_0 is special, a contradiction. If $n' \geq 3t'+3$, then by a similar discussion as above, we obtain that $\Phi(T_0) \leq f(t_0)$ and the equality holds if and only if T_0 is special, a contradiction.

Next, we consider the case $T' \in \mathcal{T}_1(n', \psi')$. Clearly, h is a quasi-pendant vertex of T'. In addition, h is not the major vertex of T'. Otherwise, T_0 is special if $T' \cong O_{P_2,P_3,T^*_{5,3}}$, and $T_0 \in \mathcal{T}_1(n_0, \psi_0)$ otherwise, which contradicts the choice of T_0. If $n' = 3t'$, then $n_0 = 3t_0$. By (1.1) and Lemma 3.1, one has

$$\begin{aligned}\Phi(T_0) &= \Phi(T') + (3^x-1)\Phi_{\overline{h}}(T') \leq 3^{t_0-x-1} + t_0 - x + 1 + (3^x-1)3^{t_0-x-1} \\ &= 3^{t_0-1} + t_0 - x + 1 \leq 3^{t_0-1} + t_0,\end{aligned}$$

and all the equalities throughout hold if and only if $\Phi_{\overline{h}}(T') = 3^{t_0-x-1}$ and $x = 1$. It follows that h is the major vertex of T', a contradiction.

If $n' = 3t'+1$, then $n_0 = 3t_0+1$. If $x = t_0 - 1$, then $T' \cong P_4$ and h must be its major vertex, a contradiction. Hence $x \leq t_0 - 2$ and $t' \geq 2$. Together with (1.1) and Lemma 3.1, one has

$$\begin{aligned}\Phi(T_0) &= \Phi(T') + (3^x-1)\Phi_{\overline{h}}(T') \leq 3^{t_0-x-1} + 1 + (3^x-1)(3^{t_0-x-2}+1) \\ &= 3^{t_0-2} + 3^x + 2\cdot 3^{t_0-x-2}.\end{aligned}$$

Let $g(x) = 3^{t_0-2} + 3^x + 2\cdot 3^{t_0-x-2}$ be a real function in x for $x \in [1, t_0-2]$. It is routine to check that the derivative function and the second derivative function of $g(x)$ are, respectively,

$$g'(x) = (3^x - 2\cdot 3^{t_0-x-2})\ln 3 \quad \text{and} \quad g''(x) = (3^x + 2\cdot 3^{t_0-x-2})(\ln 3)^2 > 0.$$

Hence

$$\begin{aligned}\Phi(T_0) &\leq g(x) \leq \max\{g(1), g(t_0-2)\} = \max\{5\cdot 3^{t_0-3}+3, 2\cdot 3^{t_0-2}+2\}\\ &= 2\cdot 3^{t_0-2}+2 < 3^{t_0-1},\end{aligned}$$

a contradiction.

If $n' \geq 3t'+2$, then $n_0 \geq 3t_0+2$. If $x = t_0-1$, then $T' \cong O_{aP_2,bP_3}$ for some nonnegative integers a, b with $a+2b+1 = n' \geq 5$ and $b \geq 1$ (since h is not the major vertex of T'). It is straightforward to check that $T_0 \cong O_{P_2,xP_4,O_{(a+1)P_2,(b-1)P_3}}$ and hence $\Phi(T_0) = 1 < 2\cdot 3^{t_0-2}$, a contradiction. Therefore, $x \leq t_0-2$ and $t' \geq 2$. In view of (1.1) and Lemma 3.1, one has

$$\begin{aligned}\Phi(T_0) &= \Phi(T') + (3^x-1)\Phi_{\overline{h}}(T') \leq 3^{t_0-x-1} + (3^x-1)3^{t_0-x-2}\\ &= 3^{t_0-2} + 2\cdot 3^{t_0-x-2} \leq 5\cdot 3^{t_0-3} < 2\cdot 3^{t_0-2},\end{aligned}$$

a contradiction.

This completes the proof of Claim 3.7. □

Claim 3.8. $y = 0$.

Proof. Suppose that $y \geq 1$. We proceed by considering the following two possible cases.

Case 1*:* $y = 1$. Let $T_1 = T_0 - (X \cup Y \cup \{h\})$ and $T_2 = T_0 - (X \cup Y)$. Then $n_1 := |V_{T_1}| = n_0 - 3x - 3$, $\psi_1 := \psi(T_1) = \psi_0 - 2x - 2$ and $n_2 := |V_{T_2}| = n_0 - 3x - 2$ and $\psi_2 := \psi(T_2) \in \{\psi_0 - 2x - 2, \psi_0 - 2x - 1\}$. Hence $t_1 := t(T_1) = t_0 - x - 1$ and $t_2 := t(T_2) \in \{t_0 - x, t_0 - x - 1\}$. Note that $x \leq t_0 - 1$. If $x = t_0 - 1$, then $t_1 = 0$ and so $T_1 \in \{P_1, P_2\}$. It follows that $T_0 \in \mathcal{T}_1(n_0, \psi_0)$, a contradiction. Hence $x \leq t_0 - 2$. Now, we proceed by distinguishing the following two subcases.

Subcase 1.1*:* $\psi_2 = \psi_0 - 2x - 2$. In this subcase, the vertex h is in no maximum dissociation set of T_0. Let $T' = T_0 - X$. Then $n' := |V_{T'}| = n_0 - 3x$ and $\psi' := \psi(T') = \psi_0 - 2x$. Thus, $t' := t(T') = t_0 - x \geq 2$. In view of Theorem 1.1, one has

$$\psi' - 2 = \psi_2 \geq \frac{2n_2}{3} = \frac{2(n'-2)}{3},$$

which is equivalent to $n' \geq 3t' + 2$. Furthermore, the vertex h does not belong to any maximum dissociation set of T'. Hence $\Phi(T') = \Phi_{\overline{h}}(T')$. Notice that every maximum dissociation set of T' not containing h can be extended in 3^x ways to a maximum dissociation set of T_0, and each maximum dissociation set in T_0 is of such a form. It implies that $\Phi(T_0) = 3^x\Phi_{\overline{h}}(T')$.

Firstly, we assume that $T' \notin \mathcal{T}_1(n', \psi')$. Since $n' \geq 3t' + 2$, one has $n_0 \geq 3t_0 + 2$. Combining with Lemma 3.2, we have $\Phi(T_0) = 3^x\Phi_{\overline{h}}(T') \leq 3^x\cdot 2\cdot 3^{t_0-x-2} = 2\cdot 3^{t_0-2} \leq f(t_0)$, and all the equalities throughout hold if and only if $n_0 \geq 3t_0+3$ and $\Phi_{\overline{h}}(T') = 2\cdot 3^{t_0-x-2}$, which is equivalent to $n' \geq 3t'+3$ and $\Phi(T') = 2\cdot 3^{t_0-x-2}$. In addition, by the choice of T_0, we know that $\Phi(T') \leq 2\cdot 3^{t_0-x-2}$ if $n' \geq 3t'+3$, and the equality holds if and only if T' is special. Hence $\Phi(T_0) = f(t_0)$ holds if and only if T' is special with $n' \geq 3t'+3$ and h is the major vertex of T'. Therefore, T_0 is special, which contradicts the choice of T_0.

Next, we consider the case $T' \in \mathcal{T}_1(n', \psi')$ with $n' \geq 3t'+2$. Recall that $\Phi(T') = \Phi_{\overline{h}}(T')$. In view of Lemma 3.1, one obtains that $T' \ncong O_{P_2,P_3,T^*_{5,3}}$ and h must be the major vertex of T'. Therefore, $T_0 \in \mathcal{T}_1(n_0, \psi_0)$, a contradiction.

Subcase 1.2*:* $\psi_2 = \psi_0 - 2x - 1$. In this subcase, $\psi_2 = \psi_1 + 1$, which implies that the vertex h belongs to all maximum dissociation sets of T_2. Hence $\Phi_h(T_2) = \Phi(T_2)$ and $T_2 \ncong P_3$. Note that $t_2 = t_0 - x - 1$. If S is a maximum dissociation set of T_2 such that $h \in S$ and $d_{T_2[S]}(h) = 0$, then it can be extended in $x+2$ ways to a maximum dissociation set of T_0; if S is a maximum dissociation set of T_2 such that $h \in S$ and $d_{T_2[S]}(h) = 1$, then it can be extended in a unique way to a maximum dissociation set of T_0; and all maximum dissociation sets of T_0 containing h are of those forms. On the other hand, a maximum dissociation set of T_1 can be extended in 3^x ways to a maximum dissociation set in T_0 that does not contain h, and each maximum dissociation set of T_0 not containing h is of that form. Therefore,

$$\begin{aligned}\Phi(T_0) &= \Phi_h(T_0) + \Phi_{\overline{h}}(T_0) = (x+2)\Phi^0_h(T_2) + \Phi^1_h(T_2) + 3^x\Phi(T_1) \\ &= 3^x\Phi(T_1) + \Phi(T_2) + (x+1)\Phi^0_h(T_2) = 3^x\Phi(T_1) + \Phi(T_2) + (x+1)\Phi_{\overline{s}}(T_2).\end{aligned} \tag{3.2}$$

If $x = t_0 - 2$, then $t_1 = t_2 = 1$. Hence $T_2 \cong O_{aP_2,bP_3}$ for some nonnegative integers a, b with $a + 2b + 1 = n_2$. Notice that h is a pendant vertex of T_2. Then T_0 must be one of the graphs as depicted in Figure 3.2. Notice that $T_1 \notin \{P_1, P_2, P_3\}$. Otherwise, either $T_0 \in \mathcal{T}_1(n_0, \psi_0)$ or T_0 is special, a contradiction. Together with $t_1 = 1$ and Theorem 1.2(ii), one has $\Phi(T_1) \leq 2$ and the equality holds if and only if $T_1 \cong P_4$.

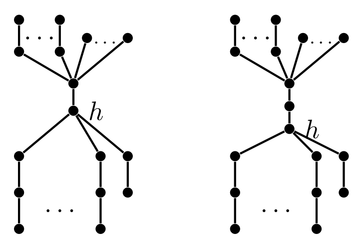


Figure 3.2: All possible structures of T_0 for $x = t_0 - 2$.

We first assume that T_0 is the first graph in Figure 3.2. If $T_1 \cong P_4$, then $T_2 \cong T^*_{5,3}$ and $n_0 = 3t_0 + 1$. In view of (3.2), we have

$$\Phi(T_0) = 2\cdot 3^x + 1 + x + 1 = 2\cdot 3^{t_0-2} + t_0 \leq 3^{t_0-1} = f(t_0),$$

and the equality holds if and only if $t_0 = 3$, i.e., $x = 1$, which implies that $n_0 = 10$ and T_0 is special, a contradiction.

If $T_1 \ncong P_4$, then $\Phi(T_1) = \Phi(T_2) = \Phi_{\overline{s}}(T_2) = 1$. Applying (3.2) again yields that

$$\Phi(T_0) = 3^x + 1 + x + 1 = 3^{t_0-2} + t_0 \leq 2 \cdot 3^{t_0-2} \leq f(t_0),$$

and $\Phi(T_0) = f(t_0)$ holds if and only if $t_0 = 3$ and $n_0 \geq 3t_0+3$, i.e., $x = 1$ and $n_0 \geq 3t_0+3$, which also implies that T_0 is special, a contradiction.

Next, we assume that T_0 is the last graph in Figure 3.2. If $T_1 \cong P_4$, then $n_0 = 3t_0 + 1$ and $T_2 \cong P_5$. Hence $\Phi(T_2) = 1$ and $\Phi_{\overline{s}}(T_2) = 0$. Based on (3.2), we get

$$\Phi(T_0) = 2 \cdot 3^x + 1 = 2 \cdot 3^{t_0-2} + 1 < 3^{t_0-1} = f(t_0),$$

a contradiction.

If $T_1 \ncong P_4$, then $\Phi(T_1) = \Phi(T_2) = 1$. In addition, $\Phi_{\overline{s}}(T_1) = 0$. Then (3.2) implies

$$\Phi(T_0) = 3^x + 1 = 3^{t_0-2} + 1 < 2 \cdot 3^{t_0-2} = f(t_0),$$

a contradiction.

So, in what follows, it suffices to consider the case $x \leq t_0 - 3$. Hence $t_0 \geq 4$ and $t_1 = t_2 \geq 2$. Note that for each nonnegative integer i, if $n_0 = 3t_0 + i$, then $n_1 = 3t_1 + i$ and $n_2 = 3t_2 + i + 1$. In view of Lemmas 3.1 and 3.2, one has $\Phi_{\overline{s}}(T_2) \leq 3^{t_0-x-2}$. Together with the choice of T_0, (1.1) and (3.2), one obtains

$$\Phi(T_0) \leq \begin{cases} 3^x(3^{t_0-x-2} + t_0 - x) + 3^{t_0-x-2} + 1 + (x+1)3^{t_0-x-2} & \text{if } n_0 = 3t_0, \\ 3^x(3^{t_0-x-2} + 1) + 3^{t_0-x-2} + (x+1)3^{t_0-x-2} & \text{if } n_0 = 3t_0 + 1, \\ 3^x \cdot 3^{t_0-x-2} + 3^{t_0-x-2} + (x+1)3^{t_0-x-2} & \text{if } n_0 \geq 3t_0 + 2. \end{cases} \tag{3.3}$$

If $n_0 = 3t_0$, then by (3.3) one has $\Phi(T_0) \leq 3^{t_0-2} + 3^x(t_0 - x) + (x+2)3^{t_0-x-2} + 1$. Let $g_1(x) = 3^{t_0-2} + 3^x(t_0 - x) + (x+2)3^{t_0-x-2} + 1$ be a real function in x for $x \in [1, t_0 - 3]$. It is routine to check that

$$g_1'(x) = -3^x + 3^x(t_0 - x)\ln 3 + 3^{t_0-x-2} - (x+2)3^{t_0-x-2}\ln 3$$

and

$$g_1''(x) = \ln 3\big(3^x((t_0 - x)\ln 3 - 2) + 3^{t_0-x-2}((x+2)\ln 3 - 2)\big) > 0.$$

Hence

$$\Phi(T_0) \leq g_1(x) \leq \max\{g_1(1), g_1(t_0 - 3)\} = 2 \cdot 3^{t_0-2} + 3t_0 - 2 < 3^{t_0-1} + t_0 = f(t_0),$$

a contradiction.

If $n_0 = 3t_0 + 1$, then by (3.3) one has $\Phi(T_0) \le 3^{t_0-2} + 3^x + (x+2)3^{t_0-x-2}$. Let $g_2(x) = 3^{t_0-2} + 3^x + (x+2)3^{t_0-x-2}$ be a real function in x for $x \in [1, t_0 - 3]$. It is straightforward to check that $g_2''(x) > 0$. Hence

$$\begin{aligned}\Phi(T_0) &\le g_2(x) \le \max\{g_2(1), g_2(t_0-3)\} = \max\{2 \cdot 3^{t_0-2} + 3, 5 \cdot 3^{t_0-3} + 3t_0 - 3\} \\ &< 3^{t_0-1} = f(t_0),\end{aligned}$$

a contradiction.

If $n_0 \ge 3t_0 + 2$, then by (3.3) one has $\Phi(T_0) \le 3^{t_0-2} + (x+2)3^{t_0-x-2}$. Let $g_3(x) = 3^{t_0-2} + (x+2)3^{t_0-x-2}$ be a real function in x for $x \in [1, t_0-3]$. It is routine to check that $g_3'(x) < 0$ and hence $g_3(x)$ is decreasing in the interval $x \in [1, t_0-3]$. Therefore,

$$\Phi(T_0) \le g_3(x) \le g_3(1) = 2 \cdot 3^{t_0-2} \le f(t_0),$$

and all equalities hold if and only if $\Phi(T_1) = \Phi(T_2) = \Phi_{\overline{s}}(T_2) = 3^{t_0-x-2}$, $x = 1$ and $n_0 \ge 3t_0 + 3$. Together with the choice of T_0, we obtain that $T_2 \in \mathcal{T}_1(n_2, \psi_2)$ and s is its major vertex. Thus, T_0 is special, which contradicts the choice of T_0.

Case 2*: $y \ge 2$.* Let $T' = T_0 - X$. Then $T' \ncong O_{P_2,P_3,T^*_{5,3}}$ and each maximum dissociation set of T_0 (resp. T') does not contain h. Therefore, $\Phi(T_0) = \Phi_{\overline{h}}(T_0)$ and $\Phi(T') = \Phi_{\overline{h}}(T')$. Furthermore, $n' := |V_{T'}| = n_0 - 3x$ and $\psi' := \psi(T') = \psi - 2x$. That is, $t' := t(T') = t_0 - x$. Clearly, $x \le t_0 - 1$. In fact, $x \le t_0 - 2$. Otherwise, $x = t_0 - 1$. Then $t' = 1$ and $T' \cong O_{aP_2,bP_3}$ for some nonnegative integers a, b with $a + 2b + 1 = n'$ and $b \ge 2$. Note that h is the major vertex of T'. Hence $T_0 \in \mathcal{T}_1(n_0, \psi_0)$, a contradiction. It follows that $t' \ge 2$.

Let $T'' = T' - (Y \cup \{h\})$. Then $n'' := |V_{T''}| = n' - 2y - 1$ and $\psi'' := \psi(T'') = \psi' - 2y$. By Theorem 1.1, one has

$$\psi' - 2y = \psi'' \ge \frac{2n''}{3} = \frac{2(n' - 2y - 1)}{3},$$

which is equivalent to $n' \ge 3t' + 2y - 2 \ge 3t' + 2$.

On the other hand, a maximum dissociation set of T' can be extended in 3^x ways to a maximum dissociation set of T_0, and all maximum dissociation sets of T_0 are of those forms. Hence $\Phi(T_0) = 3^x\Phi(T') = 3^x\Phi_{\overline{h}}(T')$. Note that h can not be the major vertex of T' if $T' \in \mathcal{T}_1(n', \psi') \setminus \{O_{P_2,P_3,T^*_{5,3}}\}$. Otherwise, $T_0 \in \mathcal{T}_1(n_0, \psi_0)$, a contradiction. Recall that $n' \ge 3t' + 2$ and $T' \ncong O_{P_2,P_3,T^*_{5,3}}$. Together with Lemmas 3.1 and 3.2, one has

$$\Phi(T_0) = 3^x\Phi_{\overline{h}}(T') \le 3^x \cdot 2 \cdot 3^{t_0-x-2} = 2 \cdot 3^{t_0-2}.$$

Hence $\Phi(T_0) \le f(t_0)$ with equality if and only if $\Phi_{\overline{h}}(T') = \Phi(T') = 2 \cdot 3^{t_0-x-2}$ and $n_0 \ge 3t_0 + 3$. Together with the choice of T_0, we obtain that T' is a special tree with $n' \ge 3t' + 3$ and h is the major vertex. It follows that T_0 is special, which is a contradiction.

This completes the proof of Claim 3.8. □

Now, we are ready to give the proof of Theorem 1.3.

Let $T_1 = T_0 - (X \cup \{h\})$ and $T_2 = T_0 - X$. Then $n_1 := |V_{T_1}| = n_0 - 3x - 1$, $\psi_1 := \psi(T_1) \in \{\psi_0 - 2x - 1, \psi_0 - 2x\}$, and $n_2 := |V_{T_2}| = n_0 - 3x$, $\psi_2 := \psi(T_2) = \psi_0 - 2x$. Hence $t_1 := t(T_1) \in \{t_0 - x, t_0 - x - 1\}$ and $t_2 := t(T_2) = t_0 - x$. If $x = t_0$, then $t_2 = 0$ and $T_2 \cong P_2$. It follows that $n_0 = 3t_0 + 2$ and $T_0 \cong O_{P_2,t_0P_4}$. Thus, $\Phi(T_0) = 1 < 2 \cdot 3^{t_0-2} + 1$, a contradiction. Hence $x \leq t_0 - 1$. Next, let us consider the following two possible cases regarding in the value of ψ_1.

Case 1*:* $\psi_1 = \psi_0 - 2x - 1$. In this case, $t_1 = t_0 - x$ and $\psi_2 = \psi_1 + 1$. Then h belongs to all the maximum dissociation sets of T_2 and T_0. Hence $\Phi(T_2) = \Phi_h(T_2)$ and $\Phi(T_0) = \Phi_h(T_0)$. If S is a maximum dissociation set of T_2 such that $d_{T_2[S]}(h) = 0$, then it can be extended in $x + 1$ ways to a maximum dissociation set of T_0; if S is a maximum dissociation set of T_2 such that $d_{T_2[S]}(h) = 1$, then it can be extended in a unique way to a maximum dissociation set of T_0. In addition, every maximum dissociation set of T_0 is the form described as above. Hence

$$\Phi(T_0) = \Phi_h(T_0) = (x + 1)\Phi_h^0(T_2) + \Phi_h^1(T_2) = \Phi(T_2) + x\Phi_h^0(T_2) = \Phi(T_2) + x\Phi_{\overline{s}}(T_2).$$

Based on Theorem 1.1, we have

$$\psi_2 - 1 = \psi_1 \geq \frac{2n_1}{3} = \frac{2(n_2 - 1)}{3},$$

which is equivalent to $n_2 \geq 3t_2 + 1$. It follows from Lemmas 3.1 and 3.2 that $\Phi_{\overline{s}}(T_2) \leq 3^{t_0-x-1}$. If $n_2 = 3t_2 + 1$, then $n_0 = 3t_0 + 1$. Based on the choice of T_0 and (1.1), we obtain

$$\Phi(T_0) = \Phi(T_2) + x\Phi_{\overline{s}}(T_2) \leq 3^{t_0-x-1} + 1 + x \cdot 3^{t_0-x-1} = (x + 1)3^{t_0-x-1} + 1.$$

Let $g(x) = (x + 1)3^{t_0-x-1} + 1$ be a real function in x for $x \in [1, t_0 - 1]$. It is routine to check that the derivative function of $g(x)$ is

$$g'(x) = 3^{t_0-x-1} - 3^{t_0-x-1}(x + 1)\ln 3 = 3^{t_0-x-1}(1 - (x + 1)\ln 3) < 0.$$

Hence $g(x)$ is a decreasing function in x for $x \in [1, t_0 - 1]$. Therefore,

$$\Phi(T_0) \leq g(x) \leq g(1) = 2 \cdot 3^{t_0-2} + 1 < 3^{t_0-1} = f(t_0),$$

a contradiction.

If $n_2 \geq 3t_2 + 2$, then $n_0 \geq 3t_0 + 2$. By the choice of T_0 and (1.1), one has

$$\Phi(T_0) = \Phi(T_2) + x\Phi_{\overline{s}}(T_2) \leq 3^{t_0-x-1} + x \cdot 3^{t_0-x-1} = (x + 1)3^{t_0-x-1}.$$

By a similar discussion as above, we know that $\Phi(T_0) \leq 2 \cdot 3^{t_0-2} \leq f(t_0)$, and all the equalities throughout hold if and only if $\Phi(T_2) = \Phi_{\overline{s}}(T_2) = 3^{t_0-x-1}$, $x = 1$ and $n_0 \geq 3t_0+3$.

It follows from the choice of T_0 that $T_2 \in \mathcal{T}_1(n_2, \psi_2)$ with $n_2 \geq 3t_2 + 3$ and s is its major vertex. Note that h is a pendant vertex of T_2. Hence $\Phi(T_0) = f(t_0)$ holds if and only if T_0 is special with $n_0 \geq 3t_0 + 3$, a contradiction.

Case 2: $\psi_1 = \psi_0 - 2x$. In this case, $t_1 = t_0 - x - 1$. If $x = t_0 - 1$, then $t_1 = 0$ and $T_1 \in \{P_1, P_2\}$. Together with $t_2 = 1$, one has $T_1 \cong P_2$. Therefore, $T_0 \cong O_{P_3,(t_0-1)P_4}$, i.e., $T_0 \in \mathcal{T}_1(n_0, \psi_0)$, a contradiction.

Next, we assume $x = t_0 - 2$. Then $t_1 = 1$ and $t_2 = 2$. Hence $T_1 \cong O_{aP_2 \cup bP_3}$ for some integers with $a + 2b + 1 = n_1$. Since $t_2 = 2$, one has $n_2 \geq 6$, $b \geq 1$ and s must be one of the quasi-pendant vertices and their pendant neighbors in T_1.

If $n_0 = 3t_0$, then $n_1 = 5$ and $T_1 \in \{O_{2P_2,P_3}, O_{2P_3}\}$. It is straightforward to check that

$$\Phi(T_0) = \begin{cases} 3^{t_0-2} + 3t_0 - 2 & \text{if } d_{T_1}(s) = 2, \\ 3^{t_0-2} + t_0 + 2 & \text{if } T_1 \cong O_{2P_2,P_3} \text{ and } d_{T_1}(s) = 1, \\ 3^{t_0-2} + 2t_0 + 1 & \text{if } T_1 \cong O_{2P_3} \text{ and } d_{T_1}(s) = 1. \end{cases}$$

Hence $\Phi(T_0) < 3^{t_0-1} + t_0$, a contradiction.

If $n_0 = 3t_0 + 1$, then $n_1 = 6$ and $T_1 \in \{O_{3P_2,P_3}, O_{P_2,2P_3}\}$. It is routine to check that

$$\Phi(T_0) = \begin{cases} 3^{t_0-2} + t_0 & \text{if } T_1 \cong O_{3P_2,P_3}, \\ 3^{t_0-2} + t_0 + 1 & \text{if } T_1 \cong O_{P_2,2P_3} \text{ and } d_{T_1}(s) = 1, \\ 3^{t_0-2} + 2t_0 - 1 & \text{if } T_1 \cong O_{P_2,2P_3} \text{ and } d_{T_1}(s) = 2. \end{cases}$$

Hence $\Phi(T_0) < 3^{t_0-1}$, a contradiction.

If $n_0 \geq 3t_0 + 2$, then $n_1 \geq 7$. It is straightforward to check that the major vertex of T_1 is not in any maximum dissociation set of T_0 and hence $\Phi(T_0) = \Phi(O_{P_3,(t_0-2)P_4}) = 3^{t_0-2} + t_0 \leq 2 \cdot 3^{t_0-2} \leq f(t_0)$, and all the equalities throughout hold if and only if $t_0 = 3$ and $n_0 \geq 3t_0 + 3$, i.e., $x = 1$ and $n_0 \geq 3t_0 + 3$. It follows that T_0 is special, a contradiction.

In what follows, we only consider the case $x \leq t_0 - 3$. Then $t_0 \geq 4$. Recall that, in this subcase, $\psi_2 = \psi_1$. Thus, for every maximum dissociation set S in T_1, one has $s \in S$ and $d_{T_1[S]}(s) = 1$. Let $N_{T_1}(s) = \{h_1, \ldots, h_k\}$. Next, we are to prove that there exists a vertex in $N_{T_1}(s)$ such that it is in all maximum dissociation set of T_1. Without loss of generality, we suppose that there are two maximum dissociation sets, say S_1 and S_2, of T_1 such that $h_1 \in S_1$ and $h_2 \in S_2$. Let $H_1, \ldots, H_k$ be all the connected components of $T_1 - s$ satisfying $h_i \in V_{H_i}$. It is easy to see that $S_1 \cap V_{H_1}$ is a maximum dissociation set of H_1 and every maximum dissociation set of H_1 contains the vertex h_1. Since $S_2 \cap V_{H_1}$ is a dissociation set of H_1 not containing h_1, one has $|S_2 \cap V_{H_1}| < |S_1 \cap V_{H_1}|$. Furthermore, together with S_2 is a maximum dissociation set of T_1, we have $|S_2 \cap V_{H_1}| = |S_1 \cap V_{H_1}| - 1$. Let $S' = (S_2 \setminus ((S_2 \cap V_{H_1}) \cup \{s\})) \cup (S_1 \cap V_{H_1})$. Then S' is a maximum dissociation set of

T_1 and $s \notin S'$, a contradiction. Thus, there exists a vertex in $N_{T_1}(s)$, say h_1, such that it is contained in all the maximum dissociation set of T_1.

If S is a maximum dissociation set in T_1, then $S_1 = (S \cup \{h\}) \setminus \{s\}$ is a maximum dissociation set of T_2 such that $d_{T_2[S_1]}(h) = 0$, and $S_2 = (S \cup \{h\}) \setminus \{h_1\}$ is a maximum dissociation set of T_2 such that $d_{T_2[S_2]}(h) = 1$. Furthermore, S is also a maximum dissociation set in T_2 that does not contain h, and every maximum dissociation set of T_2 not containing h is a maximum dissociation set of T_1. Thus, we have

$$\Phi_{\overline{h}}(T_2) = \Phi(T_1) \le \min\{\Phi_h^0(T_2), \Phi_h^1(T_2)\}.$$

On the other hand, note that $\Phi(T_2) = \Phi_{\overline{h}}(T_2) + \Phi_h^0(T_2) + \Phi_h^1(T_2)$. Hence $\Phi_{\overline{h}}(T_2) \le \Phi(T_2)/3$.

Notice that a maximum dissociation set of T_2 not containing h can be extended in 3^x ways to a maximum dissociation set of T_0; a maximum dissociation set S of T_2 such that $h \in S$ and $d_{T_2[S]}(h) = 0$ can be extended in $x + 1$ ways to a maximum dissociation set of T_0, and a maximum dissociation set S of T_2 such that $h \in S$ and $d_{T_2[S]}(h) = 1$ can be extended in a unique way to a maximum dissociation set of T_0. Furthermore, all the maximum dissociation sets of T_0 are of those forms. So,

$$\begin{aligned}
\Phi(T_0) &= 3^x \Phi_{\overline{h}}(T_2) + (x+1)\Phi_h^0(T_2) + \Phi_h^1(T_2) \\
&= \Phi(T_2) + (3^x - 1)\Phi_{\overline{h}}(T_2) + x\Phi_h^0(T_2) \\
&= \Phi(T_2) + (3^x - 1)\Phi_{\overline{h}}(T_2) + x\big(\Phi(T_2) - \Phi_{\overline{h}}(T_2) - \Phi_h^1(T_2)\big) \\
&= (x+1)\Phi(T_2) + (3^x - 1 - x)\Phi_{\overline{h}}(T_2) - x\Phi_h^1(T_2) \\
&\le (x+1)\Phi(T_2) + (3^x - 1 - x)\Phi_{\overline{h}}(T_2) - x\Phi_{\overline{h}}(T_2) \\
&= (x+1)\Phi(T_2) + (3^x - 1 - 2x)\Phi_{\overline{h}}(T_2) \\
&\le (x+1)\Phi(T_2) + \frac{3^x - 1 - 2x}{3}\Phi(T_2) = \frac{3^x + x + 2}{3}\Phi(T_2).
\end{aligned} \tag{3.4}$$

If $n_2 = 3t_2$, then $n_0 = 3t_0$. Together with the choice of T_0, (1.1) and (3.4), one has

$$\begin{aligned}
\Phi(T_0) &\le \frac{3^x + x + 2}{3}(3^{t_0 - x - 1} + t_0 - x + 1) \\
&= 3^{t_0 - 2} + 3^{x-1}(t_0 - x + 1) + 3^{t_0 - x - 2}(x+2) + \frac{(x+2)(t_0 - x + 1)}{3}.
\end{aligned}$$

Let $g_1(x) = 3^{t_0-2} + 3^{x-1}(t_0 - x + 1) + 3^{t_0-x-2}(x+2) + (x+2)(t_0 - x + 1)/3$ be a real function in x for $x \in [1, t_0 - 3]$. It is straightforward to check that

$$g_1'(x) = 3^{x-1}(t_0 - x + 1)\ln 3 - 3^{x-1} - 3^{t_0-x-2}(x+2)\ln 3 + 3^{t_0-x-2} + \frac{t_0 - 2x - 1}{3}$$

and

$$g_1''(x) = \big(3^{x-1}((t_0 - x + 1)\ln 3 - 2) + 3^{t_0-x-2}((x+2)\ln 3 - 2)\big)\ln 3 - \frac{2}{3} > 0.$$

Hence

$$\Phi(T_0) \le g_1(x) \le \max\{g_1(1), g_1(t_0-3)\} = \max\left\{2(3^{t_0-2}+t_0), 13\cdot\frac{3^{t_0-3}+t_0-1}{3}\right\}$$
$$= 2(3^{t_0-2}+t_0) < 3^{t_0-1}+t_0,$$

a contradiction.

If $n_2 = 3t_2+1$, then $n_0 = 3t_0+1$. Based on the choice of T_0, (1.1) and (3.4), one has

$$\Phi(T_0) \le \frac{3^x+x+2}{3}(3^{t_0-x-1}+1) = 3^{t_0-2}+3^{x-1}+3^{t_0-x-2}(x+2)+\frac{x+2}{3}.$$

Let $g_2(x) = 3^{t_0-2}+3^{x-1}+3^{t_0-x-2}(x+2)+(x+2)/3$ be a real function in x for $x \in [1, t_0-3]$. It is straightforward to check that $g_2''(x) > 0$ for $x \in [1, t_0-3]$. Hence

$$\Phi(T_0) \le g_2(x) \le \max\{g_2(1), g_2(t_0-3)\} = \max\left\{2(3^{t_0-2}+1), 10\cdot\frac{3^{t_0-3}+t_0-1}{3}\right\}$$
$$= 2(3^{t_0-2}+1) < 3^{t_0-1}+1,$$

a contradiction.

If $n_2 \ge 3t_2+2$, then $n_0 \ge 3t_0+2$. In view of the choice T_0, (1.1) and (3.4), one has

$$\Phi(T_0) \le \frac{3^x+x+2}{3}\cdot 3^{t_0-x-1} = 3^{t_0-2}+3^{t_0-x-2}(x+2).$$

Let $g_3(x) = 3^{t_0-2}+3^{t_0-x-2}(x+2)$ be a real function in x for $x \in [1, t_0-3]$. It is easy to see that $g_3'(x) < 0$ for $x \in [1, t_0-3]$. Hence

$$\Phi(T_0) \le g_3(x) \le g_3(1) = 2\cdot 3^{t_0-2} \le f(t_0).$$

Furthermore, $\Phi(T_0) = f(t_0)$ holds only if $\Phi(T_2) = 3^{t_0-x-1}$, $x = 1$ and $n_0 \ge 3t_0+3$. Together with the choice of T_0, we deduce that $T_2 \in \mathcal{T}_1(n_2, \psi_2)$ with $n_2 \ge 3t_2+3$ and $x = 1$. Note that h is the pendant vertex of T_2. Then T_0 must be one of the graphs depicted in Figure 3.3. Recall that T_0 is not special. Hence T_0 can only be the last graph in Figure 3.3. It is routine to check that $\Phi(T_0) = 3^{t_0-2} < f(t_0)$, which contradicts the choice of T_0.

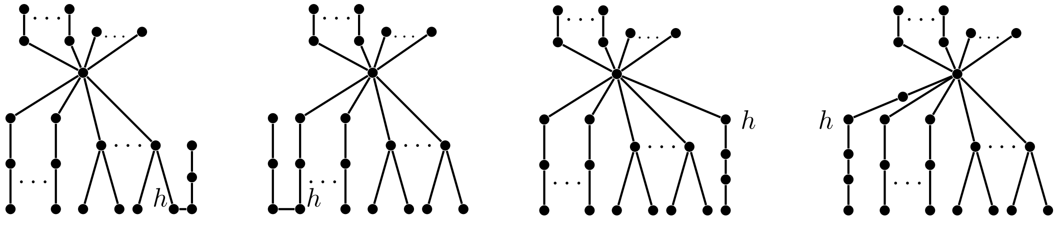


Figure 3.3: All possible structures of T_0 if $x = 1$ and $T_2 \in \mathcal{T}_1(n_2, \psi_2)$ with $n_2 \ge 3t_2+3$.

This completes the proof of Theorem 1.3. □

4. Proof of Theorem 1.4

In this section, we give the proof of Theorem 1.4, which characterizes all the forests with fixed order and dissociation number having the largest and the second largest number of maximum dissociation sets. Recall that $\mathfrak{F}(n,\psi)$ denote the set of forests with order n and dissociation number ψ satisfying that each component of the forest has order at least 3.

Proof of Theorem 1.4. It is straightforward to check that, for all forests $F \in \mathcal{F}_1(n,\psi)$, $\Phi(F)$ attains the upper bound in (1.3). Clearly, the upper bound in (1.3) is larger than $h(t)$ given in (1.4) and (1.5) for $t \geq 2$. Hence, in order to prove the theorem, it suffices to show that, if $F \in \mathfrak{F}(n,\psi) \setminus \mathcal{F}_1(n,\psi)$, then $n \geq 7$, $t \geq 2$ and $\Phi(F) \leq h(t)$ with equality if and only if $F \in \mathcal{F}_2(n,\psi)$.

Let F be a forest in $\mathfrak{F}(n,\psi) \setminus \mathcal{F}_1(n,\psi)$ such that F contains at least two components and $\Phi(F)$ is as large as possible. Assume that $T_1, T_2, \ldots, T_k$ are all the components of F satisfying $t_1 \geq t_2 \geq \cdots \geq t_k$, where $t_i = n_i - \psi_i$ with $n_i = |V_{T_i}|$ and $\psi_i = \psi(T_i)$ for $1 \leq i \leq k$. Note that each component of F is not isomorphic to P_1 and P_2. Hence $t \geq 2$ and $n \geq 3t \geq 6$ (based on Theorem 1.1). If $n = 6$, then $F \cong 2P_3 \in \mathcal{F}_1(n,\psi)$, a contradiction. So, $n \geq 7$.

It is routine to check that $\mathcal{F}_2(n,\psi) \subseteq \mathfrak{F}(n,\psi) \setminus \mathcal{F}_1(n,\psi)$, and the graphs in $\mathcal{F}_2(n,\psi)$ attain the upper bound in Theorem 1.4. Hence $\Phi(F) \geq h(t)$ holds.

(i) If $t = 2$, then F contains exactly two components such that $\psi_i = n_i - 1 \geq 2$ for $i \in \{1,2\}$. Hence $T_i \cong O_{a_iP_2,b_iP_3}$ with $a_i + 2b_i + 1 = n_i$ for $i \in \{1,2\}$. Without loss of generality, assume that $n_1 \geq n_2$.

Note that $F \notin \mathcal{F}_1(n,\psi)$. If $n = 7$, then $n_1 = 4$ and $n_2 = 3$. Hence $F \cong K_{1,3} \cup P_3$. If $n = 8$, then $n_1 = n_2 = 4$ or $n_1 = 5$ and $n_2 = 3$. In the former case, $F \in \{P_4 \cup K_{1,3}, 2K_{1,3}\}$ and so $\Phi(F) \leq 2 < 3$, a contradiction; in the latter case, by Theorem 1.2(ii) one has $\Phi(F) \leq 3$ with equality if and only if $F \cong T \cup P_3$, where $T \in \mathcal{T}_1(5,4)$. If $n \geq 9$ and $n_2 = 3$, then $F \in \mathcal{F}_1(n,\psi)$, a contradiction. If $n \geq 9$ and $n_2 = 4$, then Theorem 1.2(ii) implies $\Phi(F) \leq 2$, with equality if and only if $F \cong O_{a_1P_2,b_1P_3} \cup P_4$. If $n \geq 9$ and $n_2 \geq 5$, then applying Theorem 1.2(ii) again we obtain $\Phi(F) \leq 1 < 2$, a contradiction. Hence, if $t = 2$, then

$$F \in \begin{cases} \{K_{1,3} \cup P_3\} & \text{if } n = 7, \\ \{T \cup P_3 : T \in \mathcal{T}_1(5,4)\} & \text{if } n = 8, \\ \{T \cup P_4 : T \in \mathcal{T}_1(n-4,n-5)\} & \text{if } n \geq 9. \end{cases}$$

(ii) In what follows, we assume that $t \geq 3$. Then Theorem 1.1 implies $n \geq 9$. We proceed by considering the following four cases.

Case 1*:* $n = 3t$. In view of Theorem 1.1, one has $n_i = 3t_i$ for $1 \leq i \leq k$. Note that $F \ncong tP_3$. Then $k < t$, i.e., $t_1 \geq 2$. In order to characterize the structure of F, we need the following claim.

Claim 4.1. $t_1 = 2$ and $t_2 = \cdots = t_k = 1$.

Proof. Firstly, we are to prove $t_1 = 2$. Suppose that $t_1 \geq 3$. Then in view of Theorems 1.2 and 1.3, one has

$$\Phi(T_1) \leq 3^{t_1-1} + t_1 + 1 < 3 \cdot (3^{t_1-2} + t_1) = \Phi(P_3 \cup T),$$

where $T \in \mathcal{T}_1(n_1 - 3, \psi_1 - 2)$. Let $F_1 = P_3 \cup T \cup T_2 \cup \cdots \cup T_k$. Hence F_1 is disconnected and $\Phi(F) < \Phi(F_1)$. On the other hand, note that $t(T) = t_1 - 1 \geq 2$. Thus, $F_1 \in \mathfrak{F}(n, \psi) \setminus \mathcal{F}_1(n, \psi)$, which contradicts the choice of F. It follows that $t_1 = 2$.

Next, we show that $t_2 = \cdots = t_k = 1$. Suppose that $t_2 \geq 2$. Based on Theorems 1.2 and 1.3, one has

$$\Phi(T_2) \leq 3^{t_2-1} + t_2 + 1 < 3^{t_2} = \Phi(t_2 P_3).$$

Let $F_2 = T_1 \cup t_2 P_3 \cup T_3 \cup \cdots \cup T_k$. Thus, F_2 is disconnected and $\Phi(F) < \Phi(F_1)$. Recall that $t_1 = 2$. Then $F_2 \in \mathfrak{F}(n, \psi) \setminus \mathcal{F}_1(n, \psi)$, a contradiction. Hence $t_2 = 1$ and so $t_3 = \cdots = t_k = 1$.

This completes the proof of Claim 4.1. $\square$

In view of Claim 4.1, we know that $T_2 = \cdots = T_k \cong P_3$ and $k = t - 1$. Together with Theorem 1.2, one obtains

$$\Phi(F) = \Phi(T_1) \cdot 3^{t-2} \leq 2 \cdot 3^{t-1},$$

and the equality holds if and only if $T_1 \cong P_6$, i.e., $F \cong P_6 \cup (t-2)P_3$, as desired.

Case 2*:* $n = 3t + 1$. In this case, there exists exactly one j such that $n_j = 3t_j + 1$ for some $j \in \{1, \ldots, k\}$, and $n_i = 3t_i$ for each $i \in \{1, \ldots, k\} \setminus \{j\}$. If $k = t$, then $t_1 = \cdots = t_k = 1$. It follows that $T_j \in \{P_4, K_{1,3}\}$ and $T_i \cong P_3$ for each $i \in \{1, \ldots, k\} \setminus \{j\}$. Recall that $F \ncong P_4 \cup (t-1)P_3$. Hence $F \cong K_{1,3} \cup (t-1)P_3$ and so $\Phi(F) = 3^{t-1} < 4 \cdot 3^{t-1}$, a contradiction. Thus, $k \leq t - 1$, that is, $t_1 \geq 2$. Similar to Case 1, we are to characterize the structure of F by the following claim.

Claim 4.2. $t_1 = 2$ and $t_2 = \cdots = t_k = 1$.

Proof. We first prove $t_1 = 2$. Suppose that $t_1 \geq 3$. If $n_1 = 3t_1$, then by a similar discussion as Claim 4.1, we get a contradiction. If $n_1 = 3t_1 + 1$, then based on Theorems 1.2 and 1.3, one has

$$\Phi(T_1) \leq 3^{t_1-1} + 1 < 3 \cdot (3^{t_1-2} + 1) = \Phi(P_3 \cup T),$$

where $T \in \mathcal{T}_1(n_1 - 3, \psi_1 - 2)$. Let $F_3 = P_3 \cup T \cup T_2 \cup \cdots \cup T_k$. Hence F_3 contains at least two components and $\Phi(F) < \Phi(F_3)$. On the other hand, notice that $t(T) = t_1 - 1 \geq 2$. Therefore, $F_3 \in \mathfrak{F}(n, \psi) \setminus \mathcal{F}_1(n, \psi)$, which deduces a contradiction. Therefore, $t_1 = 2$.

Next, we show that $t_2 = \cdots = t_k = 1$. Suppose that $t_2 \geq 2$. If $n_2 = 3t_2$, then by a similar discussion as Claim 4.1, we get a contradiction. If $n_2 = 3t_2 + 1$, then by Theorems 1.2 and 1.3, we obtain

$$\Phi(T_2) \leq 3^{t_2-1} + 1 < 2 \cdot 3^{t_2-1} = \Phi(P_4 \cup (t_2 - 1)P_3).$$

Let $F_4 = T_1 \cup P_4 \cup (t_2 - 1)P_3 \cup T_3 \cup \cdots \cup T_k$. Then F_4 is disconnected and $\Phi(F) < \Phi(F_4)$. Together with $t_1 = 2$, we get $F_4 \in \mathfrak{F}(n, \psi) \setminus \mathcal{F}_1(n, \psi)$, which contradicts the choice of F. Hence $t_2 = 1$ and so $t_3 = \cdots = t_k = 1$.

This completes the proof of Claim 4.2. $\square$

In view of Claim 4.2, we know that $T_i \cong P_3$ for each $i \in \{2, \ldots, k\} \setminus \{j\}$. If $j = 1$, i.e., $n_1 = 3t_1 + 1$, then together with Claim 4.2 and Theorem 1.2, we get

$$\Phi(F) \leq (3^{t_1-1} + 1) \cdot 3^{t-t_1} = 4 \cdot 3^{t-2},$$

and the equality holds if and only if $T_1 \in \mathcal{T}_1(7, 5)$, i.e., $F \cong T_1 \cup (t-2)P_3$ with $T_1 \in \mathcal{T}_1(7, 5)$. If $j \neq 1$, i.e., $n_1 = 3t_1$, then applying Claim 4.2 and Theorem 1.2 again, one obtains

$$\Phi(F) \leq (3^{t_1-1} + t_1 + 1) \cdot (3^{t_j-1} + 1) \cdot 3^{t-t_1-t_j} = 4 \cdot 3^{t-2},$$

and the equality holds if and only if $T_1 \cong P_6$ and $T_j \cong P_4$, i.e., $F \cong P_6 \cup P_4 \cup (t - 3)P_3$.

Consequently, if $n = 3t+1$, then $F \in \{T \cup (t-2)P_3 : T \in \mathcal{T}_1(7, 5)\} \cup \{P_6 \cup P_4 \cup (t-3)P_3\}$, as desired.

Case 3*:* $n = 3t+2$. Assume that $F \cong T_1 \cup \cdots \cup T_r \cup l_1P_4 \cup l_2K_{1,3}$ for some nonnegative integers r, l_1 and l_2 with $r+l_1+l_2 = k$ and $\sum_{i=1}^{r} t_i + l_1 + l_2 = t$, where $T_i \notin \{P_4, K_{1,3}\}$ for $1 \leq i \leq r$. Hence $l_1+l_2 \leq 2$. Let $F_5 = T_1 \cup \cdots \cup T_r$. Then $F_5 \in \mathfrak{F}(n-4(l_1+l_2), \psi-3(l_1+l_2))$ and $t(F_5) = t - (l_1 + l_2)$. Based on Theorems 1.2 and 1.3, we know that if F_5 is connected, then

$$\Phi(F_5) \leq \begin{cases} 3^{t-(l_1+l_2)-1} + t - (l_1 + l_2) + 1 & \text{if } |V_{F_5}| = 3t(F_5), \\ 3^{t-(l_1+l_2)-1} + 1 & \text{if } |V_{F_5}| = 3t(F_5) + 1, \\ 3^{t-(l_1+l_2)-1} & \text{if } |V_{F_5}| \geq 3t(F_5) + 2. \end{cases} \tag{4.1}$$

Next, we consider the following three possible subcases.

• $l_1 + l_2 = 2$. Then together with Theorem 1.1 we have $n_i = 3t_i$ for $1 \leq i \leq r$. If $l_1 = 2$, then $t_1 \geq 2$ and $t \geq 4$. Otherwise, $F \cong 2P_4 \cup (t-2)P_3$, a contradiction. Therefore, $F_5 \in \mathfrak{F}(n - 8, \psi - 6) \setminus \mathcal{F}_1(n - 8, \psi - 6)$ and $t(F_5) = t - 2 \geq 2$. Together with Case 1 and (4.1), we have

$$\Phi(F) = 4\Phi(F_5) \leq 4 \cdot \max\{3^{t-3} + t - 1, 2 \cdot 3^{t-3}\} = 8 \cdot 3^{t-3} < 3^{t-1},$$

a contradiction. If $l_1 \leq 1$, then in view of Case 1 and (4.1), we get

$$\Phi(F) \leq 2\Phi(F_5) \leq 2 \cdot \max\{3^{t-3} + t - 1, 3^{t-2}\} = 2 \cdot 3^{t-2} < 3^{t-1},$$

a contradiction.

• $l_1 + l_2 = 1$. Then $F_5 \in \mathfrak{F}(n-4, \psi-3)$ and $t(F_5) = t-1$. Therefore, $|V_{F_5}| = 3t(F_5)+1$. Note that P_4 is not a component of F_5 and so $F_5 \ncong P_4 \cup (t-2)P_3$. In view of Case 2 and (4.1), one has

$$\Phi(F) \leq 2\Phi(F_5) \leq 2 \cdot \max\{3^{t-2} + 1, 4 \cdot 3^{t-3}\} = 8 \cdot 3^{t-3} < 3^{t-1},$$

a contradiction.

• $l_1 + l_2 = 0$. Then there exists an integer j with $1 \leq j \leq r$ such that $n_j = 3t_j + 2$, or there are two integers j_1 and j_2 with $1 \leq j_1 < j_2 \leq r$ such that $n_{j_1} = 3t_{j_1} + 1$ and $n_{j_2} = 3t_{j_2} + 1$. For the former case, one has $n_i = 3t_i$ if $i \in \{1, \ldots, r\} \setminus \{j\}$. Combining Theorems 1.2 and 1.3 with Case 1, we obtain

$$\Phi(F) = \Phi(T_j)\Phi(F - T_j) \leq 3^{t_j-1} \cdot \max\{3^{t-t_j-1} + t - t_j + 1, 3^{t-t_j}\} = 3^{t-1}$$

and all the equalities throughout hold if and only if $F \cong T_j \cup (t - t_j)P_3$, where $T_j \in \mathcal{T}_1(n_j, \psi_j)$. For the latter case, one has $n_i = 3t_i$ if $i \in \{1, \ldots, r\} \setminus \{j_1, j_2\}$ and $\min\{t_{j_1}, t_{j_2}\} \geq 2$. By a similar discussion as Claim 4.2, one obtains that $t_{j_1} = t_{j_2} = 2$ and $t_i = 1$ for each $i \in \{1, \ldots, r\} \setminus \{j_1, j_2\}$. Therefore, $r = t-2$ and $T_i \cong P_3$ for each $i \in \{1, \ldots, r\} \setminus \{j_1, j_2\}$. Applying Theorem 1.2 again, one obtains

$$\Phi(F) = \Phi(T_{j_1})\Phi(T_{j_2})\Phi(F - T_{j_1} - T_{j_2}) \leq 16 \cdot 3^{t-4} < 3^{t-1},$$

a contradiction.

Therefore, we have shown that if $n = 3t + 2$, then $F \cong T \cup lP_3$, where $T \in \mathcal{T}_1(n - 3l, \psi - 2l)$ with $0 < l < t$.

Case 4: $n \geq 3t + 3$. Assume that $F \cong T_1 \cup \cdots \cup T_r \cup l_1P_4 \cup l_2K_{1,3} \cup l_3P_3$ for some nonnegative integers r, l_1, l_2 and l_3 with $r + l_1 + l_2 + l_3 = k$ and $\sum_{i=1}^{r} t_i + l_1 + l_2 + l_3 = t$, where $T_i \notin \{P_3, P_4, K_{1,3}\}$ for $1 \leq i \leq r$. We claim that $l_1 + l_2 \leq 3$. Otherwise, $l_1 + l_2 > 3$. Let $F_6 = T_1 \cup \cdots \cup T_r \cup (l_1 + l_2 - 3)P_4 \cup T \cup l_3P_3$, where $T \in \mathcal{T}_1(12, 9)$. Note that F_6 is a disconnected forest in $\mathfrak{F}(n, \psi) \setminus \mathcal{F}_1(n, \psi)$. By a direct calculation, we obtain

$$\Phi(F) \leq 2^{l_1+l_2} \cdot 3^{l_3} \cdot \prod_{i=1}^{r} \Phi(T_i) < 2^{l_1+l_2-3} \cdot 9 \cdot 3^{l_3} \cdot \prod_{i=1}^{r} \Phi(T_i) = \Phi(F_6),$$

which contradicts the choice of F. In order to characterize the structure of F, we need the following two claims.

Claim 4.3. There exists at most one j in $\{1, \ldots, r\}$ such that $n_j \geq 3t_j + 2$.

Proof. Suppose that there are two components, say T_{j_1} and T_{j_2}, with $1 \le j_1 < j_2 \le r$ such that $n_{j_1} \ge 3t_{j_1} + 2$ and $n_{j_2} \ge 3t_{j_2} + 2$. Then let $F_7 = P_4 \cup T \cup (F - T_{j_1} - T_{j_2})$, where $T \in \mathcal{T}_1(n_{j_1} + n_{j_2} - 4, \psi_{j_1} + \psi_{j_2} - 3)$. Clearly, F_7 contains at least two components and $F_7 \in \mathfrak{F}(n,\psi) \setminus \mathcal{F}_1(n,\psi)$. On the other hand, combining with Theorems 1.2 and 1.3, one has

$$\Phi(F) \le 3^{t_{j_1}-1} \cdot 3^{t_{j_2}-1} \cdot \Phi(F - T_{j_1} - T_{j_2}) < 2 \cdot 3^{t_{j_1}+t_{j_2}-2}\Phi(F - T_{j_1} - T_{j_2}) = \Phi(F_7),$$

which contradicts the choice of F.

This completes the proof of Claim 4.3. □

Note that if $l_1 + l_2 > 0$, then $F \notin \mathcal{F}_1(n,\psi)$. Together with Claim 4.3, and by a similar discussion as Claims 4.1 and 4.2, we obtain the following claim immediately.

Claim 4.4. If $l_1 + l_2 > 0$, then $r \le 1$. In addition, if $r = 1$, then $n_1 \ge 3t_1 + 2$.

We firstly consider that $l_1 + l_2 = 3$. Note that $n \ge 3t + 3$. If $n = 3t + 3$, then $r = 0$ (based on Claim 4.4). Thus, $\Phi(F) \le 8 \cdot 3^{t-3}$ with equality if and only if $F \cong 3P_4 \cup (t-3)P_3$. If $n \ge 3t + 4$, then by Claim 4.4 one has $r = 1$ and $n_1 \ge 3t_1 + 2$. In view of Theorems 1.2 and 1.3, we get

$$\Phi(F) \le 3^{t_1-1} \cdot 2^{l_1} \cdot 3^{t-t_1-l_1-l_2} \le 8 \cdot 3^{t-4} < 2 \cdot 3^{t-2},$$

a contradiction.

Next, we assume that $1 \le l_1 + l_2 \le 2$. Since $n \ge 3t + 3$, together with Claim 4.4 one obtains $r = 1$ and $n_1 \ge 3t_1 + 2$. Applying Theorems 1.2 and 1.3 yields

$$\Phi(F) \le 3^{t_1-1} \cdot 2^{l_1} \cdot 3^{t-t_1-l_1-l_2} \le 2 \cdot 3^{t-2},$$

and all the equalities throughout hold if and only if $F \cong T_1 \cup P_4 \cup (t - t_1 - 1)P_3$ with $T_1 \in \mathcal{T}_1(n_1, \psi_1)$.

Now, we consider the case $l_1 + l_2 = 0$ and $r = 1$. Then $n_1 \ge 3t_1 + 3$. Note that $F \notin \mathcal{F}_1(n,\psi)$ and so $T_1 \notin \mathcal{T}_1(n_1,\psi_1)$. In view of Theorems 1.2 and 1.3, one has $\Phi(F) \le 2 \cdot 3^{t_1-2} \cdot 3^{t-t_1} = 2 \cdot 3^{t-2}$, and the equality holds if and only if $F \cong T_1 \cup (t - t_1)P_3$, where $T_1 \in \mathcal{T}_2(n_1, \psi_1)$ with $2 \le t_1 < t$.

In what follows, we assume $l_1 + l_2 = 0$ and $r \ge 2$. In view of Claim 4.3, we obtain that there exists at most one component, say T_j, of F with $j \in \{1, \dots, r\}$ and $n_j \ge 3t_j + 2$. Note that $T_i \notin \{P_3, P_4, K_{1,3}\}$ for $1 \le i \le r$. Hence $t_i \ge 2$ for each $i \in \{1, \dots, r\} \setminus \{j\}$. By a similar discussion as Claims 4.1 and 4.2, one has $t_i = 2$ for each $i \in \{1, \dots, r\} \setminus \{j\}$.

If F contains exactly one component T_j with $n_j \ge 3t_j + 2$, then $r = 2$. Otherwise, suppose that F contains at least two components, say T_{j_1} and T_{j_2}, such that $n_{j_i} \le 3t_{j_i} + 1$ for $i \in \{1, 2\}$. If $n_{j_1} = 3t_{j_1}$, then $\Phi(F) \le 6 \cdot \Phi(F - T_{j_1}) < 9 \cdot \Phi(F - T_{j_1}) = \Phi(2P_3 \cup (F - T_{j_1}))$.

Obviously, $2P_3 \cup (F - T_{j_1}) \in \mathfrak{F}(n,\psi) \setminus \mathcal{F}_1(n_1,\psi_1)$, we obtain a contradiction. If $n_{j_1} = 3t_{j_1}+1$, then $\Phi(F) \le 4\cdot\Phi(F - T_{j_1}) < 6\cdot\Phi(F-T_{j_1}) = \Phi(P_3 \cup P_4 \cup (F - T_{j_1}))$. Clearly, $P_3 \cup P_4 \cup (F - T_{j_1}) \in \mathfrak{F}(n,\psi) \setminus \mathcal{F}_1(n_1,\psi_1)$, we also get a contradiction. It follows from Theorems 1.2 and 1.3 that

$$\Phi(F) \le 3^{t_j-1}\cdot 6 \cdot 3^{t-t_j-2} = 2\cdot 3^{t-2},$$

and all the equalities throughout hold if and only if $F \cong T_1 \cup P_6 \cup (t-t_1-2)P_3$, where $T_1 \in \mathcal{T}_1(n_1,\psi_1)$.

If each component T_i of F satisfies $n_i \le 3t_i+1$, then $r \ge 3$. Without loss of generality, assume that $n_1 = 3t_1+1 = 7$. It follows that

$$\Phi(F) \le 4\cdot\Phi(F-T_1) < \Phi(P_3 \cup P_4 \cup (F - T_1)).$$

Together with $P_3 \cup P_4 \cup (F-T_1) \in \mathfrak{F}(n,\psi) \setminus \mathcal{F}_1(n_1,\psi_1)$, we get a contradiction.

We can now derive the final conclusion of this case: if $n = 3t+3$, then $F \cong 3P_4 \cup (t-3)P_3$; if $n \ge 3t+4$, then $F \cong T \cup P_4 \cup lP_3$ with $T \in \mathcal{T}_1(n-3l-4,\psi-2l-3)$ and $l < t-1$, or $F \cong T \cup lP_3$ with $T \in \mathcal{T}_2(n-3l,\psi-2l)$ and $0 < l < t-1$, or $F \cong T \cup P_6 \cup lP_3$ with $T \in \mathcal{T}_1(n-3l-6,\psi-2l-4)$ and $l < t-2$.

This completes the proof. □

5. Concluding remarks

In this paper, we first establish a lower bound on the dissociation number of a forest with fixed order, and all extremal forests are characterized. Then, we characterize all trees (resp. forests) with the largest and the second largest number of maximum dissociation sets among trees (resp. forests) with given order and dissociation number.

If we just fix the order n of a tree T and its dissociation number is taken over all possible integers, then in view of Theorems 1.2 and 1.3, we know that the upper bound of $\Phi(T)$ is decreasing with respect to $\psi(T)$ for $\psi(T) \in [2n/3, n]$. The following result is an immediate consequence of Theorems 1.2 and 1.3, which determines all trees with fixed order having the largest and second largest number of maximum dissociation sets, and the first part is obtained in [27].

Corollary 5.1. *Let T a tree on n (≥ 4) vertices. Then*

$$\Phi(T) \le \begin{cases} 3^{\frac{n}{3}-1} + \frac{n}{3} + 1 & \text{if } n \equiv 0 \pmod 3,\\ 3^{\frac{n-1}{3}-1} + 1 & \text{if } n \equiv 1 \pmod 3,\\ 3^{\frac{n-2}{3}-1} & \text{if } n \equiv 2 \pmod 3.\end{cases}$$

Equality holds if and only if $T \in \mathcal{T}_1(n)$, where

$$\mathcal{T}_1(n) = \begin{cases} \{O_{P_3,(\frac{n}{3}-1)P_4}\} & \textit{if } n \equiv 0 \pmod 3, \\ \{O_{P_2,P_3,t'P_4,(\frac{n-1}{3}-t'-1)K_{1,3}} : 0 \le t' \le \frac{n-1}{3} - 1\} & \textit{if } n \equiv 1 \pmod 3, \\ \{O_{xP_2,yP_3,t'P_4,(\frac{n-2}{3}-t'-1)K_{1,3}} : x + 2y = 4 & \\ \quad \textit{and } 0 \le t' \le \frac{n-2}{3} - 1\} \cup \{O_{P_2,P_3,T^*_{5,3}}\} & \textit{if } n \equiv 2 \pmod 3. \end{cases}$$

Furthermore, if $T \notin \mathcal{T}_1(n)$, then

$$\Phi(T) \le \begin{cases} 2 & \textit{if } n = 8, \\ 3^{\frac{n}{3}-1} + \frac{n}{3} & \textit{if } n \equiv 0 \pmod 3, \\ 3^{\frac{n-1}{3}-1} & \textit{if } n \equiv 1 \pmod 3, \\ 2 \cdot 3^{\frac{n-2}{3}-2} + 1 & \textit{if } n \equiv 2 \pmod 3 \textit{ and } n \ne 8. \end{cases}$$

Equality holds if and only if $T \in \mathcal{T}_2(n)$, where

$$\mathcal{T}_2(n) = \begin{cases} \{O_{3P_2,P_5}, O_{3P_2,T^*_{5,3}}, O_{P_2,P_3,P_5}\} & \textit{if } n = 8, \\ \{O_{2P_2,K_{1,3}}, O_{P_3,(\frac{n}{3}-2)P_4,K_{1,3}}\} & \textit{if } n \equiv 0 \pmod 3, \\ \{O_{3P_2,t'P_4,(\frac{n-1}{3}-t'-1)K_{1,3}} : 0 \le t' \le \frac{n-1}{3} - 1\} & \\ \quad \cup \{P_7, O_{P_3,P_4,T^*_{5,3}}\} & \textit{if } n \equiv 1 \pmod 3, \\ \{O_{P_2,P_3,T^*_{5,3},t'P_4,(\frac{n-2}{3}-t'-2)K_{1,3}} : 0 \le t' \le \frac{n-2}{3} - 2\} & \textit{if } n \equiv 2 \pmod 3 \textit{ and } n \ne 8. \end{cases}$$

Next, if we just fix the dissociation number ψ of a tree T and its order n is taken over all possible integers, then by Theorems 1.2 and 1.3, one obtains that the upper bound of $\Phi(T)$ is increasing with respect to n for $n \in [1, 3\psi/2]$. The subsequent result follows from Theorems 1.2 and 1.3, which characterizes all trees with fixed dissociation number having the largest and second largest number of maximum dissociation sets, and the first part is given in [26].

Corollary 5.2. *Let T a tree with dissociation number ψ. Then*

$$\Phi(T) \le \begin{cases} 1 & \textit{if } \psi = 1, \\ 3^{\frac{\psi-1}{2}-1} + 1 & \textit{if } \psi \textit{ is odd and } \psi > 1, \\ 3^{\frac{\psi}{2}-1} + \frac{\psi}{2} + 1 & \textit{if } \psi \textit{ is even.} \end{cases}$$

Equality holds if and only if $T \in \mathcal{T}'_1(\psi)$, where

$$\mathcal{T}'_1(\psi) = \begin{cases} \{P_1\} & \textit{if } \psi = 1, \\ \{O_{P_2,P_3,t'P_4,(\frac{\psi-1}{2}-t'-1)K_{1,3}} : 0 \le t' \le \frac{\psi-1}{2} - 1\} & \textit{if } \psi \textit{ is odd and } \psi > 1, \\ \{O_{P_3,(\frac{\psi}{2}-1)P_4}\} & \textit{if } \psi \textit{ is even.} \end{cases}$$

Furthermore, if $T \notin \mathcal{T}_1'(\psi)$, then $\psi \geq 2$ and

$$\Phi(T) \leq \begin{cases} 1 & \text{if } \psi = 2, \\ 3^{\frac{\psi-1}{2}-1} & \text{if } \psi \text{ is odd}, \\ 3^{\frac{\psi}{2}-1} + \frac{\psi}{2} & \text{if } \psi \text{ is even and } \psi > 2. \end{cases}$$

Equality holds if and only if $T \in \mathcal{T}_2'(\psi)$, where

$$\mathcal{T}_2'(\psi) = \begin{cases} \{P_2\} & \text{if } \psi = 2, \\ \{O_{3P_2,t'P_4,(\frac{\psi-1}{2}-t'-1)K_{1,3}} : 0 \leq t' \leq \frac{\psi-1}{2} - 1\} & \\ \quad \cup \{P_7, O_{P_3,P_4,T^*_{5,3}}\} & \text{if } \psi \text{ is odd}, \\ \{O_{2P_2,K_{1,3}}, O_{P_3,(\frac{\psi}{2}-2)P_4,K_{1,3}}\} & \text{if } \psi \text{ is even and } \psi > 2. \end{cases}$$

Similarly, all forests with fixed order (resp. dissociation number) having the largest and the second largest number of maximum dissociation sets can be deduced by Theorem 1.4.

Corollary 5.3. *Let F be a forest on $n \geq 6$ vertices with at least two components, and each component of F has order at least 3. Then*

$$\Phi(F) \leq \begin{cases} 3^{\frac{n}{3}} & \text{if } n \equiv 0 \pmod 3, \\ 2 \cdot 3^{\frac{n-1}{3}-1} & \text{if } n \equiv 1 \pmod 3, \\ 4 \cdot 3^{\frac{n-2}{3}-2} & \text{if } n \equiv 2 \pmod 3. \end{cases}$$

Equality holds if and only if $F \in \mathcal{F}_1(n)$, where

$$\mathcal{F}_1(n) = \begin{cases} \{\frac{n}{3}P_3\} & \text{if } n \equiv 0 \pmod 3, \\ \{P_4 \cup (\frac{n-1}{3} - 1)P_3\} & \text{if } n \equiv 1 \pmod 3, \\ \{2P_4 \cup (\frac{n-2}{3} - 2)P_3\} & \text{if } n \equiv 2 \pmod 3. \end{cases}$$

Furthermore, if $F \notin \mathcal{F}_1(n)$, then $n \geq 7$ and

$$\Phi(F) \leq \begin{cases} 3 & \text{if } n = 7, \\ 2 \cdot 3^{\frac{n}{3}-1} & \text{if } n \equiv 0 \pmod 3, \\ 4 \cdot 3^{\frac{n-1}{3}-2} & \text{if } n \equiv 1 \pmod 3 \text{ and } n \neq 7, \\ 3^{\frac{n-2}{3}-1} & \text{if } n \equiv 2 \pmod 3. \end{cases}$$

Equality holds if and only if $F \in \mathcal{F}_2(n)$, where

$$\mathcal{F}_2(n) = \begin{cases} \{K_{1,3} \cup P_3\} & \text{if } n = 7, \\ \{P_6 \cup (\frac{n}{3} - 2)P_3\} & \text{if } n \equiv 0 \pmod 3, \\ \{T \cup (\frac{n-1}{3} - 2)P_3 : T \in \mathcal{T}_1(7)\} & \\ \quad \cup \{P_6 \cup P_4 \cup (\frac{n-1}{3} - 3)P_3\} & \text{if } n \equiv 1 \pmod 3 \text{ and } n \neq 7, \\ \{T \cup lP_3 : T \in \mathcal{T}_1(n-3l) \text{ with } 1 \leq l < \frac{n-2}{3}\} & \text{if } n \equiv 2 \pmod 3. \end{cases}$$

Corollary 5.4. *Let F be a forest with dissociation number $\psi \geq 4$, and F contains at least two components each of which has order at least 3. Then*

$$\Phi(F) \leq \begin{cases} 3^{\frac{\psi}{2}} & \text{if } \psi \text{ is even}, \\ 2 \cdot 3^{\frac{\psi-1}{2}-1} & \text{if } \psi \text{ is odd}. \end{cases}$$

Equality holds if and only if $F \in \mathcal{F}_1'(\psi)$, where

$$\mathcal{F}_1'(\psi) = \begin{cases} \{\frac{\psi}{2}P_3\} & \text{if } \psi \text{ is even}, \\ \{P_4 \cup (\frac{\psi-1}{2} - 1)P_3\} & \text{if } \psi \text{ is odd}. \end{cases}$$

Furthermore, if $F \notin \mathcal{F}_1'(\psi)$, then $\psi \geq 5$ and

$$\Phi(F) \leq \begin{cases} 3 & \text{if } \psi = 5, \\ 2 \cdot 3^{\frac{\psi}{2}-1} & \text{if } \psi \text{ is even}, \\ 4 \cdot 3^{\frac{\psi-1}{2}-2} & \text{if } \psi \text{ is odd and } \psi \geq 7. \end{cases}$$

Equality holds if and only if $F \in \mathcal{F}_2'(\psi)$, where

$$\mathcal{F}_2'(\psi) = \begin{cases} \{K_{1,3} \cup P_3\} & \text{if } \psi = 5, \\ \{P_6 \cup (\frac{\psi}{2} - 2)P_3\} & \text{if } \psi \text{ is even}, \\ \{T \cup (\frac{\psi-1}{2} - 2)P_3 : T \in \mathcal{T}_1'(5)\} & \\ \quad \cup \{P_6 \cup P_4 \cup (\frac{\psi-1}{2} - 3)P_3\} & \text{if } \psi \text{ is odd and } \psi \geq 7. \end{cases}$$

On the other hand, motivated by [10, 11, 17, 18, 31], which characterized graphs with the maximal number of maximal independent sets, it is interesting to characterize graphs having the maximal number of maximal dissociation sets among some families of graphs. We will do it in the near future.

Acknowledgments

We take this opportunity to thank the anonymous referees for their careful reading of the manuscript and suggestions which have immensely helped us in getting the article to its present form. This work is financially supported by the National Natural Science Foundation of China (Grant Nos. 12171190, 11671164) and the excellent doctoral dissertation cultivation grant from Central China Normal University (Grant No. 2022YBZZ033).

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