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The number of dominating sets in *d*-ary trees

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Abstract
An (unrooted) *d-ary tree* is a tree in which every internal vertex has degree $d+1$. In this paper, we show for every fixed $d \geq 2$ that *d*-ary caterpillars have the minimum number of dominating sets among *d*-ary trees of a given order. We also determine the maximum number of dominating sets in binary trees (the special case $d = 2$) and classify the extremal trees, which are also unique.

Keywords Binary tree · *d*-ary tree · Dominating set · Number of dominating sets

Mathematics Subject Classification 05C05 · 05C69

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1 Introduction

A *dominating set D* is a set of vertices in a graph *G* such that every vertex is *dominated*, i.e., it is an element of *D* or has a neighbour in *D*. The books [4–6] give a comprehensive survey on domination in graphs. For a graph *G* on *n* vertices, the number of dominating sets of *G*, $\delta(G)$, has the trivial bounds $1 \leq \delta(G) \leq 2^n - 1$, with equality for the empty and complete graphs respectively. Bród and Skupień [2] studied the number of dominating sets in trees. They showed that the star of order *n*, with $2^{n-1} + 1$ dominating sets, has the maximum number of dominating sets in a tree on *n* vertices (for $n = 4$ and $n = 5$, the path has the same number). As a lower bound, we have

$$\delta(T) \geq \begin{cases} 5^{\frac{n}{3}}, & n \equiv 0 \mod 3, \\ 9 \cdot 5^{\frac{n-4}{3}}, & n \equiv 1 \mod 3, \\ 3 \cdot 5^{\frac{n-2}{3}}, & n \equiv 2 \mod 3, \end{cases}$$

which is attained with equality by a rich class of trees. Wagner [16] showed that this lower bound still holds for arbitrary connected graphs and graphs without isolated vertices, see also [14]. There are also similar results on minimal dominating sets [3, 10], minimal 2-dominating sets [9] and total dominating sets [7, 8, 11].

A vertex of degree 1 in a tree is a *leaf*. All other vertices are called *internal vertices*. A *binary tree* (more precisely, *unrooted binary tree*) is a tree in which all internal vertices are exactly of degree 3 (see for instance [15]). Such trees arise for example in the context of phylogenetics. More generally, if all internal vertices of a tree are exactly of degree $d + 1$, it is known as a *d-ary tree*.

A *rooted d-ary tree* has a distinguished root of degree *d*, while all other internal vertices have degree $d + 1$. Here and in the following, whenever we only write "*d*-ary tree" without further specification, we refer to unrooted *d*-ary trees.

The focus of this paper is the number of dominating sets in *d*-ary trees of a given order, with the goal to determine the maximum and minimum values and the corresponding extremal trees. Similar results have been obtained for the number of subtrees [15], the number of independent sets and the number of matchings [1]. See also [12, 13] for analogous results on the number of maximal independent (equivalently, independent dominating) sets and total dominating sets.

In the following section, we will show that the minimum number of dominating sets of a *d*-ary tree with *k* internal vertices is $(2^d + 1)^2(2^{d-1} + 1)^{k-2}$. The minimum is attained by the *d-ary caterpillar*, i.e., a *d*-ary tree in which the internal vertices form a path, as shown in Fig. 1. See Theorem 2.5. In Sect. 3, the binary trees with maximum number of dominating

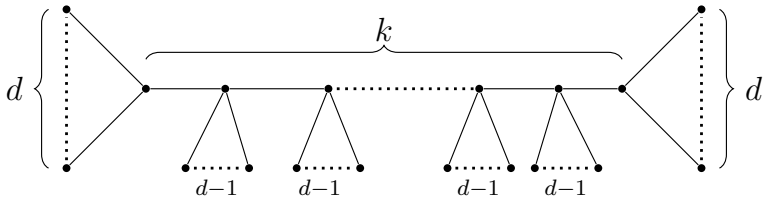


Fig. 1 A *d*-ary caterpillar with *k* internal vertices

sets are established in Theorems 3.8 and 3.9. The binary trees attaining the maximum are also always unique.

For our proofs, we need several auxiliary quantities associated with rooted (*d*-ary) trees. Let S be a rooted tree, with root v. We consider three different types of vertex subsets that are dominating except possibly for v. The vertex v can be included in such a set or not. If v is an element, then it is of course automatically dominated. Otherwise, if v is not included in such a set, it can be dominated by other vertices or not. This gives a total of three combinations that are indicated by subscripts in the notation we use: the first subscript is 1 if v is included and 0 otherwise; the second subscript is 1 if v is dominated (i.e., if v or one of its neighbours is included in the set), and 0 otherwise. Thus the three possible combinations are as follows:

- $\delta_{11}(S, v)$ is the number of dominating sets of S that include v;
- $\delta_{01}(S, v)$ is the number of dominating sets of S that do not include v;
- $\delta_{00}(S, v)$ is the number of vertex subsets of S where neither v nor any of its neighbours is included and all vertices but v are dominated.

Note that $\delta(S) = \delta_{11}(S, v) + \delta_{01}(S, v)$. For short, we will often write S_{ab} instead of $\delta_{ab}(S, v)$. For example, in the trivial case that S consists of a single vertex v, we have

$$S_{11} = \delta_{11}(S, v) = 1, S_{01} = \delta_{01}(S, v) = 0, S_{00} = \delta_{00}(S, v) = 1.$$

It is clear that $\delta_{11}(S, v) > 0$, since the set consisting of all vertices is always dominating. Likewise, $\delta_{01}(S, v) > 0$ for all trees S with more than one vertex, since the set consisting of all vertices except for v is always dominating. However, as we will see, $\delta_{00}(S, v)$ can be 0 even in nontrivial cases. Lemma 2.1 characterizes this situation.

2 *d*-ary trees with minimum number of dominating sets

As a first result, we obtain the minimum number of dominating sets in *d*-ary trees and characterize the extremal cases. Here and in the rest of this paper, an internal vertex will be called a *support vertex* if it is adjacent to at least one leaf, and a *leafless vertex* otherwise.

Lemma 2.1 *For every rooted tree S with root v, we have $\delta_{00}(S, v) = 0$ if and only if v is a support vertex.*

Proof If v is a leaf or a leafless internal vertex, then $V(S) - N[v]$ (the set consisting of all vertices except for v and its neighbours) is a set that is counted by $\delta_{00}(S, v)$, thus $\delta_{00}(S, v) > 0$. If v is a support vertex, then there exists at least one leaf neighbour u. In a set D that is counted by $\delta_{00}(S, v)$, neither u nor v can be included. This however means that u is not dominated, which is a contradiction. Thus $\delta_{00}(S, v) = 0$ in this case. □

Rooted d-ary caterpillars are rooted *d*-ary trees where the internal vertices form a path, as shown in Fig. 2. They will play a major role in the proof of the main result of this section. The following lemma provides the values of δ_{11}, δ_{01} and δ_{00} for a rooted *d*-ary caterpillar as well as the total number of dominating sets in an (unrooted) *d*-ary caterpillar.

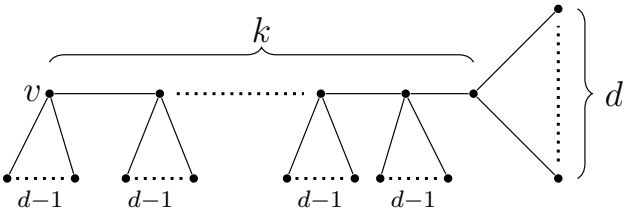


Fig. 2 A rooted d-ary caterpillar with root v

Lemma 2.2 *Let S be a rooted d-ary caterpillar with root v and $k \geq 1$ internal vertices (as in Fig. 2). Then we have*

$$\delta_{11}(S) = \begin{cases} 2^d, & k = 1, \\ 2^{d-1}(2^d+1)(2^{d-1}+1)^{k-2}, & k > 1, \end{cases}$$

$$\delta_{01}(S) = \begin{cases} 1, & k = 1, \\ (2^d+1)(2^{d-1}+1)^{k-2}, & k > 1, \end{cases}$$

$$\delta_{00}(S) = 0.$$

Furthermore, for every d-ary caterpillar T with $k \geq 2$ internal vertices (see Fig. 1), we have

$$\delta(T) = (2^d+1)^2(2^{d-1}+1)^{k-2}.$$

Proof Note that every internal vertex of a rooted or unrooted d-ary caterpillar is a support vertex. For every internal vertex w, a dominating set D must either contain w or all its leaf neighbours so that all leaves are dominated. Conversely, if this condition holds for every internal vertex w, then D is indeed dominating. In the case of a rooted caterpillar, this gives us $2^{d-1}+1$ possibilities for every internal vertex other than the internal vertex furthest from the root v (or v itself if $k = 1$), where we have $2^d + 1$ possibilities. For an unrooted caterpillar, we have $2^{d-1}+1$ possible choices for each internal vertex other than the two ends, and $2^d + 1$ for each of the ends. The stated formulas for $\delta_{11}(S)$, $\delta_{01}(S)$ and $\delta(T)$ follow. We already know from Lemma 2.1 that $\delta_{00}(S) = 0$. □

Suppose L, R and W are rooted trees with roots v_l, v_r and v_w respectively. With the abbreviations introduced earlier in the introductory section (i.e., $L_{11} = \delta_{11}(L)$, etc.), let us set

$$\mathcal{L} = L_{11} + L_{01} + L_{00}, \quad \mathcal{R} = R_{11} + R_{01} + R_{00} \quad \text{and} \quad \mathcal{W} = W_{11} + W_{01} + W_{00}. \tag{1}$$

Our next lemma gives formulas for the number of dominating sets in trees that are decomposed in a certain way. When an edge e of a tree T is removed, each of the two connected components can be considered as a rooted tree (rooted at one of the ends of e). Such a rooted tree is then called a *branch* of T.

Lemma 2.3 *Suppose that a tree T can be decomposed as shown in Fig. 3 (left), where the two branches L and R are rooted trees with roots v_l and v_r respectively, and S has a distinguished vertex v. We have*

$$\delta(T) = \mathcal{L}\mathcal{R}S_{11} + \delta(L)\delta(R)S_{01} + (\delta(L)\delta(R) - L_{01}R_{01})S_{00}. \tag{2}$$

As a special case, consider a tree T' that can be decomposed into a tree S with a distinguished vertex *v*, a branch *W* with root v_w, and a single leaf *u*, as in Fig. 3 (right). We have

$$\delta(T') = 2\mathcal{W}S_{11} + \delta(W)(S_{01} + S_{00}). \tag{3}$$

Proof First consider any dominating set D of T, and let $D' = D \cap V(S)$. Then D' dominates all vertices of S except possibly v (which can be dominated by v_l or v_r instead, unlike the other vertices of S). Hence we distinguish three possible cases that depend on D'.

- Case 1: D' is a set that contains v and is thus counted by S_{11}. In this case, v_l and v_r are dominated by v. The part of D that belongs to L can either dominate all of L or all but v_l, giving us $\delta(L) + L_{00} = L_{11} + L_{01} + L_{00} = \mathcal{L}$ possibilities in T. Likewise, there are $\mathcal{R}$ possibilities for the part of D that belongs to R, for a total of

$$\mathcal{L}\mathcal{R}S_{11}$$

possible combinations.

- Case 2: D' is a set that dominates all of S, but does not contain v, so it is counted by S_{01}. Then the rest of D can consist of arbitrary dominating sets in L and R, so there are

$$\delta(L)\delta(R)S_{01}$$

possible combinations.

- Case 3: D' is a set that dominates all of S except for v, and is thus counted by S_{00}. Since v is not dominated in D', either v_l or v_r needs to be included. So the rest of D consists of dominating sets in L and R, with either v_l or v_r (or both) included. There are $\delta(L)\delta(R) - L_{01}R_{01}$ pairs of such dominating sets in L and R, so we have

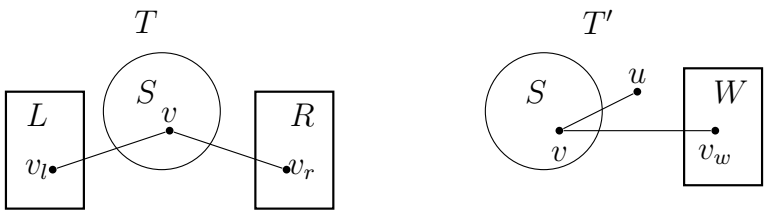


Fig. 3 The trees T and T' in Lemma 2.3

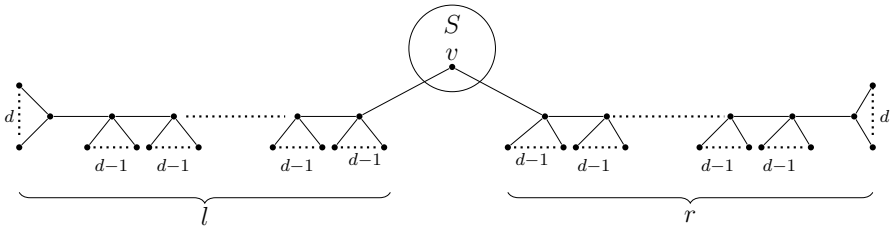


Fig. 4 The tree T in Lemma 2.4

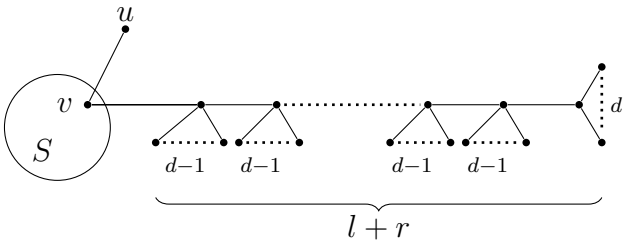


Fig. 5 The tree T' in Lemma 2.4

$$(\delta(L)\delta(R) - L_{01}R_{01})S_{00}$$

possible combinations in this case.
Adding the three cases, we obtain Eq. (2).

Equation (3) is obtained as the special case where L is a single vertex and $R = W$. We only have to set $\mathcal{L} = 2$, $\delta(L) = 1$ and $L_{01} = 0$ in (2). □

Lemma 2.4 *In the setting of Lemma 2.3, suppose that T is a d-ary tree where the branches L and R are rooted d-ary caterpillars with l and r internal vertices respectively ($l, r \geq 1$, see Fig. 4). Then*

$$\delta(T) = (2^{d-1}+1)^{l+r-4}\Bigg((2^d+1)^2(2^{d-1}+1)^2(S_{11}+S_{01}) + \begin{cases} (2^{2d}+2^{d+1})(2^{d-1}+1)^2S_{00}, & l=r=1 \\ (2^{2d-1}+3\cdot 2^{d-1})(2^d+1)(2^{d-1}+1)S_{00}, & l=1 or r=1, but not both \\ 2^d(2^d+1)^2(2^{d-2}+1)S_{00}, & l,r>1 \end{cases}\Bigg). \tag{4}$$

Still in the setting of Lemma 2.3, suppose that T' is a d-ary tree where W is a rooted d-ary caterpillar branch with $l + r$ internal vertices (as in Fig. 5). Then we have

$$\delta(T') = (2^d+1)(2^{d-1}+1)^{l+r-1}\Big(2S_{11}+S_{01}+S_{00}\Big). \tag{5}$$

Furthermore, $\delta(T) \geq \delta(T')$, with equality if and only if S is a star centred at v, i.e., every neighbour of v in S is a leaf.

Proof By Lemma 2.2, we have

$$L_{11} = \begin{cases} 2^d, & l = 1, \\ 2^{d-1}(2^d+1)(2^{d-1}+1)^{l-2}, & l > 1, \end{cases}$$
$$L_{01} = \begin{cases} 1, & l = 1, \\ (2^d+1)(2^{d-1}+1)^{l-2}, & l > 1, \end{cases}$$

$$R_{11} = \begin{cases} 2^d, & r = 1, \\ 2^{d-1}(2^d+1)(2^{d-1}+1)^{r-2}, & r > 1, \end{cases}$$
$$R_{01} = \begin{cases} 1, & r = 1, \\ (2^d+1)(2^{d-1}+1)^{r-2}, & r > 1, \end{cases}$$
$$W_{11} = 2^{d-1}(2^d+1)(2^{d-1}+1)^{l+r-2},$$
$$W_{01} = (2^d+1)(2^{d-1}+1)^{l+r-2},$$

and finally $L_{00} = R_{00} = W_{00} = 0$. Plugging these values into (2) and (3), we arrive at (4) and (5), respectively.

We now prove the final part of the lemma. If the $d-1$ neighbours of v in S are all leaves, then T is isomorphic to T', thus $\delta(T) = \delta(T')$. Assume that at least one of the neighbours of v in S is not a leaf. Setting $\Delta = \delta(T) - \delta(T')$, we want to show that $\Delta > 0$. By (4) and (5), we have

$$\Delta = (2^{d-1}+1)^{l+r-4}\big(\alpha_1 S_{11} + \alpha_2 S_{01} + \alpha_3 S_{00}\big),$$

where

$$\alpha_1 = -(2^d+1)(2^{d-1}+1)^2,$$
$$\alpha_2 = 2^{d-1}(2^d+1)(2^{d-1}+1)^2 = -2^{d-1}\alpha_1,$$

and finally

$$\alpha_3 = \begin{cases} (2^{d-1}+1)^3(2^d-1), & l = r = 1, \\ (2^d+1)(2^{d-1}+1)(2^{2d-2}+2^{d-1}-1), & l = 1 \text{ or } r = 1, \text{but not both}, \\ (2^d+1)(2^{3d-3}+2^{2d-1}-2^{d-1}-1), & l, r > 1. \end{cases}$$

Since $(2^{d-1}+1)^{l+r-4} > 0$, we are done if we can show that

$$\alpha_1 S_{11} + \alpha_2 S_{01} + \alpha_3 S_{00} = \alpha_1 S_{11} - 2^{d-1}\alpha_1 S_{01} + \alpha_3 S_{00} > 0. \tag{6}$$

Let us further decompose S into its root v and rooted d-ary trees $S^1, S^2, \ldots, S^{d-1}$ with roots $v_1, v_2, \ldots, v_{d-1}$ respectively, where $v_1, v_2, \ldots, v_{d-1}$ are the neighbours of v in S (see Fig. 6).

Let $S^* = S - v = \bigcup_{i=1}^{d-1} S^i$. We consider four different types of vertex subsets of the forest S^* that are dominating except possibly for the vertices $v_1, v_2, \ldots, v_{d-1}$. We distinguish according to whether or not at least one of these vertices is included, and whether or

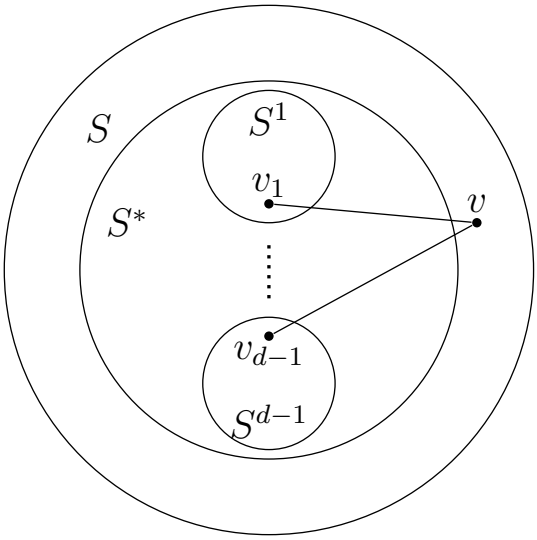


Fig. 6 The rooted d-ary tree S in the proof of Lemma 2.4

not all of them are dominated by another vertex in the set. This gives a total of four combinations that are indicated by subscripts in the notation we use: the first subscript is 1 if at least one of the vertices $v_1, v_2, \ldots, v_{d-1}$ is included, and 0 otherwise; the second subscript is 1 if $v_1, v_2, \ldots, v_{d-1}$ are all dominated, and 0 otherwise. Thus the four possible combinations are as follows:

- S^*_{11} is the number of dominating sets of S^* that include at least one of the vertices $v_1, v_2, \ldots, v_{d-1}$;
- S^*_{01} is the number of dominating sets of S^* that do not include any of the vertices $v_1, v_2, \ldots, v_{d-1}$;
- S^*_{10} is the number of vertex subsets of S^* including at least one of the vertices $v_1, v_2, \ldots, v_{d-1}$, where all vertices other than $v_1, v_2, \ldots, v_{d-1}$ are dominated, and at least one of $v_1, v_2, \ldots, v_{d-1}$ is not dominated;
- S^*_{00} is the number of vertex subsets of S^* where none of the vertices $v_1, v_2, \ldots, v_{d-1}$ is included, all vertices other than $v_1, v_2, \ldots, v_{d-1}$ are dominated, and at least one of $v_1, v_2, \ldots, v_{d-1}$ is not dominated.

The restriction of a dominating set of S that contains v to S^* can be any of these four types, thus

$$S_{11} = S^*_{11} + S^*_{01} + S^*_{10} + S^*_{00},$$

and similarly

$$S_{01} = S^*_{11} \text{ and } S_{00} = S^*_{01}.$$

In view of these identities, (6) becomes

$$-\alpha_1\big((2^{d-1}-1)S^*_{11} - S^*_{10} - S^*_{00}\big) + (\alpha_1+\alpha_3)S^*_{01} > 0. \tag{7}$$

We have $-\alpha_1 = (2^d+1)(2^{d-1}+1)^2 > 0$, and

$$\alpha_1+\alpha_3 = \begin{cases} (2^{d-1}+1)^2(2^{2d-1}-2^{d-1}-2), & l=r=1, \\ (2^d+1)(2^{d-1}+1)(2^{2d-2}-2), & l=1 \text{ or } r=1, \text{but not both}, \\ (2^d+1)(2^{d-2}+1)(2^{2d-1}-2^d-2), & l,r>1, \end{cases}$$

which is clearly positive in all cases as $d \geq 2$. Since $S^*_{01} \geq 0$ holds trivially, the final term in (7) is nonnegative, so we can focus on the remaining expression, more specifically the factor $(2^{d-1}-1)S^*_{11} - S^*_{10} - S^*_{00}$.

Let $\mathcal{F}$ be the set of all vertex sets counted by S^*_{10} or S^*_{00}, and let $\mathcal{H}$ be the set of all sets that are counted by S^*_{11}. We define a map $f : \mathcal{F} \to \mathcal{H}$ as follows: for every F in $\mathcal{F}$, $f(F)$ is obtained from F by adding all vertices in the set $\{v_1, v_2, \ldots, v_{d-1}\}$ that are not dominated by F. The resulting set $f(F)$ is clearly a dominating set of S^* as all vertices other than $v_1, v_2, \ldots, v_{d-1}$ are already dominated in F. Moreover, $f(F)$ includes at least one of the vertices $v_1, v_2, \ldots, v_{d-1}$, so it is indeed an element of $\mathcal{H}$, making the map well-defined.

Let $H \in \mathcal{H}$. We consider the preimage of H under f. Every set $F \in f^{-1}(H)$ is obtained by removing one or more of the vertices $v_1, v_2, \ldots, v_{d-1}$ from H. Since there are only $2^{d-1}-1$ nonempty subsets of these vertices, it follows that $|f^{-1}(H)| \leq 2^{d-1}-1$. Equality can only hold if H contains all the vertices $v_1, v_2, \ldots, v_{d-1}$. So it readily follows that $|\mathcal{F}| \leq (2^{d-1}-1)|\mathcal{H}|$, or equivalently

$$(2^{d-1}-1)S^*_{11} - S^*_{10} - S^*_{00} \geq 0.$$

We have thus already shown that the left side of (7) is nonnegative, and it remains to prove that it cannot be 0. If this were the case, then two things would have to hold: $S^*_{01} = 0$, and $|\mathcal{F}| = (2^{d-1}-1)|\mathcal{H}|$, meaning that every set in $\mathcal{H}$ has exactly $2^{d-1}-1$ preimages under f. If none of the S^i is a single vertex, then the set consisting of all vertices of S^* except for $v_1, v_2, \ldots, v_{d-1}$ is a dominating set, thus $S^*_{01} > 0$ in this case. Otherwise, by the assumption that the neighbours of v in S are not all leaves, we must have $d > 2$, and at least one S^i (without loss of generality S^1) is not a single leaf. Now the set consisting of all vertices of S^* except for v_1 is a set that lies in $\mathcal{H}$, but since it only contains $d-2$ of the neighbours of v, the size of its preimage under f is at most $2^{d-2}-1 < 2^{d-1}-1$. In either case, we have completed the proof of (7) and thus the lemma. □

We can now present the main theorem of this section.

Theorem 2.5 *The d-ary caterpillar is the unique tree with the minimum number of dominating sets among all d-ary trees of a given order.*

Proof Let T be a d-ary tree that is not a d-ary caterpillar. Let T^{int} be the tree formed by the internal vertices of T. This tree is not a path by assumption, so there exists at least one internal vertex, say w, such that two of the branches of T^{int} whose roots are adjacent to w are paths. One way to find w is as follows: contract every maximal path of T^{int} whose internal vertices have degree 2 in T^{int} to a single edge. The result is a tree T^{int}_* without vertices of degree 2. In this tree T^{int}_*, pick the second to last vertex of any diametrical path. Since its degree is at least 3 and all but one of the neighbours of this vertex are leaves, it must have at least two leaf neighbours. The corresponding vertex in T^{int} has the desired property, since

edges ending in a leaf in T_*^{int} correspond to path branches in T^{int}. By implication, the two corresponding branches in T are rooted d-ary caterpillars as in Fig. 4. Suppose we transform T by replacing these two by a leaf and a single caterpillar branch as in Fig. 5, creating a tree T'. By Lemma 2.4, $\delta(T) > \delta(T')$. This shows that T cannot have the minimum number of dominating sets, which proves that the minimum must be attained by a d-ary caterpillar. □

3 Binary trees with many dominating sets

In this section, we consider the maximum of the number of dominating sets, which is more difficult to obtain. For this reason, we will have to restrict ourselves to the special case $d = 2$, i.e., to binary trees. The full structure of the extremal trees will be characterized in Theorem 3.8 and Theorem 3.9. It turns out that they are unique up to isomorphism.

The first lemma in this section provides some auxiliary inequalities. We state it for general d, even though we will only require the special case $d = 2$ of binary trees.

Lemma 3.1 *If S is a rooted d-ary tree with root v and $|S| > 1$, then*

$$2^d\delta_{00}(S,v) \le \delta_{11}(S,v) \quad \text{and} \quad (2^d-1)\delta_{00}(S,v) \le \delta_{01}(S,v) < \delta_{11}(S,v).$$

Proof For every dominating set that does not contain v, we can add v to obtain a dominating set that does, so clearly $\delta_{11}(S,v) \ge \delta_{01}(S,v)$. Since the set $V(S) - N(v)$ is dominating, thus counted by $\delta_{11}(S,v)$, but $V(S) - N[v]$ is not dominating, the inequality is strict, i.e., $\delta_{11}(S,v) > \delta_{01}(S,v)$.

Next, if v is a support vertex then $\delta_{00}(S,v) = 0$, thus trivially $\delta_{11}(S,v) \ge 2^d\delta_{00}(S,v)$ and $\delta_{01}(S,v) \ge (2^d-1)\delta_{00}(S,v)$. Now suppose that v is a leafless internal vertex. Then for every set that is counted by $\delta_{00}(S,v)$, we can add any nonempty subset of the neighbours of v to get a set that is counted by $\delta_{01}(S,v)$. Since v has d neighbours, we have $2^d - 1$ possible sets, thus $\delta_{01}(S,v) \ge (2^d-1)\delta_{00}(S,v)$. Similarly, for every set that is counted by $\delta_{00}(S,v)$, we can add v plus any subset of $N(v)$ to get a set that is counted by $\delta_{11}(S,v)$. Therefore, $\delta_{11}(S,v) \ge 2^d\delta_{00}(S,v)$. □

The next lemma provides recursions for the quantities $\delta_{ij}(S,v)$. Again, we formulate it in somewhat greater generality than is required for the purpose of this section.

Lemma 3.2 *Let S be a rooted tree with root v, and let $S^1, S^2, \ldots, S^k$ be the branches of v in S. Let v_j be the neighbour of v in S^j (see Fig. 7). With the abbreviations introduced in the first section (i.e., $S_{11} = \delta_{11}(S,v)$, etc.), we have the following formulas:*

$$S_{11} = \prod_{j=1}^{k}(S_{11}^j + S_{01}^j + S_{00}^j), \tag{8}$$

$$S_{01} = \prod_{j=1}^{k}(S_{11}^j + S_{01}^j) - \prod_{j=1}^{k} S_{01}^j, \tag{9}$$

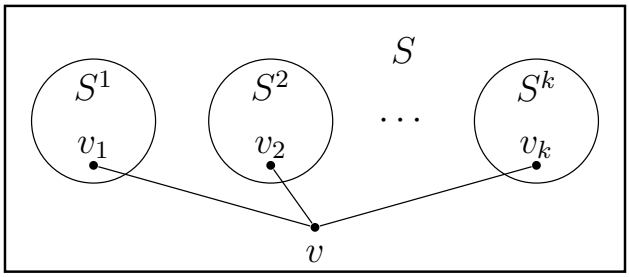


Fig. 7 A rooted tree S with root v

$$S_{00} = \prod_{j=1}^{k} S_{01}^j. \tag{10}$$

Furthermore, if $k = 2$ and both S^1 and S^2 consist of more than one vertex, then

$$3S_{01} > S_{11}. \tag{11}$$

Proof First consider a dominating set D of S that includes v. Then $D^j = D \cap V(S^j)$ is a vertex subset of S^j that is either dominating or dominates all of S^j except for v_j (compare the proof of Lemma 2.3). The total number of such sets is $S_{11}^j + S_{01}^j + S_{00}^j$.

Conversely, given a collection of sets $D^1, D^2, \ldots, D^k$ in $S^1, S^2, \ldots, S^k$ respectively such that D^j dominates either all of S^j or all but v^j for each j, one can add v to their union to obtain a dominating set of S containing v. Thus (8) holds.

Next consider a dominating set D of S that does not include v. For v to be dominated, at least one of the restrictions $D^j = D \cap V(S^j)$ must contain v_j. Moreover, each D^j must be dominating in S^j. The rest of the argument is the same as in the previous case, and we obtain (9).

Lastly, consider a dominating set D of $S - v$ that does not dominate v. Then neither v nor any of its neighbours v_j can be included, and the restriction $D^j = D \cap V(S^j)$ has to be a dominating set of S^j for every j. Again, the converse holds, and we have (10).

Let us finally prove (11). Set $\Delta = 3S_{01} - S_{11}$. By (8) and (9), we have

$$\begin{aligned}\Delta &= 3(S_{11}^1 + S_{01}^1)(S_{11}^2 + S_{01}^2) - 3S_{01}^1 S_{01}^2 - (S_{11}^1 + S_{01}^1 + S_{00}^1)(S_{11}^2 + S_{01}^2 + S_{00}^2) \\ &= 2(S_{11}^1 S_{11}^2 + S_{11}^1 S_{01}^2 + S_{01}^1 S_{11}^2) - S_{11}^1 S_{00}^2 - S_{00}^1 S_{11}^2 - (S_{01}^1 + S_{00}^1)(S_{01}^2 + S_{00}^2).\end{aligned}$$

Now by Lemma 3.1, we have $S_{00}^1 \le \frac{1}{4} S_{11}^1$ and $S_{00}^2 \le \frac{1}{4} S_{11}^2$. Thus

$$\begin{aligned}\Delta &\ge 2S_{11}^1 S_{11}^2 + 2S_{11}^1 S_{01}^2 + 2S_{01}^1 S_{11}^2 - \frac{9}{16} S_{11}^1 S_{11}^2 - S_{01}^1 S_{01}^2 - \frac{1}{4} S_{01}^1 S_{11}^2 - \frac{1}{4} S_{11}^1 S_{01}^2 \\ &= \frac{23}{16} S_{11}^1 S_{11}^2 + \frac{7}{4} S_{11}^1 S_{01}^2 + \frac{7}{4} S_{01}^1 S_{11}^2 - S_{01}^1 S_{01}^2.\end{aligned}$$

Since (again by Lemma 3.1) $S^1_{01} \le S^1_{11}$ and $S^2_{01} \le S^2_{11}$, it follows that Δ must be positive, completing the proof. □

We will make use of tree transformations again. For this purpose, we need a version of Lemma 2.3 for birooted trees: in the following lemma, S is a tree with two distinguished vertices (roots) u and v. We write S^{ab}_{cd} for the number of vertex subsets of S where all vertices, except possibly u and v, are dominated and the indices a, b, c, d indicate the status of these two vertices: $a = 1$ ($c = 1$, respectively) means that we count sets where u (v) is included. Otherwise, $a = 0$ ($c = 0$). Likewise, $b = 1$ ($d = 1$, respectively) means that we count sets where u (v) is dominated. Otherwise, $b = 0$ ($d = 0$). For example, S^{11}_{01} is the number of dominating vertex subsets of the tree S that contain u, but not v. Similarly, S^{01}_{00} is the number of vertex subsets of S that dominate all vertices except for v and contain neither u nor v. Observe that $\delta(S) = S^{11}_{11} + S^{11}_{01} + S^{01}_{11} + S^{01}_{01}$.

Lemma 3.3 *Suppose that a binary tree T can be decomposed as shown in Fig. 8 (top left), where L and R are rooted binary trees with roots l and r respectively, S has distinguished vertices u and v, and x_1 and y_1 are leaves adjacent to support vertices x and y respectively. With the notation introduced in (1), we have the formula*

$$\begin{aligned}\delta(T) = {} & \big(4\mathcal{LR} + 2\mathcal{L}\delta(R) + 2\mathcal{R}\delta(L) + \delta(L)\delta(R)\big)\big(S^{11}_{11} + S^{01}_{11} + S^{11}_{01} + S^{01}_{01}\big) \\ & + \big(4\mathcal{LR} + 2\mathcal{L}\delta(R)\big)\big(S^{00}_{11} + S^{00}_{01}\big) + \big(4\mathcal{LR} + 2\mathcal{R}\delta(L)\big)\big(S^{11}_{00} + S^{01}_{00}\big) \\ & + 4\mathcal{LR}S^{00}_{00}.\end{aligned} \tag{12}$$

Suppose now that T has a decomposition as before, but without the tree S and instead an edge between x and y (one can consider S as empty in this case). Then we have

$$\delta(T) = 4\mathcal{LR} + 2\mathcal{L}\delta(R) + 2\mathcal{R}\delta(L) + \delta(L)\delta(R). \tag{13}$$

Next, consider the tree T' obtained by removing the edges xx_1 and yr from T and replacing them by xr and yx_1, thus exchanging R and the leaf x_1 (as in Fig. 8, top right). Then we have the formula

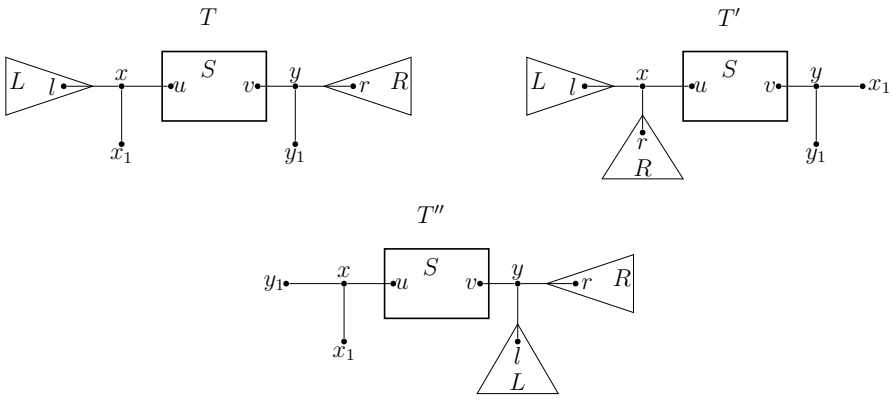


Fig. 8 The trees T, T' and T'' in Lemma 3.3

$$\begin{aligned}\delta(T') = {} & 5\big(\mathcal{LR} + \delta(L)\delta(R)\big)\big(S_{11}^{11} + S_{01}^{11}\big) + 5\big(\mathcal{LR} + \delta(L)\delta(R) - L_{01}R_{01}\big)\big(S_{11}^{01} + S_{01}^{01}\big) \\ & + 5\mathcal{LR}\big(S_{11}^{00} + S_{01}^{00}\big) + 4\big(\mathcal{LR} + \delta(L)\delta(R)\big)S_{00}^{11} \\ & + 4\big(\mathcal{LR} + \delta(L)\delta(R) - L_{01}R_{01}\big)S_{00}^{01} + 4\mathcal{LR}S_{00}^{00}.\end{aligned} \tag{14}$$

If there is an edge between x and y instead of the tree S, we have

$$\delta(T') = 5\mathcal{LR} + 5\delta(L)\delta(R) - L_{01}R_{01}. \tag{15}$$

Likewise, consider the tree T'' obtained by removing the edges yy_1 and xl from T and replacing them by yl and xy_1, thus exchanging L and the leaf y_1 (as in Fig. 8, bottom). Then we have

$$\begin{aligned}\delta(T'') = {} & 5\big(\mathcal{LR} + \delta(L)\delta(R)\big)\big(S_{11}^{11} + S_{11}^{01}\big) + 5\big(\mathcal{LR} + \delta(L)\delta(R) - L_{01}R_{01}\big)\big(S_{01}^{11} + S_{01}^{01}\big) \\ & + 5\mathcal{LR}\big(S_{00}^{11} + S_{00}^{01}\big) + 4\big(\mathcal{LR} + \delta(L)\delta(R)\big)S_{11}^{00} \\ & + 4\big(\mathcal{LR} + \delta(L)\delta(R) - L_{01}R_{01}\big)S_{01}^{00} + 4\mathcal{LR}S_{00}^{00}.\end{aligned} \tag{16}$$

If there is an edge between x and y instead of the tree S, then T' is isomorphic to T'', thus $\delta(T') = \delta(T'')$.

In either case (with the tree S or with an edge between x and y), if both L and R are nontrivial rooted binary trees, i.e., if they each have more than one vertex, then $\delta(T') + \delta(T'') > 2\delta(T)$ and thus $\max(\delta(T'), \delta(T'')) > \delta(T)$.

Proof We start by determining the number $\delta(T)$ of dominating sets of T in the case that the tree S is nonempty. For any dominating set D of T, let $D' = D \cap V(S)$ be the restriction to S. Note that D' has to dominate all of S, except possibly u and v, which can be dominated by x and y, respectively. We distinguish different types of dominating sets depending on whether u and v are dominated by D'.

First, suppose that D' dominates u and v. If $x \in D$, then x_1 can be included in D or not, and the restriction to L can be any of the sets counted by $\mathcal{L}$, so this case contributes $2\mathcal{L}$. Otherwise, if $x \notin D$, x_1 needs to be included in D, and the restriction to L needs to be dominating, so this case contributes $\delta(L)$. This gives us $2\mathcal{L} + \delta(L)$ possibilities for $L \cup \{x, x_1\}$. Likewise, there are $2\mathcal{R} + \delta(R)$ possibilities for $R \cup \{y, y_1\}$. In total, the number of combinations in this case is

$$\big(2\mathcal{L} + \delta(L)\big)\big(2\mathcal{R} + \delta(R)\big)\big(S_{11}^{11} + S_{11}^{01} + S_{01}^{11} + S_{01}^{01}\big),$$

which is the first term of (12).

Next, suppose that D' dominates v, but not u. Then x has to be an element of D. Similar reasoning as before gives us

$$2\mathcal{L}\big(2\mathcal{R} + \delta(R)\big)\big(S_{11}^{00} + S_{01}^{00}\big)$$

possible combinations, which is the second term of (12). The argument for the third term is analogous.

Lastly, suppose D' neither dominates u nor v. Then both x and y need to be elements of D, and we obtain

$$4\mathcal{L}\mathcal{R}S_{00}^{00}$$

possible dominating sets. The combination of the four cases gives us (12). Equation (13) follows similarly, by distinguishing whether or not x and y are contained in D.

Now consider the tree T'. For any dominating set D of T', let $D' = D \cap V(S)$. We consider the same four cases as before, but additionally distinguish whether u is contained in D or not (if it is dominated).

Suppose first that D' dominates u and v, and that $u \in D$. There are five possible dominating subsets of $\{x_1, y, y_1\}$ that can be added to D', and on the other hand there are $\mathcal{LR}$ possibilities for the restrictions to L and R if $x \in D$ (so that l and r are readily dominated), and $\delta(L)\delta(R)$ possibilities otherwise. In total, this gives

$$5\big(\mathcal{L}\mathcal{R} + \delta(L)\delta(R)\big)\big(S_{11}^{11} + S_{01}^{11}\big)$$

dominating sets, explaining the first term of (14).

Suppose D' dominates u and v, and that $u \notin D$. The only difference to the previous case is that either l or r needs to be included in D if x is not. Thus there are now

$$5\big(\mathcal{L}\mathcal{R} + \delta(L)\delta(R) - L_{01}R_{01}\big)\big(S_{11}^{01} + S_{01}^{01}\big)$$

possible combinations, accounting for the second term of (14).

The remaining four cases are treated in a similar fashion: we have $5\mathcal{L}\mathcal{R}\big(S_{11}^{00} + S_{01}^{00}\big)$ dominating sets where D' dominates v, but not u. In this case, necessarily $x \in D$. There are $4\big(\mathcal{L}\mathcal{R} + \delta(L)\delta(R)\big)S_{00}^{11}$ dominating sets where D' dominates u, but not v, and $u \in D$. Here, necessarily $y \in D$. Likewise, there are $4\big(\mathcal{L}\mathcal{R} + \delta(L)\delta(R) - L_{01}R_{01}\big)S_{00}^{01}$ dominating sets where D' dominates u, but not v, and $u \notin D$. Lastly, if neither u nor v is dominated by D', then necessarily $x, y \in D$, and we have $4\mathcal{L}\mathcal{R}S_{00}^{00}$ dominating sets.

Adding all these cases, we arrive at (14). Again, (15) follows by a similar argument. The proof of (16) is completely analogous (by symmetry). It remains to show that if $|L|, |R| > 1$, then $\delta(T') + \delta(T'') > 2\delta(T)$ in both cases. Let us first consider the decomposition involving the tree S. Set $\Delta = \delta(T') + \delta(T'') - 2\delta(T)$. By (12), (14) and (16), we have

$$\Delta = \alpha_1 S_{11}^{11} + \alpha_2(S_{11}^{01} + S_{01}^{11}) + \alpha_3 S_{01}^{01} + \alpha_4 S_{11}^{00} + \alpha_5 S_{01}^{00} + \alpha_6 S_{00}^{11} + \alpha_7 S_{00}^{01},$$

where the coefficients $\alpha_1, \alpha_2, \ldots, \alpha_7$ are given as follows:

$$\begin{aligned}
\alpha_1 &= 2\mathcal{L}\mathcal{R} - 4L_{00}\delta(R) - 4R_{00}\delta(L),\\
\alpha_2 &= 2\mathcal{L}\mathcal{R} - 4L_{00}\delta(R) - 4R_{00}\delta(L) - 5L_{01}R_{01},\\
\alpha_3 &= 2\mathcal{L}\mathcal{R} - 4L_{00}\delta(R) - 4R_{00}\delta(L) - 10L_{01}R_{01},\\
\alpha_4 &= \mathcal{L}\mathcal{R} - 4L_{00}\delta(R),\\
\alpha_5 &= \mathcal{L}\mathcal{R} - 4L_{00}\delta(R) - 4L_{01}R_{01},\\
\alpha_6 &= \mathcal{L}\mathcal{R} - 4R_{00}\delta(L),\\
\alpha_7 &= \mathcal{L}\mathcal{R} - 4R_{00}\delta(L) - 4R_{01}L_{01}.
\end{aligned}$$

We prove that the coefficients $\alpha_1, \alpha_2, \alpha_4$ and α_6 are all nonnegative. To this end, we first rewrite α_1 as follows by substituting $\mathcal{L} = \delta(L) + L_{00} = L_{11} + L_{01} + L_{00}$ and $\mathcal{R} = \delta(R) + R_{00} = R_{11} + R_{01} + R_{00}$:

$$\begin{aligned}
\alpha_1 &= 2\delta(L)\delta(R) - 2\delta(L)R_{00} - 2L_{00}\delta(R) + 2L_{00}R_{00}\\
&= 2(\delta(L) - L_{00})(\delta(R) - R_{00})\\
&= 2(L_{11} + L_{01} - L_{00})(R_{11} + R_{01} - R_{00}).
\end{aligned}$$

By Lemma 3.1, we have $L_{11} \geq L_{01}$ and $L_{11} \geq 4L_{00}$, thus $L_{11} \geq \frac{3}{4}L_{01} + L_{00}$ and analogously $R_{11} \geq \frac{3}{4}R_{01} + R_{00}$. It follows that

$$\alpha_1 \geq 2 \cdot \left(\tfrac{7L_{01}}{4}\right)\left(\tfrac{7R_{01}}{4}\right) > 6L_{01}R_{01}. \tag{17}$$

We can immediately conclude that α_1 and $\alpha_2 = \alpha_1 - 5L_{01}R_{01}$ are nonnegative. Next, using again the inequalities $L_{11} \geq 4L_{00}$ and $R_{11} \geq R_{01}$ from Lemma 3.1, combined with the trivial inequalities $\mathcal{L} \geq \delta(L) = L_{11} + L_{01}$ and $\mathcal{R} \geq \delta(R) = R_{11} + R_{01}$, we have

$$\begin{aligned}
\alpha_4 = \mathcal{L}\mathcal{R} - 4L_{00}\delta(R) &\geq \delta(L)\delta(R) - 4L_{00}\delta(R) = (L_{11} + L_{01} - 4L_{00})\delta(R)\\
&\geq L_{01}\delta(R) = L_{01}(R_{11} + R_{01}) \geq 2L_{01}R_{01}.
\end{aligned} \tag{18}$$

An analogous argument shows that $\alpha_6 \geq 2L_{01}R_{01}$, so in particular α_4 and α_6 are nonnegative. Since we have now established that $\alpha_2, \alpha_4, \alpha_6 \geq 0$, it follows that

$$\Delta \geq \alpha_1 S_{11}^{11} + \alpha_3 S_{01}^{01} + \alpha_5 S_{01}^{00} + \alpha_7 S_{00}^{01}. \tag{19}$$

By (17) and (18), we have the following three inequalities:

$$\begin{aligned}
\alpha_3 &= \alpha_1 - 10L_{01}R_{01} \geq 6L_{01}R_{01} - 10L_{01}R_{01} = -4L_{01}R_{01},\\
\alpha_5 &= \alpha_4 - 4L_{01}R_{01} \geq 2L_{01}R_{01} - 4L_{01}R_{01} = -2L_{01}R_{01},\\
\alpha_7 &= \alpha_6 - 4L_{01}R_{01} \geq 2L_{01}R_{01} - 4L_{01}R_{01} = -2L_{01}R_{01}.
\end{aligned}$$

We plug these and (17) into (19) to obtain

$$\begin{aligned}
\Delta &\geq 6L_{01}R_{01}S_{11}^{11} - 4L_{01}R_{01}S_{01}^{01} - 2L_{01}R_{01}(S_{01}^{00} + S_{00}^{01})\\
&= 2L_{01}R_{01}(3S_{11}^{11} - 2S_{01}^{01} - S_{01}^{00} - S_{00}^{01}).
\end{aligned} \tag{20}$$

For every set that is counted by one of S_{01}^{01}, S_{01}^{00}, S_{00}^{01} or S_{00}^{00} we can add u and v to it to obtain a set that is counted by S_{11}^{11}, and this an injective relation. Thus,

$$S_{11}^{11} \geq S_{01}^{01} + S_{01}^{00} + S_{00}^{01} + S_{00}^{00}. \tag{21}$$

Combining (20) and (21), we find that $\Delta \geq 2L_{01}R_{01}S_{11}^{11}$. Since $|L| > 1$, we have $L_{01} > 0$ (the set consisting of all vertices in L except for l is counted by L_{01}), and likewise the assumption $|R| > 1$ implies $R_{01} > 0$. Finally, the set consisting of all vertices of S is counted by S_{11}^{11}, so $S_{11}^{11} > 0$ and thus $\Delta > 0$.

Now we consider the case that there is an edge between x and y instead of the tree S. In this case, we have

$$\begin{aligned}\Delta &= 2\delta(T') - 2\delta(T)\\ &= 2(\mathcal{L}\mathcal{R} + 4\delta(L)\delta(R) - 2\mathcal{L}\delta(R) - 2\delta(L)\mathcal{R} - L_{01}R_{01})\\ &= 2(\mathcal{L}\mathcal{R} - 2L_{00}\delta(R) - 2\delta(L)R_{00} - L_{01}R_{01}).\end{aligned}$$

By Lemma 3.1, we have $L_{11} \geq L_{01}$ as well as $L_{11} \geq 4L_{00}$ and $L_{01} \geq 3L_{00}$. It follows that $\mathcal{L} = L_{11} + L_{01} + L_{00} \geq 8L_{00}$ and $\mathcal{L} \geq \delta(L) = L_{11} + L_{01} \geq 2L_{01}$. Analogously, $\mathcal{R} \geq 8R_{00}$ and $\mathcal{R} \geq 2R_{01}$. Thus

$$\begin{aligned}\Delta &= 2(\mathcal{L}\mathcal{R} - 2L_{00}\delta(R) - 2\delta(L)R_{00} - L_{01}R_{01})\\ &\geq 2\Big(\mathcal{L}\mathcal{R} - 2\frac{\mathcal{L}}{8}\mathcal{R} - 2\mathcal{L}\frac{\mathcal{R}}{8} - \frac{\mathcal{L}}{2}\frac{\mathcal{R}}{2}\Big)\\ &= \frac{\mathcal{L}\mathcal{R}}{2} > 0.\end{aligned}$$

□

From Lemma 3.3, we immediately get the following partial characterization of binary trees with maximum number of dominating sets.

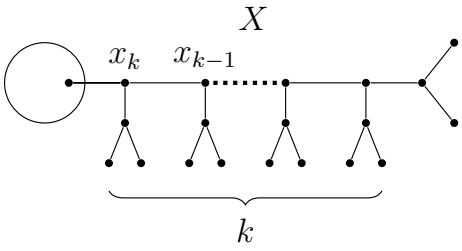
Proposition 3.4 *In a binary tree T with maximum number of dominating sets among all binary trees of the same order, there cannot be two internal vertices adjacent to exactly one leaf each. In other words, with at most one exception all internal vertices are leafless or adjacent to two leaves.*

Proof If there were two such vertices x and y in T, then we could decompose it as in Lemma 3.3. One of the trees T' and T'' (which both are of the same order as T) would have more dominating sets than T, which is an immediate contradiction. □

Suppose that a binary tree T of order $n > 4$ has the property that no internal vertex is adjacent to exactly one leaf. Then the tree formed by the internal vertices of T is also a binary tree. The number of internal vertices must be even, implying that $n = 4k + 2$ ($2k$ internal vertices and $2k + 2$ leaves). If, on the other hand, there is exactly one internal vertex adjacent to exactly one leaf, then the number of internal vertices must be odd, and $n = 4k$ ($2k - 1$ internal vertices and $2k + 1$ leaves).

In the following, by a binary branch of *type X* (or *X*-branch), we mean a branch whose shape is as shown in Fig. 9. We define the *length* of such an *X*-branch as the number of leaf-

Fig. 9 A branch of a binary tree of type X



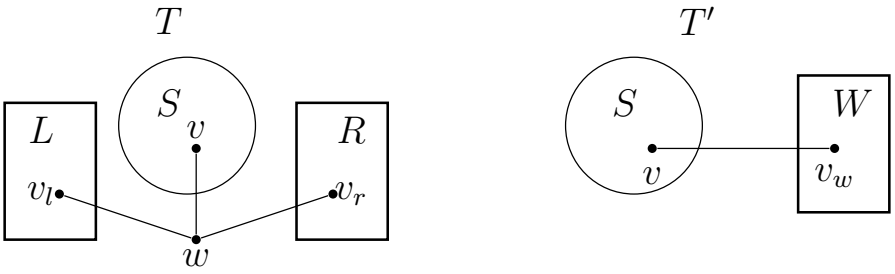


Fig. 10 The trees T and T' in Lemma 3.6

less vertices (indicated as k in the figure). An X-branch of length k will be denoted as X_k, and its natural root as x_k. We will need the following auxiliary result on X-branches.

Lemma 3.5 *The following recursions hold for $k \geq 1$:*

$$\begin{aligned}
\delta_{11}(X_k, x_k) &= 5(\delta_{11}(X_{k-1}, x_{k-1}) + \delta_{01}(X_{k-1}, x_{k-1}) + \delta_{00}(X_{k-1}, x_{k-1})),\\
\delta_{01}(X_k, x_k) &= 5\delta_{11}(X_{k-1}, x_{k-1}) + 4\delta_{01}(X_{k-1}, x_{k-1}),\\
\delta_{00}(X_k, x_k) &= \delta_{01}(X_{k-1}, x_{k-1}),
\end{aligned}$$

with initial values $\delta_{11}(X_0, x_0) = 4$, $\delta_{01}(X_0, x_0) = 1$ and $\delta_{00}(X_0, x_0) = 0$.

Proof For the recursions, we can apply Lemma 3.2, where S^1 is X_{k-1} (and v_1 is the root x_{k-1}), and S^2 is a star on three vertices, with v_2 as its centre. The initial values for X_0 are easily determined directly. □

The proof of the following lemma is very similar to that of Lemma 2.3, and it is therefore omitted.

Lemma 3.6 *Suppose that a tree T can be decomposed as shown in Fig. 10 (left), where L and R are rooted trees with roots v_l and v_r, respectively, and S has a distinguished vertex v. Then we have the formula*

$$\delta(T) = S_{11}\big(\mathcal{LR} + \delta(L)\delta(R)\big) + S_{01}\big(\mathcal{LR} + \delta(L)\delta(R) - L_{01}R_{01}\big) + S_{00}\mathcal{LR}. \qquad (22)$$

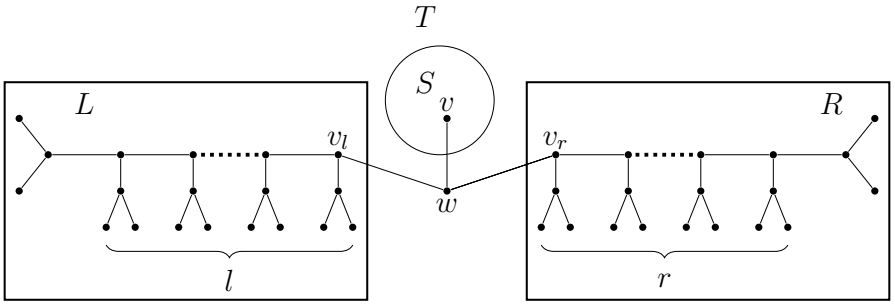
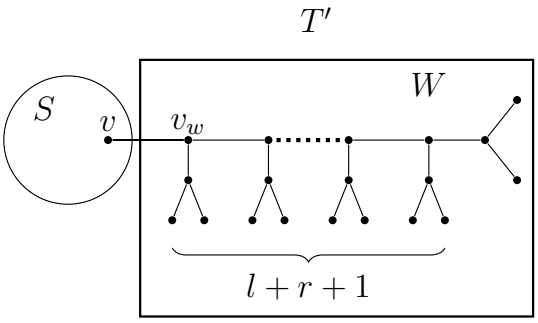


Fig. 11 The binary tree T with X-branches L and R

Fig. 12 The binary tree T' with an X-branch W



Similarly, consider a tree T' that can be decomposed into a tree S with a distinguished vertex v and a branch W with root v_w, as in Fig. 10 (right). We have the formula

$$\delta(T') = S_{11}\mathcal{W} + S_{01}\delta(W) + S_{00}W_{11}. \tag{23}$$

Lemma 3.7 *In the setting of Lemma 3.6, suppose that S is a rooted binary tree, and that L and R are two X-branches X_l and X_r, with $l, r \geq 1$ (see Fig. 11). Suppose also that W is an X-branch of length $l + r + 1$ (see Fig. 12). If $|S| = 1$ (i.e., v is a leaf), we have $\delta(T) > \delta(T')$. If $|S| = 3$, T and T' are isomorphic. In all other cases, $\delta(T) < \delta(T')$.*

Proof Let us use the notation $a_k = \delta_{11}(X_k, x_k)$, $b_k = \delta_{01}(X_k, x_k)$ and $c_k = \delta_{00}(X_k, x_k)$. By Lemma 3.5, these quantities satisfy

$$a_r = 5(a_{r-1} + b_{r-1} + c_{r-1}), \tag{24}$$

$$b_r = 5a_{r-1} + 4b_{r-1}, \tag{25}$$

$$c_r = b_{r-1}. \tag{26}$$

Plugging (25) and (26) (the latter with the index shifted by 1) into (24), we have

$$a_r = b_r + b_{r-1} + 5b_{r-2}, \quad \text{for } r \geq 2. \tag{27}$$

Plugging this into (25) (after replacing r by $r-1$) gives

$$b_r = 9b_{r-1} + 5b_{r-2} + 25b_{r-3}, \quad \text{for } r \geq 3. \tag{28}$$

By (26) and (28), we have

$$c_r = 9c_{r-1} + 5c_{r-2} + 25c_{r-3}, \quad \text{for } r \geq 3. \tag{29}$$

Finally, (27) and (28) yield

$$a_r = 9a_{r-1} + 5a_{r-2} + 25a_{r-3}, \quad \text{for } r \geq 3. \tag{30}$$

Let the coefficients of S_{11}, S_{01} and S_{00} in Eq. (22) be $f(l, r)$, $g(l, r)$ and $h(l, r)$, respectively. Observe that

$$\begin{aligned} h(l,r) &= (a_l + b_l + c_l)(a_r + b_r + c_r) \\ &= (9a_{l-1} + 5a_{l-2} + 25a_{l-3} + 9b_{l-1} + 5b_{l-2} + 25b_{l-3} + 9c_{l-1} + 5c_{l-2} + 25c_{l-3}) \\ &\quad \cdot (a_r + b_r + c_r) \\ &= 9h(l-1,r) + 5h(l-2,r) + 25h(l-3,r), \quad \text{for } l \geq 3. \end{aligned} \tag{31}$$

Similarly,

$$\begin{aligned} f(l,r) &= h(l,r) + (a_l + b_l)(a_r + b_r) \\ &= 9h(l-1,r) + 5h(l-2,r) + 25h(l-3,r) \\ &\quad + (9a_{l-1} + 5a_{l-2} + 25a_{l-3} + 9b_{l-1} + 5b_{l-2} + 25b_{l-3})(a_r + b_r) \\ &= 9f(l-1,r) + 5f(l-2,r) + 25f(l-3,r), \quad \text{for } l \geq 3, \end{aligned} \tag{32}$$

and by an analogous calculation

$$\begin{aligned} g(l,r) &= f(l,r) - b_l b_r \\ &= 9g(l-1,r) + 5g(l-2,r) + 25g(l-3,r), \quad \text{for } l \geq 3. \end{aligned} \tag{33}$$

Let $P(l, r)$ and $Q(l, r)$ denote the right side of (22) and (23), respectively (regarded as functions of l and r). Note that $P(l,r) = P(r,l)$ and $Q(l,r) = Q(r,l)$ by symmetry. By (31), (32) and (33), we have

$$\begin{aligned} P(l,r) &= f(l,r)S_{11} + g(l,r)S_{01} + h(l,r)S_{00} \\ &= 9P(l-1,r) + 5P(l-2,r) + 25P(l-3,r), \quad \text{for } l \geq 3. \end{aligned} \tag{34}$$

On the other hand, the recursions (28), (29) and (30) yield

$$\begin{aligned} Q(l,r) &= (a_{l+r+1} + b_{l+r+1} + c_{l+r+1})S_{11} + (a_{l+r+1} + b_{l+r+1})S_{01} + a_{l+r+1}S_{00} \\ &= 9Q(l-1,r) + 5Q(l-2,r) + 25Q(l-3,r), \quad \text{for } l \geq 3. \end{aligned} \tag{35}$$

We will now prove by induction on l and r that for $l, r \geq 1$, $Q(l,r) > P(l,r)$ if v is not a leaf, and otherwise $Q(l,r) < P(l,r)$. Observe first that

$$
\begin{aligned}
Q(1,1) - P(1,1) &= -71S_{11} + 284S_{01} - 25S_{00},\\
Q(1,2) - P(1,2) &= -634S_{11} + 2536S_{01} - 600S_{00},\\
Q(1,3) - P(1,3) &= -6061S_{11} + 24244S_{01} - 5525S_{00},\\
Q(2,2) - P(2,2) &= -5586S_{11} + 22344S_{01} - 9050S_{00},\\
Q(2,3) - P(2,3) &= -53444S_{11} + 213776S_{01} - 84450S_{00},\\
Q(3,3) - P(3,3) &= -511301S_{11} + 2045204S_{01} - 787675S_{00}.
\end{aligned}
$$

Thus, for $l, r \leq 3$, we have

$$Q(l,r) - P(l,r) = -A(l,r)S_{11} + 4A(l,r)S_{01} - C(l,r)S_{00},$$

where $A(l,r), C(l,r) > 0$ and $3A(l,r) > C(l,r)$. We consider the following cases:

Case 1: v is a leaf. Then $S_{11} = 1, S_{01} = 0, S_{00} = 1$, and thus

$$Q(l,r) - P(l,r) = -A(l,r) - C(l,r) < 0.$$

Case 2: v is a support vertex. Then $S_{00} = 0$ (Lemma 2.1), thus

$$Q(l,r) - P(l,r) = A(l,r)(4S_{01} - S_{11}).$$

It is easy to see that T and T' are isomorphic if $|S| = 3$, and indeed $4S_{01} - S_{11} = 0$ in this case, so $Q(l,r) = P(l,r)$. Otherwise, let $\tilde{S}$ be the branch of S that remains when v and its leaf neighbour are removed. By Lemma 3.2, we have $S_{01} = \tilde{S}_{11} + \tilde{S}_{01}$ and $S_{11} = 2(\tilde{S}_{11} + \tilde{S}_{01} + \tilde{S}_{00})$. Thus

$$4S_{01} - S_{11} = 2(\tilde{S}_{11} + \tilde{S}_{01} - \tilde{S}_{00}),$$

and since $|\tilde{S}| > 1$, this is positive by Lemma 3.1, so it follows that $Q(l,r) > P(l,r)$.

Case 3: v is a leafless internal vertex. By Lemma 3.1, $S_{01} \geq 3S_{00}$, and by Lemma 3.2, $3S_{01} > S_{11}$. Thus

$$
\begin{aligned}
Q(l,r) - P(l,r) &= -A(l,r)S_{11} + 4A(l,r)S_{01} - C(l,r)S_{00}\\
&\geq -A(l,r)S_{11} + 4A(l,r)S_{01} - 3A(l,r)S_{00}\\
&= A(l,r)(3S_{01} - S_{11} + S_{01} - 3S_{00}) > 0.
\end{aligned}
$$

We have thus proven the statement for $l, r \leq 3$ and proceed now by induction. We only consider the case that v is a leaf, the other being analogous. Assume that for all $1 \leq l, r \leq k-1$, $Q(l,r) < P(l,r)$. By the recursions (34) and (35), we have, for $1 \leq j \leq k-1$,

$$
\begin{aligned}
&Q(k,j) - P(k,j)\\
&= 9(Q(k-1,j) - P(k-1,j)) + 5(Q(k-2,j) - P(k-2,j)) + 25(Q(k-3,j) - P(k-3,j)),
\end{aligned}
$$

so it follows from the induction hypothesis that $Q(k,j) < P(k,j)$. By symmetry, we also deduce that $Q(j,k) < P(j,k)$. Applying the recursions one more time, we have

$$Q(k,k) - P(k,k)$$
$$= 9(Q(k-1,k) - P(k-1,k)) + 5(Q(k-2,k) - P(k-2,k)) + 25(Q(k-3,k) - P(k-3,k)),$$

so that $Q(k,k) < P(k,k)$ if v is a leaf. Thus the statement holds for all $1 \leq l, r \leq k$, completing the induction. □

We are now ready to prove our main theorems.

Theorem 3.8 *Let n be a multiple of 4, and suppose that the binary tree T has the maximum number of dominating sets among all binary trees of order n.*

- If $n = 4$, then T is a star, and $\delta(T) = 9$.
- If $n \geq 8$, then T is of the form shown in Fig. 13, with two X-branches whose lengths l and r are given as follows:
  - If $n = 8$, then $l = r = 0$, and $\delta(T) = 75$.
  - If $n = 12$, then $l = 0$ and $r = 1$ (or vice versa), and $\delta(T) = 745$.
  - If $n = 16$, then $l = r = 1$ and $\delta(T) = 7401$.
  - If $n \geq 20$, then $l = 2$ and $r = \frac{n}{4} - 4$ (or vice versa). If we set $\delta(T) = M_n$, then we have the recursive formula

$$M_n = 9M_{n-4} + 5M_{n-8} + 25M_{n-12}, \quad \text{for } n \geq 32, \tag{36}$$

with $M_{20} = 72579$, $M_{24} = 711891$ and $M_{28} = 6952539$.

Proof The case $n = 4$ is trivial, so we assume that $n \geq 8$. We know from Proposition 3.4 that there is exactly one internal vertex w that is adjacent to exactly one leaf. Let this leaf be v. We decompose the tree T as in Fig. 10 (left). The first step is to show that both L and R have to be X-branches. Assume to the contrary that at least one of them is not.

Among all branches of T contained in either L or R, pick one that is not a single leaf or an X-branch and is minimal with this property (such a branch must exist, as L or R satisfies the requirement). Let this branch be B. It can be split into its root x_b and two sub-branches B_1 and B_2. By minimality of B, each of the two sub-branches is either a single leaf or an X-branch. If B_1 and B_2 are both single leaves, then B is an X-branch of length 0, which is a contradiction. If only one of them is a single leaf, then x_b has precisely one leaf neighbour, which is also impossible (as w is the only vertex with this property by assumption). Thus B_1 and B_2 are both X-branches. If either B_1 or B_2 is an X-branch of length 0 (i.e., a star on three vertices), then B is an X-branch, and we reach another contradiction.

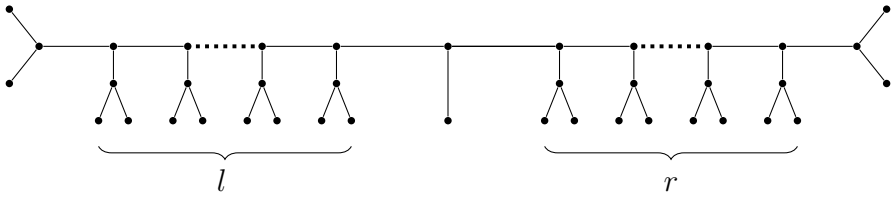


Fig. 13 The optimal binary tree when $4|n$ and $n \geq 8$

So both B_1 and B_2 are X-branches of length ≥ 1. This puts us exactly in the setting of Lemma 3.7, with x_b taking the role of w in that lemma. The tree S is neither a single leaf nor a star of order 3 in our situation, as its order is at least $\min(|L|, |R|) + 2 > 3$. Thus we can transform T by merging B_1 and B_2 into a single X-branch, which yields a new tree T' with $\delta(T') > \delta(T)$ by Lemma 3.7. This contradicts our assumptions on T. So we have shown that L and R must in fact be X-branches. This means that T is of the form in Fig. 13, and it only remains to determine the values of l and r.

Note that T can be regarded as the tree in Fig. 11 if we take S as a single vertex. Thus we can apply the formula (22) for the number of dominating sets of T. We have $S_{11} = 1, S_{01} = 0, S_{00} = 1$, and substituting these values into (22) yields

$$\delta(T) = 2\mathcal{LR} + \delta(L)\delta(R) = 2(a_l + b_l + c_l)(a_r + b_r + c_r) + (a_l + b_l)(a_r + b_r). \quad (37)$$

Here, $n = (4\,l + 3) + (4r + 3) + 2$, thus $l + r = \frac{n}{4} - 2$. Let us write $T(l, r)$ for the right side of (37). Note that $T(r, l) = T(l, r)$. Moreover, for fixed r, $T(l, r)$ is a linear combination of the sequences a_l, b_l, c_l that all satisfy the same linear recursion (see (28), (29) and (30)). Thus $T(l, r)$ satisfies this linear recursion as well:

$$T(l, r) = 9T(l - 1, r) + 5T(l - 2, r) + 25T(l - 3, r), \quad \text{for } l \geq 3. \quad (38)$$

Now observe that

$$T(0, 0) = 75,$$
$$T(1, 0) = 745,$$

and

$$T(1, 1) = 7401 > T(2, 0) = T(0, 2) = 7305.$$

This readily proves the claim for $n \leq 16$. To conclude the proof, we show by induction on $w = l + r = \frac{n}{4} - 2$ that $T(w - 2, 2) \geq T(w - m, m)$ for all w, m with $0 \leq m \leq w \leq 5$, with equality if and only if either $m = 2$ or $w - m = 2$. Observe first that we have

$$T(2, 1) = T(1, 2) = 72579 > T(3, 0) = T(0, 3) = 71345$$

as well as

$$T(2, 2) = 711891 > \max(T(3, 1), T(4, 0)) \quad \text{and} \quad T(3, 2) = 6952539 > \max(T(4, 1), T(5, 0)).$$

Thus for $3 \leq w \leq 5$ and $0 \leq m \leq w$, we always have $T(w - 2, 2) \geq T(w - m, m)$, with equality if and only if either $m = 2$ or $w - m = 2$. Next assume that the statement holds for all w with $3 \leq w \leq k - 1$, where k is some integer ≥ 6. We want to show that $T(k - 2, 2) \geq T(k - m, m)$ holds for all m with $0 \leq m \leq k$, with inequality if and only if either $m = 2$ or $k - m = 2$. By symmetry, it suffices to consider $m \leq \frac{k}{2}$, so that $k - m \geq \frac{k}{2} \geq 3$. In view of the recursion for $T(l, r)$ and the induction hypothesis, we have

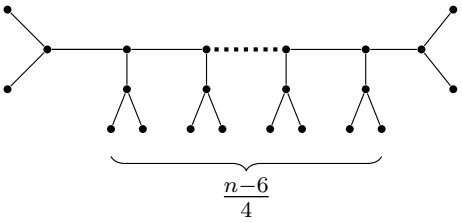


Fig. 14 The optimal binary tree when $n \equiv 2 \mod 4$

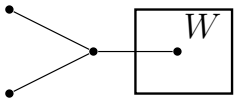


Fig. 15 Decomposition with branch W

$$\begin{aligned} T(k-m,m) &= 9T(k-m-1,m) + 5T(k-m-2,m) + 25T(k-m-3,m) \\ &\leq 9T(k-3,2) + 5T(k-4,2) + 25T(k-5,2) \\ &= T(k-2,2), \end{aligned}$$

with equality if and only if $m = 2$. This completes the induction and thus the proof of the theorem. The recursion (36) follows from (38). □

In the case that $n \equiv 2 \mod 4$, the proof of the main result is similar to that of Theorem 3.8 (and in fact easier).

Theorem 3.9 *Let $n \equiv 2 \mod 4$, $n \geq 6$, and suppose that the binary tree T has the maximum number of dominating sets among all binary trees of order n. Then T is of the form shown in Fig. 14. If we set $\delta(T) = M_n$, then we have the recursive formula*

$$M_n = 9M_{n-4} + 5M_{n-8} + 25M_{n-12}, \quad for n \geq 18, \tag{39}$$

with $M_6 = 25$, $M_{10} = 249$ and $M_{14} = 2451$.

Proof Every binary tree T with at least three vertices can be decomposed as shown in Fig. 15. This is true since T will always have an internal vertex that is a leaf in the subtree induced by its internal vertices and therefore has two leaf neighbours. By an analogous argument as in the proof of Theorem 3.8, the branch W has to be an X-branch, or consist of a root and two sub-branches that are both X-branches (the case where equality can hold in Lemma 3.7). In either case, T is of the form shown in Fig. 14.

It only remains to determine a recursion for the number of dominating sets. The binary tree T in Fig. 14 is isomorphic to the tree shown in Fig. 12 if we take S to be a star of order 3 (with v as its centre). Thus we can apply the formula (23) for $\delta(T)$. We have $S_{11} = 4$, $S_{01} = 1$ and $S_{00} = 0$, which we can substitute into (23) to obtain

$$\delta(T) = 4\mathcal{W} + \delta(W).$$

If we let $w = \frac{n-6}{4}$ be the length of W, this becomes

Table 1 Maximum number of dominating sets in small binary trees

n	2	4	6	8	10	12	14	16	20	24	28
$M_n = \max_{\|T\|=n} \delta(T)$	3	9	25	75	249	745	2451	7401	72579	711891	6952589

$$\delta(T) = 4(a_w + b_w + c_w) + (a_w + b_w).$$

Since a_w, b_w, c_w satisfy the same linear recursion (see again (28), (29) and (30)), this is also the case for this linear combination, so (39) follows. The initial values for $w \leq 2$ ($n \leq 14$) are easily determined directly. □

In summary, the maximum number M_n of dominating sets in a binary tree with n vertices is given by Table 1 for $n \leq 16$ and $n \in \{20, 24, 28\}$, and otherwise by the recursion

$$M_n = 9M_{n-4} + 5M_{n-8} + 25M_{n-12}.$$

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