Graphs with few total dominating sets

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Abstract

We give a lower bound for the number of total dominating sets of a graph together with a characterization of the extremal graphs, for trees as well as arbitrary connected graphs of given order. Moreover, we obtain a sharp lower bound involving both the order and the total domination number, and characterise the extremal graphs as well.
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1 Introduction

A dominating set D is a set of vertices of a graph G with the property that every vertex of G either lies in D or has a neighbour in D. Total domination is an even stronger property: D is called a total dominating set of G if *every* vertex of G has a neighbour in D, whether or not it lies in D itself. The most classical and well-studied graph parameter in the context of (total) domination is the *(total) domination number*: the domination number $\gamma(G)$ of a graph G is the smallest cardinality of a dominating set, and likewise the total domination number $\gamma_t(G)$ is the smallest cardinality of a total dominating set. Numerous upper and lower bounds and other results on these numbers have been obtained over the years – we refer to the books [4, 5] by Haynes, Hedetniemi and Slater and the more recent book [6] by Henning and Yeo, which focuses on total domination, for a comprehensive treatment of the subject. Comparatively little work has been done

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on the *number* of (total) dominating sets. These two belong to the class of graph parameters based on counting subsets with specific properties; other well-studied examples are the number of independent sets and the number of matchings—see [10] for a recent survey including these and other examples.

As for the number $\partial(G)$ of dominating sets of a graph G, one has the trivial bounds

$$1 \leq \partial(G) \leq 2^n - 1,$$

with equality for the empty and complete graphs respectively. Bród and Skupień [1] studied the number of dominating sets in trees. The maximum of $2^{n-1} + 1$ for trees with n vertices is attained only by the star (except for the cases $n = 4$ and $n = 5$, when the path also attains the maximum). The lower bound, on the other hand, is not only more complicated—the trees attaining it are no longer unique. We will observe a similar phenomenon for total domination in this paper. As shown in [11], the lower bound for trees is also sharp for arbitrary connected graphs and even graphs without isolated vertices. See also the recent paper by Skupień [9]. For trees, similar results can also be found for the number of efficient dominating sets, minimal dominating sets and minimal 2-dominating sets (see [2, 7, 8]) – in these cases, the maximum is more interesting, though.

The focus of this paper is the number of total dominating sets of a graph, which we will denote by $\partial_t(G)$. We have similarly trivial bounds:

$$0 \leq \partial_t(G) \leq 2^n - n - 1,$$

with equality for a graph with at least one isolated vertex and the complete graph respectively. For trees, the upper bound is still quite simple, but it already illustrates some of our main ideas:

Proposition 1 *We have*

$$\partial_t(T) \leq 2^{n-1} - 1$$

for every tree T with n vertices, with equality only for the star.

Proof. The statement is trivial for $n = 1$ and $n = 2$, so let us assume that $n \geq 3$. Every tree T with at least three vertices has two or more leaves, thus at least one vertex adjacent to a leaf (we will call such a vertex a support vertex); we denote this vertex by v. This vertex v has to be part of every total dominating set. This leaves us with only 2^{n-1} possible sets, of which $\{v\}$ is clearly not a total dominating set (v is not dominated). Thus $\partial_t(T) \leq 2^{n-1} - 1$, and equality can only hold if v is the only vertex adjacent to a leaf. This only holds for the star. ■

Just as for the number of dominating sets, the lower bound is more interesting. In the following section, we will show that the minimum number of total dominating sets of a tree (connected graph, or even arbitrary graph without components of order 1 or 2) with n vertices is of order $\Theta(9^{n/7})$. A precise bound, along with the characterisation of the extremal graphs, is given in Theorems 5, 7 and 8. In Theorems 16 and 18, we obtain a sharp lower bound for $\partial_t(G)$ that takes the total dominating number into account as well. See Section 3 for details.

2 The general lower bound

In this section, we determine the minimum number of total dominating sets of a connected graph with n vertices for arbitrary n. In fact, we will show that the lower bound we obtain remains valid for disconnected graphs as long as we exclude trivial components of one vertex (for which there is no total dominating set) or two vertices (for which the only total dominating set consists of both vertices).

It turns out to be advantageous to prove the lower bound for trees first (Theorem 5), and to generalise it to connected graphs (Theorem 7) and arbitrary graphs (Theorem 8) later. *Leaves* and *support vertices* will play an important role: we call a vertex with only a single neighbour a leaf, even if the graph is not a tree. The unique neighbour of a leaf is called a support vertex. The trivial observation that every support vertex has to be contained in every total dominating set of a graph will become very useful in the following.

As we will see, the extremal graphs are obtained as unions of *subdivided stars*: the subdivided star $S(K_{1,r})$ is obtained from a star $K_{1,r}$ with r leaves by subdividing each edge into two edges (thus introducing an additional vertex on each edge).

Let us now begin our discussion by considering trees. We will write $m_n = \min\{\partial_t(T) : |T| = n\}$ for the minimum number of total dominating sets of a tree with n vertices, and $\mathcal{T}_n = \{T : |T| = n,\ \partial_t(T) = m_n\}$ for the set of all trees that attains this minimum. We start with a very useful lemma on merging trees.

Lemma 2 *Let T_1 and T_2 be two trees and v_1, v_2 vertices of T_1 and T_2 respectively. Consider the tree T obtained by adding the edge v_1v_2 to the union $T_1 \cup T_2$. We have*

$$\partial_t(T) \geq \partial_t(T_1)\partial_t(T_2),$$

and equality holds if and only if v_1 and v_2 are at distance 2 from a leaf in T_1 and T_2, respectively.

Proof. Obviously, every total dominating set of $T_1 \cup T_2$ is also a total dominating set of T, which readily proves the inequality: note that $\partial_t(T_1 \cup T_2) = \partial_t(T_1)\partial_t(T_2)$, since every total dominating set of $T_1 \cup T_2$ is the union of a total dominating set of T_1 and a total dominating set of T_2, and vice versa. It remains to determine the cases of equality.

Assume first that both v_1 and v_2 have the required property. Consider any total dominating set D of T, and assume that its restriction to T_1 is not total dominating. The only reason this could happen is that v_1 is dominated by v_2 in T, but not by any other neighbour. One of these neighbours, however, is a support vertex in T_1 by our assumption. If this support vertex is not present in D, then its leaf neighbour is not dominated, and we reach a contradiction. Thus the only total dominating sets of T are obtained as unions of total dominating sets of T_1 and T_2.

Now suppose, for instance, that there is no leaf in T_1 whose distance to v_1 is 2. Then none of v_1's neighbours in T_1 is a support vertex in T. It is easy to verify in this case that $D = T \setminus N_{T_1}(v_1)$ (i.e., all vertices of T except for v_1's neighbours in T_1) is a total dominating set of T, but the restriction of D to T_1 is clearly not (v_1 is not dominated). Thus $\partial_t(T) > \partial_t(T_1)\partial_t(T_2)$ in this case, and by symmetry the same argument applies to v_2. ■

The next lemma already gives a recursive characterisation of trees in $\mathcal{T}_n$, i.e. trees that attain the minimum number of total dominating sets.

Lemma 3 *Suppose that $T \in \mathcal{T}_n$ for some integer $n \geq 3$. Then one of the following holds:*

- *T is a subdivided star $S(K_{1,(n-1)/2})$. This is only possible if n is odd.*
- *T is a subdivided star $S(K_{1,n/2})$ with one leaf removed, i.e., $T = S(K_{1,n/2}) \setminus \{v\}$ for some leaf v of $S(K_{1,n/2})$. This is only possible if n is even.*
- *For some edge $e = v_1v_2$ of T, the two components T_1 and T_2 of $T \setminus \{e\}$ (indices chosen such that $v_1 \in T_1$, $v_2 \in T_2$) satisfy $T_1 \in \mathcal{T}_k$, $T_2 \in \mathcal{T}_{n-k}$ for some $k \in \{3, 4, \ldots, n-3\}$, and there exist leaves u_1, u_2 in T_1 and T_2 respectively such that the distance between u_i and v_i in T_i is 2.*

Proof. Suppose first that there exists an edge e with the property that the two components of $T \setminus \{e\}$, which we call T_1 and T_2, both contain at least three vertices. Let k be the number of vertices of T_1 (so that $n-k$ is the number of vertices of T_2). By Lemma 2, we have

$$\partial_t(T) \geq \partial_t(T_1 \cup T_2) = \partial_t(T_1)\partial_t(T_2) \geq m_k m_{n-k}. \tag{1}$$

On the other hand, if we take any two trees $S_1 \in \mathcal{T}_k$ and $S_2 \in T_{n-k}$ and select two vertices $u_1 \in S_1$ and $u_2 \in S_2$ such that they are both at distance 2 from some leaf (this is possible for any tree of order at least 3, see also the proof of Lemma 14 later), then the tree S obtained from $S_1 \cup S_2$ by adding the edge u_1u_2 satisfies $\partial_t(S) = \partial_t(S_1)\partial_t(S_2) = m_k m_{n-k}$ by Lemma 2.

Since we know now that equality can hold in (1), it has to hold for every tree $T \in \mathcal{T}_n$, i.e., every tree that attains the minimum. Then it is clear that $T_1 \in \mathcal{T}_k$

and $T_2 \in \mathcal{T}_{n-k}$, and again by Lemma 2, the ends of e both have distance 2 from some leaf in their respective components.

We are left with the possibility that no such edge e exists. This is impossible if the diameter of T is at least 5, since then the middle edge of a diameter (one of the two middle edges if the length is even) would have the desired property. Let us consider the remaining cases:

- If the diameter is 2, then T is a star, and $\partial_t(T) = 2^{n-1} - 1$.
- If the diameter is 3, then $\partial_t(T) = 2^{n-2}$.
- If the diameter is 4, then we are dealing with a star with some subdivided edges (for all other trees of diameter 4, there exists an edge e as desired). Let k be the number of non-subdivided edges and ℓ the number of subdivided edges, so that $k + 2\ell + 1 = n$. We have $\partial_t(T) = 2^{k+\ell}$ if $k \neq 0$ and $\partial_t(T) = 2^{\ell} + 1$ if $k = 0$.

The minimum is achieved for either $k = 0$ or $k = 1$ in the last case, depending on whether n is odd or even, and the trees achieving the minimum are as described in the statement of the lemma (for $n = 3$ or $n = 4$, the diameter is less than 4, but the statement remains true). The respective minima are $2^{n/2}$ (n even) and $2^{(n-1)/2} + 1$ (n odd). ■

Corollary 4 *Set $s(n) = 2^{n/2}$ if n is even and $s(n) = 2^{(n-1)/2} + 1$ if n is odd. From Lemma 3, we immediately obtain the following recursive characterization of m_n:*

$$m_n = \min\Big(\{s(n)\} \cup \{m_k m_{n-k} \,:\, 3 \leq k \leq n-3\}\Big).$$

This corollary enables us to determine m_n algorithmically for small values of n, and a pattern readily emerges. The following theorem characterizes m_n almost completely (with only finitely many exceptions):

Theorem 5 *Define c_k by the following table:*

c_0	c_1	c_2	c_3	c_4	c_5	c_6
1	$17^4/9^5$	$17/9$	$17^5/9^6$	$17^2/9^2$	5	$17^3/9^3$

For every tree T with n vertices, we have $\partial_t(T) \geq c_k \cdot 9^{\lfloor n/7 \rfloor}$, where $k \equiv n \bmod 7$. Equality holds if and only if T is constructed as follows:

- *If $n \equiv 0 \bmod 7$, then T has to be the union of $\frac{n}{7}$ copies of the subdivided star $S(K_{1,3})$, whose centres are connected to form a tree in an arbitrary way.*
- *If $n \equiv 1 \bmod 7$, then T has to be the union of $\frac{n-36}{7}$ copies of the subdivided star $S(K_{1,3})$ and four copies of the subdivided star $S(K_{1,4})$, connected in the same way as in the first case,*

- *If* $n \equiv 2 \bmod 7$*, then* T *has to be the union of* $\frac{n-9}{7}$ *copies of the subdivided star* $S(K_{1,3})$ *and one copy of the subdivided star* $S(K_{1,4})$*, connected in the same way as in the first case,*

- *If* $n \equiv 3 \bmod 7$*, then* T *has to be the union of* $\frac{n-45}{7}$ *copies of the subdivided star* $S(K_{1,3})$ *and five copies of the subdivided star* $S(K_{1,4})$*, connected in the same way as in the first case,*

- *If* $n \equiv 4 \bmod 7$*, then* T *has to be the union of* $\frac{n-18}{7}$ *copies of the subdivided star* $S(K_{1,3})$ *and two copies of the subdivided star* $S(K_{1,4})$*, connected in the same way as in the first case,*

- *If* $n \equiv 5 \bmod 7$*, then* T *has to be the union of* $\frac{n-5}{7}$ *copies of the subdivided star* $S(K_{1,3})$ *and one copy of the subdivided star* $S(K_{1,2})$*, connected in the same way as in the first case,*

- *If* $n \equiv 6 \bmod 7$*, then* T *has to be the union of* $\frac{n-27}{7}$ *copies of the subdivided star* $S(K_{1,3})$ *and three copies of the subdivided star* $S(K_{1,4})$*, connected in the same way as in the first case.*

In particular, $m_n = c_k \cdot 9^{\lfloor n/7 \rfloor}$ *(where* $k \equiv n \bmod 7$*) for all* $n \geq 39$*. See Figure 1 for an example of a tree* T *with* 39 *vertices that satisfies* $\partial_t(T) = m_{39}$*.*

Proof. We prove the result by induction on n. The claim is easily verified directly for small values of n, say up to $n = 10$. It is also easy to see that equality holds in all cases that are listed, making use of Lemma 2 and the fact that $\partial_t(S(K_{1,r})) = 2^r + 1$. Note also that $2^{n/2} \geq 2^{(n-1)/2} + 1 > c_k \cdot 9^{\lfloor n/7 \rfloor}$ for all $n \geq 10$, so the first two cases of Lemma 3 do not apply for $n \geq 10$. This means that $m_n = m_k m_{n-k}$ for some k.

Suppose that $k \equiv i \bmod 7$ and $n - k \equiv j \bmod 7$ ($0 \leq i, j \leq 6$). There are two possibilities:

- If $i + j < 7$, then one checks first that $c_i c_j \geq c_{i+j}$, so that

  $$m_n = m_k m_{n-k} \geq c_i 9^{\lfloor k/7 \rfloor} \cdot c_j 9^{\lfloor (n-k)/7 \rfloor} = c_i c_j 9^{\lfloor n/7 \rfloor} \geq c_{i+j} 9^{\lfloor n/7 \rfloor},$$

  which proves the desired inequality. Equality holds for $(i, j) \in \{(0, r) : 0 \leq r \leq 6\} \cup \{(r, 0) : 0 \leq r \leq 6\} \cup \{(1, 2), (2, 1), (2, 2), (2, 4), (4, 2)\}$. In each case, the induction hypothesis, combined with Lemma 2, shows that T has to have the form described in the statement of the theorem for equality to hold.

- If $i + j \geq 7$, then one checks first that $c_i c_j \geq 9 c_{i+j-7}$, so that

  $$m_n = m_k m_{n-k} \geq c_i 9^{\lfloor k/7 \rfloor} \cdot c_j 9^{\lfloor (n-k)/7 \rfloor} = c_i c_j 9^{\lfloor n/7 \rfloor - 1} \geq c_{i+j-7} 9^{\lfloor n/7 \rfloor},$$

which proves the desired inequality again. Equality holds for $(i, j) \in \{(2,6),(6,2),(4,4),(4,6),(6,4)\}$. In each case, the induction hypothesis, combined with Lemma 2, shows that T has to have the form described in the statement of the theorem for equality to hold.

■

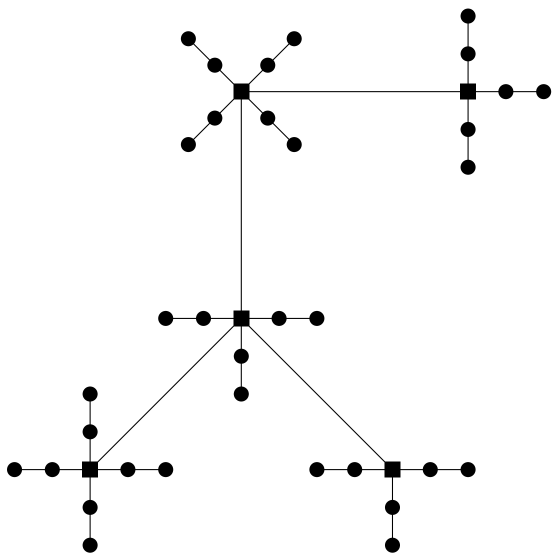

Figure 1: A tree with 39 vertices that attains the minimum m_{39}. The centres of the subdivided stars are indicated by squares.

Remark 6 *The only values of n for which $m_n = c_k \cdot 9^{\lfloor n/7 \rfloor}$ ($k \equiv n \bmod 7$) does not hold are* 1, 2, 3, 4, 6, 8, 10, 11, 13, 15, 17, 20, 22, 24, 29, 31, 38. *In these cases, the values of m_n are given in the following table:*

n	1	2	3	4	6	8	10	11	13
m_n	0	1	3	4	8	15	25	33	65
n	15	17	20	22	24	29	31	38	
m_n	125	225	561	1089	2025	9537	18225	162129	

With the exceptions $n = 1$, $n = 2$, $n = 4$ and $n = 6$, the trees that attain the bound m_n are either subdivided stars or obtained by gluing together several subdivided stars as in the statement of Theorem 5.

It is obvious that a spanning subgraph H of a graph G can have at most as many total dominating sets as G (since every total dominating set in H is automatically a total dominating set in G). It turns out that equality can hold even if $H \neq G$. It is interesting to compare this to the situation for independent sets: if H is a spanning subgraph of G and $H \neq G$, then H must always have strictly more independent sets than G. The following theorem characterizes all connected graphs that attain the lower bound for the number of total dominating sets:

Theorem 7 *Define c_k as in Theorem 5. For every connected graph G with $n \geq 3$ vertices we have $\partial_t(G) \geq c_k \cdot 9^{\lfloor n/7 \rfloor}$, where $k \equiv n \bmod 7$. Equality holds if and only if G is constructed in the same way as the trees in Theorem 5, except that the centres of the subdivided stars can form an arbitrary connected graph, see Figure 2 for an example*

Proof. Since G has at least as many total dominating sets as any of its spanning trees T, the bound follows trivially from Theorem 5. Equality can only hold if T is one of the trees described in the statement of this lemma. It remains to determine when $\partial_t(G) = \partial_t(T)$ can hold if T is such a tree.

Note that additional edges between the centres of subdivided stars do not increase the number of total dominating sets. Each centre of a subdivided star is adjacent to at least one support vertex, which has to be contained in every total dominating set. Therefore all the centres are always dominated automatically as well, which means that additional edges between centres are irrelevant.

However, no other edges can be added without increasing the number of total dominating sets. Suppose that there is an edge in G that is not an edge of T and that has a leaf v of T as one of its ends. Let w be the unique neighbour of v in T. The set $V(G) \setminus \{w\}$ is a total dominating set of G, but not of T, so $\partial_t(G) > \partial_t(T)$, and equality cannot hold in the theorem.

Likewise, suppose that there is an edge in G that is not an edge of T and that has a support vertex v of T as one of its ends. Let w_1, w_2 be the neighbours of v in T. The set $V(G) \setminus \{w_1, w_2\}$ is a total dominating set of G, but not of T, so again $\partial_t(G) > \partial_t(T)$. ■

Interestingly enough, the lemma even remains true if disconnected graphs are allowed, as long as there are no isolated vertices and no components of order 2.

Theorem 8 *The lower bound in Theorem 7 remains true if G is a graph whose components all have at least three vertices. Equality holds for the same graphs as in Theorem 5 and Theorem 7, except that the centres of the subdivided stars can induce an arbitrary graph.*

Proof. We prove the result by induction on the number r of components of G. The case $r = 1$ is already given by Theorem 7. For the induction step, note first that

$$\partial_t(G) = \prod_{j=1}^{k} \partial_t(G_j)$$

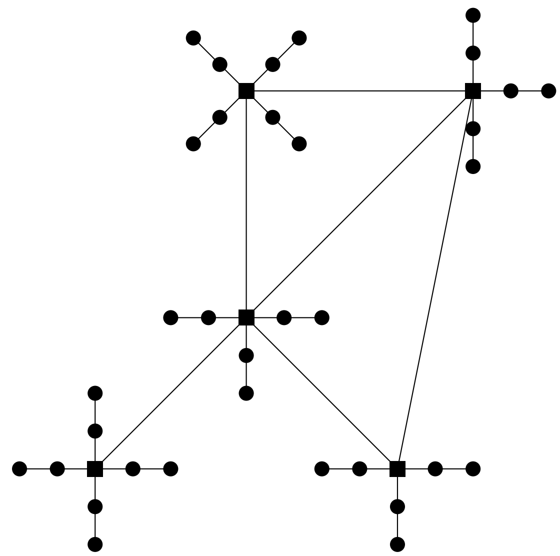

Figure 2: A connected graph with 39 vertices that attains the minimum. Note the two additional edges compared to Figure 1 that do not change the number of total dominating sets.

if $G_1, G_2, \ldots, G_k$ are the connected components of a graph G. Let H_1 be one of the components of G, and let $H_2 = G \setminus H_1$ be the rest. We can apply the induction hypothesis to H_1 and H_2. Let k be the number of vertices of H_1, and accordingly $n-k$ the number of vertices of H_2. Suppose that $k \equiv i \bmod 7$ and $n-k \equiv j \bmod 7$ $(0 \leq i,j \leq 6)$. It was already mentioned in the proof of Theorem 5 that $c_i c_j \geq c_{i+j}$ if $i+j<7$ and $c_i c_j \geq 9c_{i+j-7}$ otherwise.

In the former case ($i+j<7$), we obtain

$$\partial_t(G) = \partial_t(H_1)\partial_t(H_2) \geq c_i 9^{\lfloor k/7 \rfloor} \cdot c_j 9^{\lfloor (n-k)/7 \rfloor} = c_i c_j 9^{\lfloor n/7 \rfloor} \geq c_{i+j} 9^{\lfloor n/7 \rfloor},$$

and in the latter ($i+j \geq 7$)

$$\partial_t(G) = \partial_t(H_1)\partial_t(H_2) \geq c_i 9^{\lfloor k/7 \rfloor} \cdot c_j 9^{\lfloor (n-k)/7 \rfloor} = c_i c_j 9^{\lfloor n/7 \rfloor - 1} \geq c_{i+j-7} 9^{\lfloor n/7 \rfloor}.$$

In either case, the cases of equality are the same as in the proof of Theorem 5, and the induction hypothesis shows that equality holds if and only if G has the form described in the statement of the theorem. ■

3 Number of total dominating sets versus total domination number

In this section, we extend our results further by taking the total domination number into account as well. Similar results have been determined for the number of dominating sets and the domination number [11], or the number of independent sets and the independence number [3]. The graphs that attain the minimum in Theorems 5, 7 and 8 have a total domination number of approximately $\frac{4n}{7}$. In the following, we will determine the graphs that minimise the number of total dominating sets when the order and the total domination number are fixed at the same time. When the total domination number is comparatively low, this is almost trivial:

Theorem 9 *For every connected graph G with $n \geq 3$ vertices and total domination number k, we have the inequality*

$$\partial_t(G) \geq 2^{n-k}.$$

Equality can only hold if $k \leq \frac{n}{2}$, and in this case it holds if and only if G has a minimum total dominating set consisting solely of support vertices (equivalently, if every vertex is either a support vertex or adjacent to a support vertex).

Proof. Consider an arbitrary minimum total dominating set D of G; clearly, every superset of D is still total dominating, and there are 2^{n-k} such supersets. This gives us immediately the lower bound, and it remains to determine the cases of equality. Equality can only hold if every total dominating set has to contain D. In particular, for every $v \in D$, the set $V(G) \setminus \{v\}$ cannot be total dominating. This means that v must have a neighbour w that is only adjacent to v and is therefore not dominated by $V(G) \setminus \{v\}$. In other words, v has to be a support vertex. Since $n \geq 3$, no vertex of D can be both a leaf and a support vertex. So if every vertex of D has a leaf neighbour associated to it, D cannot contain more than half of the vertices. This completes the proof. ∎

Remark 10 *The inequality is also true for disconnected graphs without isolated vertices (or even disconnected graphs with isolated vertices if we interpret k as ∞ and 2^{n-k} as $2^{-\infty} = 0$ in this case). The statement on equality remains true for disconnected graphs if every connected component has at least three vertices (since one can apply it to every connected component).*

Theorem 9 settles the problem if the total domination number k is at most $\frac{n}{2}$, and even for $k > \frac{n}{2}$ if we allow connected components consisting of only two vertices. A more interesting situation arises if there are no such connected components and $k > \frac{n}{2}$. As a first observation, we find that the problem can be reduced to trees in this case:

Lemma 11 *Let G be a connected graph. There exists a spanning tree T of G such that $\gamma_t(T) = \gamma_t(G)$ and $\partial_t(T) \leq \partial_t(G)$.*

Proof. The inequality $\partial_t(T) \leq \partial_t(G)$ is trivial and holds for every spanning tree T of G, since every total dominating set of T is also a total dominating set of G. Thus it suffices to prove that there exists a spanning tree of G with the same total domination number. Take any total dominating set D of G; its vertices must induce a graph without isolated vertices. Therefore, we can find a spanning forest of D that only contains edges of G and still does not have isolated vertices. For every vertex of G that does not lie in D, there must be a neighbour in D (since D is a total dominating set), so we can add an edge to a vertex of D for each vertex outside of D. The result is a spanning forest of G, which we can extend to a spanning tree by adding edges between connected components until we obtain a tree T. Note that D is still a total dominating set of T, so $\gamma_t(T) \leq |D| = \gamma_t(G)$. On the other hand, the inequality $\gamma_t(T) \geq \gamma_t(G)$ is trivial (again, since every total dominating set of T is a total dominating set of G), so we are done. ■

Our next lemmas show how trees can be split and pieced together:

Lemma 12 *Every tree that is not a star has a minimum total dominating set that does not contain any leaves.*

Proof. Consider a minimum total dominating set D containing the least possible number of leaves. Let v be any leaf contained in D, and let w be its unique neighbour. The only possible reason for v to be contained in D is to dominate w. If our tree is not a star, w must have a non-leaf neighbour x. If x is contained in D, we can remove v from D, contradicting minimality of D. Otherwise, we can replace v by x in D, obtaining a minimum total dominating set with fewer leaves. This gives us another contradiction, so D cannot contain any leaves at all. ■

Lemma 13 *Let T be a tree with at least three non-leaves, and suppose that the non-leaves do not induce a star. There exists an edge of T such that its removal yields two trees T_1 and T_2 with at least three vertices for which*

$$\gamma_t(T) = \gamma_t(T_1) + \gamma_t(T_2).$$

Proof. Consider a minimum total dominating set D of T that only consists of non-leaves. Such a set exists by the previous lemma. We distinguish three different cases:

Case 1: Suppose that D consists of all non-leaves. Since D does not induce a star, there exists an edge whose removal splits T into two trees T_1 and T_2 each of which contains at least two vertices of D. Both T_1 and T_2 must also contain leaves of T, so they have at least three vertices each. It remains to show that $\gamma_t(T) = \gamma_t(T_1) + \gamma_t(T_2)$. The inequality $\gamma_t(T) \leq \gamma_t(T_1) + \gamma_t(T_2)$ is trivial since $T_1 \cup T_2$ is a subgraph of T. On the other hand, $D \cap T_1$ and $D \cap T_2$ contain all non-leaves of T_1 and T_2 respectively, so by the previous lemma, we have

$$\gamma_t(T_1) \leq |D \cap T_1| \qquad \text{and} \qquad \gamma_t(T_2) \leq |D \cap T_2|.$$

It follows that

$$\gamma_t(T) = |D| = |D \cap T_1| + |D \cap T_2| \geq \gamma_t(T_1) + \gamma_t(T_2),$$

which completes the proof in this case.

Case 2: Suppose that there are some non-leaves not contained in D. Let $\overline{D}$ be the set of all such non-leaves, and assume first that there are two adjacent vertices v and w in $\overline{D}$.

If we remove the edge vw from T, we obtain two trees T_1 and T_2. Both of them must contain at least two vertices of D (one vertex each to dominate v and w respectively, and one more in each tree to dominate those), so T_1 and T_2 have at least three vertices each. Again, it remains to prove that $\gamma_t(T) = \gamma_t(T_1)+\gamma_t(T_2)$, and the inequality $\gamma_t(T) \leq \gamma_t(T_1)+\gamma_t(T_2)$ is trivial. On the other hand, since v and w are not elements of D, the edge vw is immaterial and D is still a total dominating set of $T_1 \cup T_2$. Hence we have equality:

$$\gamma_t(T) = \gamma_t(T_1) + \gamma_t(T_2),$$

as required.

Case 3: Now suppose that there are non-leaves not contained in D, but no two of them are adjacent. Take any vertex v contained in the set $\overline{D}$ of non-leaves that do not belong to D.

Since v is not a leaf, it has at least two neighbours. None of them can be a leaf, since v would have to be contained in D to make D a total dominating set. Hence all neighbours of v are vertices in D. Let w be any such neighbour. As in the previous case, we remove vw to obtain two trees T_1 and T_2. Both need to contain at least two elements of D (a neighbour of v and another vertex to dominate the neighbour) as well as at least one leaf of T, thus at least three vertices. Once again, D is still a total dominating set of $T_1 \cup T_2$: the edge vw could only be relevant for dominating v, but v has at least one more neighbour in D and is thus still dominated. Hence we also have

$$\gamma_t(T) = \gamma_t(T_1) + \gamma_t(T_2)$$

in this case.

■

Lemma 14 *Let T_1 and T_2 be any two trees with at least three vertices. There exist two vertices v_1 and v_2 in T_1 and T_2 respectively such that the tree T obtained from the union of T_1 and T_2 by adding an edge between v_1 and v_2 satisfies*

$$\gamma_t(T) = \gamma_t(T_1) + \gamma_t(T_2) \qquad \text{and} \qquad \partial_t(T) = \partial_t(T_1)\partial_t(T_2).$$

Proof. Since T_1 and T_2 both have at least three vertices, there exist vertices v_1 and v_2 in T_1 and T_2 that are at distance 2 from a leaf (start at any leaf, and take any neighbour of the leaf's unique neighbour other than the leaf itself). As shown in the proof of Lemma 2, the tree T obtained by adding the edge v_1v_2 to the union of T_1 and T_2 has the property that all total dominating sets of T are the union of a total dominating set of T_1 and a total dominating set of T_2, and vice versa. The desired statement follows immediately. ■

Now we are able to provide a recursive characterisation of "optimal" trees (trees minimising the number of total dominating sets). Let $m(n,k)$ be the minimum number of total dominating sets of a tree (or arbitrary connected graph in view of Lemma 11) with n vertices and total domination number k.

Lemma 15 *Let T be an optimal tree with n vertices and total domination number k, i.e. $\partial_t(T) = m(n,k)$. Then one of the following statements holds:*

- *the non-leaves of T induce a star (possibly a degenerate star with only one or two vertices),*
- *One can remove an edge from T such that the resulting trees T_1 and T_2 satisfy the following, where $|T_1| = n_1$, $|T_2| = n_2$, $\gamma_t(T_1) = k_1$ and $\gamma_t(T_2) = k_2$:*
  - $n = n_1 + n_2$ *and* $k = k_1 + k_2$,
  - T_1 *and* T_2 *are optimal trees, i.e.* $\partial_t(T_1) = m(n_1,k_1)$ *and* $\partial_t(T_2) = m(n_2,k_2)$,
  - $m(n,k) = \partial_t(T) = \partial_t(T_1)\partial_t(T_2) = m(n_1,k_1)m(n_2,k_2)$.

Proof. If the non-leaves do not induce a star, we can split T into two trees T_1 and T_2 with at least three vertices and $\gamma_t(T) = k = k_1 + k_2 = \gamma_t(T_1) + \gamma_t(T_2)$ by Lemma 13. Of course, $|T| = n = n_1 + n_2 = |T_1| + |T_2|$ holds trivially. By Lemma 2, we have

$$m(n,k) = \partial_t(T) \geq \partial_t(T_1)\partial_t(T_2) \geq m(n_1,k_1)m(n_2,k_2). \tag{2}$$

On the other hand, if we take two optimal trees S_1 and S_2 with $|S_1| = n_1$, $|S_2| = n_2$, $\gamma_t(S_1) = k_1$ and $\gamma_t(S_2) = k_2$, we can (by Lemma 14) add an edge between S_1 and S_2 to obtain a tree S with $|S| = |S_1| + |S_2| = n_1 + n_2 = n$, $\gamma_t(S) = \gamma_t(S_1) + \gamma_t(S_2) = k_1 + k_2 = k$ and

$$\partial_t(S) = \partial_t(S_1)\partial_t(S_2) = m(n_1, k_1)m(n_2, k_2),$$

so equality must hold in (2) for T to be optimal. This means that $\partial_t(T_1) = m(n_1, k_1)$, $\partial_t(T_2) = m(n_2, k_2)$ and

$$m(n, k) = \partial_t(T) = \partial_t(T_1)\partial_t(T_2) = m(n_1, k_1)m(n_2, k_2),$$

which proves the lemma. ∎

Now we are ready to determine $m(n, k)$ for all possible values of n and k and to characterise the extremal graphs:

Theorem 16 *Define the function* $f : [0, \frac{2}{3}] \to \mathbb{R}$ *by*

$$f(x) = (1 - x)\log 2$$

if $x \leq \frac{1}{2}$, *and by*

$$f(x) = \big((2r + 1)x - (r + 1)\big)\log(2^{r-1} + 1) + \big(r - (2r - 1)x\big)\log(2^r + 1)$$

if $\frac{r+1}{2r+1} < x \leq \frac{r}{2r-1}$ *for an integer* $r \geq 2$. *For every connected graph* G *with* $n \geq 3$ *vertices and total domination number* k, *we have*

$$\partial_t(G) \geq \exp\left(f\left(\frac{k}{n}\right) \cdot n\right). \tag{3}$$

Equality holds

- *for* $k \leq \frac{n}{2}$: *if and only if every vertex is either a support vertex or adjacent to a support vertex, and there are exactly* k *support vertices,*

- *for* $\frac{r+1}{2r+1}n < k \leq \frac{r}{2r-1}n$, *where* r *is an integer* ≥ 2: *if and only if* G *is the union of* $(2r + 1)k - (r + 1)n$ *subdivided stars* $S(K_{1,r-1})$ *and* $rn - (2r - 1)k$ *subdivided stars* $S(K_{1,r})$, *with additional edges between the centres that form a connected graph, but no further additional edges. Note that* $S(K_{1,1})$ *is a path with three vertices; either leaf of* $S(K_{1,1})$ *counts as a centre in this context. See Figure 3 for an example with* 21 *vertices and domination number* 13.

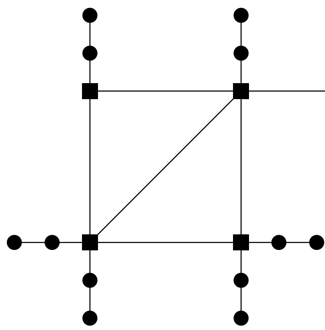

Figure 3: A connected graph with 21 vertices and domination number 13 that attains the minimum. As in Figure 1, centres of subdivided stars are indicated by squares.

Remark 17 *The function f is well-defined since*

$$\left[0, \frac{1}{2}\right] \cup \bigcup_{r=2}^{\infty} \left(\frac{r+1}{2r+1}, \frac{r}{2r-1}\right] = \left[0, \frac{2}{3}\right],$$

where the union is disjoint, and it is also easily seen to be continuous (see Figure 4).

It also deserves to be mentioned that every tree (thus every connected graph) with $n \geq 3$ vertices has a total domination number of at most $\frac{2n}{3}$. This can be seen e.g. by means of Lemma 13 and induction. Thus it is sufficient to define $f(x)$ for $x \leq \frac{2}{3}$.

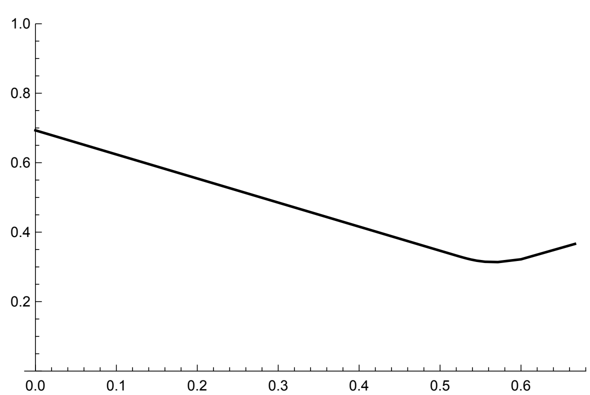

Figure 4: The function $f(x)$ in Theorem 16.

Proof. Let us start with the crucial observation that the function f is convex. This is easy to verify: since f is piecewise linear, it is sufficient to show that the gradients, which are given by

$$\frac{f(r/(2r-1)) - f((r+1)/(2r+1))}{r/(2r-1) - (r+1)/(2r+1)} = (2r+1)\log(2^{r-1}+1) - (2r-1)\log(2^r-1),$$

are decreasing in r, and that the limit as $r \to \infty$ is $-\log 2$, which is the gradient on the interval $[0, \frac{1}{2}]$. Both are simple exercises.

For $k \leq \frac{n}{2}$, the statement is already given by Theorem 9. For $k > \frac{n}{2}$, we use induction. The inequality and the cases of equality are readily verified for $n \in \{3, 4, 5\}$. Now suppose that $n \geq 6$. By Lemma 11, it suffices to prove the inequality for a spanning tree T of G. By Lemma 15, there are two possibilities:

- The non-leaves of T induce a star: each of the non-leaves must be adjacent to at least one leaf. Hence the number of non-leaves is at most $\frac{n+1}{2}$. If it is $\frac{n}{2}$ or less, then $k \leq \frac{n}{2}$ by Lemma 12, which has already been discussed. So the number of non-leaves is exactly $\frac{n+1}{2}$, which is only possible if G is an extended star: $G = S(K_{1,r})$, where $n = 2r + 1$. In this case, we have $\gamma_t(G) = r + 1$ and $\partial_t(G) = 2^r + 1$, so

$$\partial_t(G) = 2^r + 1 = \exp\left(f\left(\frac{r+1}{2r+1}\right) \cdot (2r+1)\right)$$

  by definition of f.

- Otherwise, we can split T into two trees T_1 and T_2 by removing an edge. Let these two trees have n_1 and n_2 vertices respectively, and let their total domination numbers be k_1 and k_2 respectively. We have

$$\begin{aligned}
\partial_t(T) &= \partial_t(T_1)\partial_t(T_2) \\
&\geq \exp\left(f\left(\frac{k_1}{n_1}\right)n_1\right)\left(f\left(\frac{k_2}{n_2}\right)n_2\right) \\
&= \exp\left(\left(f\left(\frac{k_1}{n_1}\right)\frac{n_1}{n} + f\left(\frac{k_2}{n_2}\right)\frac{n_2}{n}\right) \cdot n\right) \\
&\geq \exp\left(\left(f\left(\frac{k_1}{n_1} \cdot \frac{n_1}{n} + \frac{k_2}{n_2} \cdot \frac{n_2}{n}\right) \cdot n\right)\right. \\
&= \exp\left(f\left(\frac{k_1 + k_2}{n}\right) \cdot n\right) = \exp\left(f\left(\frac{k}{n}\right) \cdot n\right)
\end{aligned}$$

  by the induction hypothesis and convexity of f. For equality to hold, $\frac{k_1}{n_1}$, $\frac{k_2}{n_2}$ and $\frac{k}{n}$ have to belong to an interval on which f is linear, i.e. an interval of the form $[\frac{r+1}{2r+1}, \frac{r}{2r-1}]$. We can also use the induction hypothesis on the shape of T_1 and T_2 to show that T must also have the shape described in the statement of the theorem (Lemma 2 is used to prove that the edge between T_1 and T_2 must connect two centres of extended stars for equality to hold). Moreover, we can show in the same way as in the proof of Theorem 7 that arbitrary edges between centres of extended stars can be added without changing the total dominating sets (and thus ∂_t and γ_t), but no other edges can be added without increasing ∂_t.

  Conversely, it is easily verified that every graph with the structure described in the statement of the theorem satisfies (3) with equality.

■

Theorem 16 remains correct for disconnected graphs, provided that each connected component has at least three vertices. This is obtained by applying Theorem 16 to each connected component and using the convexity of f once again:

Theorem 18 *Let f be defined as in Theorem 16. For every graph G with n vertices and total domination number k whose connected components have at least three vertices, the following inequality holds:*

$$\partial_t(G) \geq \exp\left(f\left(\frac{k}{n}\right) \cdot n\right).$$

Equality holds

- *for $k \leq \frac{n}{2}$: if and only if every vertex is either a support vertex or adjacent to a support vertex, and there are exactly k support vertices,*
- *for $\frac{r+1}{2r+1}n < k \leq \frac{r}{2r-1}n$, where r is an integer ≥ 2: if and only if G is the union $(2r+1)k - (r+1)n$ subdivided stars $S(K_{1,r-1})$ and $rn - (2r-1)k$ subdivided stars $S(K_{1,r})$, with an arbitrary set of edges connecting centres of these subdivided stars, but no other edges.*

Remark 19 *Noticing that f attains its minimum at $\frac{4}{7}$, Theorems 7 and 8 can also be obtained as corollaries of Theorems 16 and 18 respectively with some additional work.*

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