Separation numbers of trees

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Abstract

Let G be a graph on n vertices. Given a bijection $f : V(G) \to \{1, 2, \dots, n\}$, let $|f| = \min\{|f(u) - f(v)| : uv \in E(G)\}$. The *separation number* $s(G)$ (also known as *antibandwidth* [1, 7]) of G is then $\max\{|f|\}$ over all such bijections f of G. We study the case when G is a forest, obtaining the following results.

1. Let F be a forest in which each component is a star. Then $s(F) = \frac{n-\mu}{2}$, where μ is the minimum value of $||X| - |Y||$ over all bipartitions (X, Y) of F.

2. Let d be the maximum degree of a tree T on n vertices. Then
a) $s(T) \geq \frac{n}{2} - c_1\sqrt{nd}$, and
b) $s(T) \geq \frac{n}{2} - c_2 d^2 \log_d n$,
where c_1 and c_2 are absolute constants.

We give constructions showing that the bound a) is asymptotically tight when d is in the range $n^{\frac{1}{3}} < d \leq \frac{n}{12}$, while b) is asymptotically tight when d is in the range $n^q \leq d \leq n^{\frac{1}{3}}$, where $0 < q < \frac{1}{3}$ is any fixed constant, and when $d \geq 4$ is an absolute constant.

We also show that for $h \geq 3$ and odd $d \geq 3$, we have $s(T_h^d) = \frac{n}{2} - \Theta(d^2 + dh)$, where T_h^d is the symmetric d-ary tree of height h, improving the estimates obtained in [1].

1 Introduction

We let $[a, b]$ denote the set of integers x with $a \leq x \leq b$. By a *labeling* for a graph G on n vertices we mean a bijection $f : V(G) \to [1, n]$. Let $|f|$ denote $min\{|f(x) - f(y)| : xy \in E(G)\}$, and let $s(G) = max\{|f|\}$ over all labelings. We call $s(G)$ the *separation number* of G. In this paper we seek tight bounds on this parameter when G is a forest, in terms of n and the maximum degree d.

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The separation of G is sometimes called the *antibandwidth* of G since it can viewed as dual to the well known *bandwidth* $B(G)$ of a graph G (defined as the minimum of $\max\{|f(x)-f(y)| : xy \in E(G)\}$ over all labelings f of G). Thus the study of $B(G)$ concerns minimizing the longest "stretch" $|f(x) - f(y)|$ of any edge xy under f, while the study of $s(G)$ concerns maximizing the shortest such "stretch". The separation problem was first studied in [3], where the primary concern was to study the complexity of this problem and its variants. There it was observed that the corresponding decision problem "given a graph G, is $s(G) > k$?" is NP-complete, even for the case $k = 1$ (by a simple reduction from the hamiltonian path problem). The main results gave reductions of certain multiprocessor job scheduling problems to variants of the separation problem. Given in [6] are bounds for the separation of grids, (where in [7], using the term "antibandwidth" for separation, one of the bounds was shown to be exact) and an asymptotically optimal lower bound for the separation of hypercubes (refined further in [7]). In [4] a generalization was considered, where we map a graph G into a graph H, and let $s(G, H)$ be the maximum, over all injections $f : V(G) \to V(H)$, of the minimum of $dist_H(f(x), f(y))$, over all edges xy of G (where $dist_H$ refers to distance in H). The parameter $s(G, H)$ was studied in the case where $G = K_p$ and H is a tree, and also where $G = K_{p,q}$ and H is a hypercube. Bounds for $s(G, H)$ in terms of eigenvalues for certain pairs G, H were developed in [5]. In [2] $s(G, H)$ was studied for the case when G is a path or a power of a path and H is a two dimensional grid, with applications to data storage.

In this paper, we study $s(T)$ for arbitrary trees T and obtain asymptotically tight estimates of $s(T)$ in terms of the order n and the maximum degree d of T. Note the trivial upper bound $s(G) \leq \lfloor \frac{n}{2} \rfloor$, when G has no isolated vertices, since the vertex mapped to $\lfloor \frac{n}{2} \rfloor + 1$ has a neighbor. Thus we will derive asymptotically tight lower bounds in the form $s(T) \geq \frac{n}{2} - f(n, d)$, for some function f of n and d. Earlier and independent of our work, Calamoneri et al. [1] studied the special case of $T = T_h^d$, where T_h^d is a symmetric d-ary tree of height h. They proved that $s(T_h^d) = \frac{n+1-d}{2}$ when d is even and that $\frac{n}{2} - O(d^2 h) \leq s(T_h^d) \leq \frac{n}{2} - O(h)$ when d is odd. At the end of the last section, we will improve these estimates to show that $\frac{n}{2} - O(d^2 + dh) \leq s(T_h^d) \leq \frac{n}{2} - O(d^2 + dh)$ when d is odd.

We consider only simple graphs without isolated vertices. For finite sets X, Y, we refer to $||X| - |Y||$ as the *discrepancy* of (X, Y). Given a bipartite graph G, let the *discrepancy* of G, denoted by $\mu(G)$, be the minimum discrepancy value over all bipartitions (X, Y) of G. We say that G is *balanced* if $\mu(G) = 0$. A subset S of $V(G)$ is called a *balancing set* for G if $\mu(G - S) = 0$ or 1. For a vertex v of a graph G let $N_G(v)$ denote the set of neighbors of v. For a subset W of $V(G)$ we let $N_G(W)$ denote $\cup_{v \in W} N_G(v)$. When the context is clear, we will drop the subscript G. For graph theoretic notations not defined here, see [8].

2 Basic results and star forests

We first prove a simple but useful lemma, already implicit in [6], including the proof here for completeness. Observe that in a forest F with bipartition (X, Y) where $|X| \geq |Y|$, X has a vertex of degree at most one in F. This is because the average degree $\frac{|E(F)|}{|X|}$ among vertices in X is at most $\frac{|X|+|Y|-1}{|X|} \leq \frac{2|X|-1}{|X|} < 2$.

Lemma 2.1 *Let T be a forest with a bipartition (X, Y) where $p = |X| \geq |Y| = q$. Then one can order the vertices in X as $x_1, x_2, \ldots, x_p$ and the vertices in Y as $y_1, y_2, \ldots, y_q$ such that if $x_i y_j \in E(T)$ then $j \leq i$.*

Proof. Suppose the claim fails for some bipartition (X, Y) and T, and consider a failing case with q as small as possible. Clearly $q > 0$. By earlier discussion, some vertex x_1 in X has at most one neighbor. Let y_1 denote that neighbor if $N(x_1) \neq \emptyset$, else letting y_1 be any vertex in Y_1. Then $T - \{x_1, y_1\}$ is a forest with bipartition $(X - x_1, Y - y_1)$ with $|X - x_1| \geq |Y - y_1|$, so by minimality the claim holds for this bipartition. Thus one can order the vertices in $X - x_1, Y - y_1$ as $x_2, x_3, \ldots, x_p$ and $y_2, y_3, \ldots, y_q$ respectively such that if $x_i y_j \in E(T)$ then $j \leq i$. Since x_1 has no neighbor other than y_1, the orderings $x_1, x_2, \ldots, x_p$ and $y_1, y_2, \ldots, y_q$ verify the claim for (X, Y), completing the proof. ∎

For completeness, we reprove the resulting lower bound on $s(T)$ for forests T.

Lemma 2.2 *[6] Let T be a forest on n vertices with discrepancy $\mu = \mu(T)$. Let (X, Y) be an arbitrary bipartition of T where $|X| \geq |Y|$. Then*
(a) $s(T) \geq |Y|$, and
(b) $s(T) \geq \frac{n-\mu}{2}$.

Proof. (a) Suppose $|X| = p$, $|Y| = q$. By Lemma 2.1, we can name the vertices in X as $x_1, \ldots, x_p$ and the vertices in Y as $y_1, \ldots, y_q$ such that $j \leq i$ for each edge $x_i y_j \in E(T)$. Define labeling $f : V(T) \to [1, p + q]$ as follows. For each $i = 1, 2, \ldots, q$, let $f(y_i) = i$ and $f(x_i) = q + i$. If $p > q$, assign labels in $[2q + 1, p + q]$ to $x_{q+1}, \ldots, x_p$ in an arbitrary way. Consider any edge $uv \in E(T)$ where $u \in X$ and $v \in Y$. If $u \in \{x_{q+1}, \ldots, x_p\}$, then $f(u) - f(v) \geq 2q + 1 - q = q + 1$. If $u = x_i$ for some $i \in \{1, \ldots, q\}$ then $v = y_j$ for some $j \leq i$ and $f(u) - f(v) = (q + i) - j \geq q$. Thus we have $|f| \geq q$, so $s(T) \geq |Y|$.

(b) Let (X, Y) be a bipartition of T with $|X| - |Y| = \mu$. Since $|X| + |Y| = n$, we have $|Y| = (n - \mu)/2$. So $s(T) \geq |Y| = (n - \mu)/2$. ∎

Let f be a labeling of G. Define an orientation D_f (which we abbreviate by D when f is fixed) of G by orienting each edge $uv \in E(G)$ from u to v if $f(u) < f(v)$ or from v to u if $f(v) < f(u)$. Call a vertex with in-degree 0 in D a *source*, a vertex with out-degree 0 in D a *sink*, and a vertex with both in-degree and out-degree at least one in D a *level vertex*. Let $A = A(f), B = B(f), C = C(f)$ denote the sets of sources, sinks, and level vertices, respectively in D_f. Let $d_C = d_C(f) = \max\{d(x) : x \in C\}$. We will drop the reference to f when the context is clear.

Lemma 2.3 *Let G be a bipartite graph with no isolated vertex. Let f be a labeling of G. Then $|f| \leq \min\{|A(f)|, |B(f)|\}$. If $C(f) \neq \emptyset$, then $|f| \leq \frac{n-d_C(f)+1}{2}$.*

Proof. Let $A = A(f), B = B(f), C = C(f)$. Since G has no isolated vertex, some vertex has a positive out-degree in D_f; let x be one with largest f-label. Then the $n - f(x)$ vertices whose f-labels are larger than $f(x)$ are sinks. Thus, $n - f(x) \leq |B|$. Let y be an out-neighbor of x. Then $f(x) < f(y) \leq n$. We have $|f| \leq f(y) - f(x) \leq n - f(x) \leq |B|$. Similarly, by considering the vertex with the smallest f-label that has a positive in-degree, we have $|f| \leq |A|$. It follows that $|f| \leq \min\{|A|, |B|\}$.

Suppose that $C \neq \emptyset$. Let x be a level vertex with $d(x) = d_c(f)$. Let u be an in-neighbor of x with largest f-label and v an out-neighbor of x with smallest f-label. Then $f(u) < f(x) < f(v)$. By our choice, the $f(v) - f(u) - 1$ vertices receiving labels in $(f(u), f(v))$ are non-neighbors of x. Hence, $f(v) - f(u) - 1 \leq n - d(x)$. So, $f(v) - f(u) < n - d(x) + 1$. Note that $(f(v) - f(x)) + (f(x) - f(u)) = f(v) - f(u)$. Thus, we have $|f| \leq \min\{f(v) - f(x), f(x) - f(u)\} \leq \frac{n-d(x)+1}{2} = \frac{n-d_C+1}{2}$. ■

We now derive a general upper bound on $s(G)$ that allows us to determine the exact value of $s(G)$ in some cases. Let $\gamma(G)$ denote the minimum cardinality of a balancing set of G. If G is already balanced, then we let $\gamma(G) = 0$. Clearly $\gamma(G) \leq \mu(G)$ for any bipartite graph G. The *penult degree* $d^*(G)$ of G is defined as follows. If G has no vertex of degree larger than one then $d^*(G) = 1$; otherwise $d^*(G)$ is the least vertex degree in G that is larger than one.

Theorem 2.4 *Let G be a bipartite graph on n vertices with no isolated vertices. Then*

(a) $s(G) \leq (n - \gamma(G))/2$, and

(b) $s(G) \leq \max\{\frac{n-d^*(G)+1}{2}, \frac{n-\mu(G)}{2}\}$.

Proof. Let f be a labeling of G with $|f| = s(G)$, and consider the orientation $D = D_f$. Let $A = A(f), B = B(f), C = C(f)$. Let $a = |A|, b = |B|$. Note that each of A and B is independent in G. By Lemma 2.3, we have $|f| \leq \min\{a, b\}$. By symmetry, we may assume that $a \geq b$. By removing the c level vertices and $a - b$ sources, we can split the remaining vertices into two independent sets of equal sizes. Hence, $\gamma(G) \leq c + a - b$. Since $a + b + c = n$, we have $b \leq (n - \gamma(G))/2$. So, $s(G) = |f| \leq b \leq (n - \gamma(G))/2$, proving the first statement.

For the second statement, suppose first that D has no level vertices. Then (A, B) is a bipartition of G. We have $|f| \leq \min\{a, b\}$. Since $a + b = n$ and $|a - b| \geq \mu(G)$, we have $\min\{a, b\} \leq \frac{n-\mu(G)}{2}$. Hence $s(G) = |f| \leq \frac{n-\mu(G)}{2}$ as desired. Suppose instead that $C \neq \emptyset$. Note that $d_C \geq d^*$. By Lemma 2.3. $s(G) = |f| \leq \frac{n-d_C+1}{2} \leq \frac{n-d^*(G)+1}{2}$, as desired. ■

Lemma 2.2 and Theorem 2.4 immediately yield the following.

Corollary 2.5 *Let T be a forest on n vertices. Then $\frac{n-\mu(G)}{2} \leq s(T) \leq \frac{n-\gamma(G)}{2}$.*

Corollary 2.6 *Let T be a forest on n vertices. If $d^*(T) \geq \mu(T) + 1$, then $s(T) = \frac{n-\mu(T)}{2}$.*

If T is a forest with $\mu(T) = \gamma(T)$ then Corollary 2.5 yields $s(T) = \frac{n-\mu(T)}{2}$. In general, however, $\mu(T)$ and $\gamma(T)$ can differ drastically. In such cases, Corollary 2.6 could be useful. For instance, if T is a star with m leaves, then $\mu(T) = m - 1$ while $\gamma(T) \leq 2$. Also, $d^*(T) = m = \mu(T) + 1$. So by Corollary 2.6 and $n = m + 1$, we have $s(T) = \frac{n-\mu(T)}{2} = 1$. It is natural to ask whether $s(T) = \frac{n-\mu(T)}{2}$ is still valid when T is a *star forest*, i.e., a vertex-disjoint union of stars. Neither Corollary 2.5 nor Corollary 2.6 gives a definite answer. In the next theorem we prove that this equality indeed holds for star forests.

Theorem 2.7 *Let T be a star forest. Let $\mu = \mu(T)$. Then $s(T) = \frac{n-\mu}{2}$.*

Proof. By Lemma 2.2, it remains to show that $s(T) \le \frac{n-\mu}{2}$. Let f be a labeling of T with $|f| = s(T)$. We need to show that $|f| \le \frac{n-\mu}{2}$. Consider $D = D_f$. If there is a level vertex with degree at least $\mu + 1$, then by Lemma 2.3, $|f| \le \frac{n-d_C+1}{2} \le \frac{n-\mu}{2}$ and we are done.

Thus we may assume that every level vertex has degree at most μ. Note that each level vertex has degree at least 2 and is the center of a star component of T. Let T_0 be the subforest of T obtained by removing each star component that has a level vertex at the center. Let $F_1, F_2, \ldots, F_p$ denote the star components removed. For each i, let l_i denote the number of leaves in F_i; we have $l_i \le \mu$ by our earlier assumption. Let $m = \Sigma_{i=1}^{p} l_i - p$.

Claim 1. $\mu(T_0) \ge \mu + m$.

Proof of Claim 1. Suppose that $\mu_0 = \mu(T_0) \le \mu - 1 + m$. We derive a contradiction by showing that we can obtain a bipartition of T with discrepancy at most $\mu - 1$. Let (X, Y) be a bipartition of T_0 with discrepancy μ_0, where $|X| \ge |Y|$. Let q be the largest integer such that $|X| + q \ge |Y| + \Sigma_{i=1}^{q} l_i$. Let X' be the set containing X and the centers of $F_1, \ldots, F_q$ and Y' be the set containing Y and the leaves of $F_1, \ldots, F_q$. Let $T' = T_0 \cup F_1 \cup \cdots \cup F_q$. Then (X', Y') is a bipartition of T', and by the definition of q, $|X'| \ge |Y'|$. Suppose first that $q = p$. In this case, $T' = T$. We have $|X'| - |Y'| = (|X| + p) - (|Y| + \Sigma_{i=1}^{p} l_i) = |X| - |Y| - m = \mu_0 - m \le \mu - 1$. So (X', Y') is a bipartition of T with discrepancy at most $\mu - 1$, a contradiction. Hence, we may assume that $q < p$. By our choice of q, $|X| + q + 1 < |Y| + \Sigma_{i=1}^{q+1} l_i$. That is, $|X'| + 1 < |Y'| + l_{q+1} \le |Y'| + \mu$. Thus, (X', Y') is a bipartition of T' with discrepancy at most $\mu - 1$. Now, one by one we add $F_{q+1}, F_{q+2}, \ldots, F_p$ to T', always placing the center of an added star component in the larger part and leaves in the smaller part of the current bipartition. It is easy to see that in the end we obtain a bipartition of T with discrepancy at most $\mu - 1$, a contradiction. Thus $\mu_0 = \mu(T_0) \ge \mu + m$, completing the proof of Claim 1.

Let $A = A(f), B = B(f)$.

Claim 2. $\min\{|A|, |B|\} \le \frac{n-\mu}{2}$.

Proof of Claim 2. By our assumption, each vertex in T_0 is either a source or sink in D. Let $A_0 = V(T_0) \cap A$ and $B_0 = V(T_0) \cap B$. Then (A_0, B_0) is a bipartition of T_0. By Claim 1, $||A_0| - |B_0|| \ge \mu + m$. For each $i \in \{1, \ldots, p\}$, the center of F_i is a level vertex while its l_i leaves are in $A \cup B$ with at least one in each of A and B. Hence $|V(F_i) \cap A|$ and $|V(F_i) \cap B|$ differ by at most $l_i - 1$. Hence, $||A| - |B|| \ge ||A_0| - |B_0|| - \Sigma_{i=1}^{p}(l_i - 1) \ge (\mu + m) - m = \mu$. Since $|A| + |B| \le n$, we have $\min\{|A|, |B|\} \le \frac{n-\mu}{2}$, completing the proof of Claim 2.

By Lemma 2.3, $s(G) = |f| \le \min\{|A|, |B|\} \le \frac{n-\mu}{2}$, as required. ■

3 A good measure of separation in trees

In this short section, we establish a connection between the separation number of a tree and a parameter involving independent sets of T.

Theorem 3.1 *Let W be an independent set in a tree T. Let (A, B) be a bipartition of $T - W$ with $|A| \leq |B|$. Then $s(T) \geq |A| - |N(W)|$.*

Proof. Let $A' = A - N(W)$ and $B' = B - N(W)$. The forest F induced in T by $A' \cup B'$ has (A', B') as a bipartition. Let $m = min\{|A'|, |B'|\}$. In particular, $m \geq |A'| \geq |A| - |N(W)|$. By Lemma 2.2 and its proof, F has a labeling g with $|g| \geq m$ in which without loss of generality all of A' appears before B'. Take the linear ordering of $V(F)$ associated with g, insert W between A' and B', insert $A \cap N(W)$ before A', and $B \cap N(W)$ after B', where within each of $A \cap N(W)$, W and $B \cap N(W)$ the ordering is arbitrary. Let f be the resulting labeling of T. Since $m \geq |A| - |N(W)|$, it suffices to show that $|f| \geq m$.

Let uv be an edge in T with $f(v) - f(u) = |f|$. We are done if either all of A' or all of B' lies between u and v in f, since then $f(v) - f(u) \geq \min\{|A'|, |B'|\} = m$. It is easy to see, from the definition of f and the independence of A, W, B, that the only remaining case is when $u \in A'$ and $v \in B'$. But then $f(v) - f(u) \geq g(v) - g(u) \geq m$, completing the proof. ■

For each independent set W in T, let $\varphi(W) = \frac{1}{2}\mu(T - W) + \frac{1}{2}|W| + |N(W)|$. Let $\varphi(T) = \min\{\varphi(W) : W \text{ is an independent set of } T\}$. The next two theorems show that $\varphi(T)$ provides a good measure of how far $s(T)$ is from the trivial upper bound $\frac{n}{2}$. As a result, we can get good bounds on $s(T)$ by finding good bounds on $\varphi(T)$.

Theorem 3.2 *Let T be an n-vertex tree. Then $s(T) \geq \frac{n}{2} - \varphi(T)$.*

Proof. Let W be independent in T with $\varphi(W) = \varphi(T)$. Let (A, B) be a bipartition of $T - W$, with $|A| \leq |B|$ and $|B| - |A| = \mu(T - W) = \mu$. We have $|A| \geq \frac{n - |W| - \mu}{2}$. By Theorem 3.1, $s(T) \geq |A| - |N(W)| \geq \frac{n}{2} - \frac{\mu}{2} - \frac{|W|}{2} - |N(W)| = \frac{n}{2} - \varphi(W) = \frac{n}{2} - \varphi(T)$. ■

Theorem 3.3 *Let T be an n-vertex tree. Then $s(T) \leq \lfloor \frac{n}{2} \rfloor + 1 - \lfloor \frac{\varphi(T)}{5} \rfloor \leq \frac{n}{2} + 2 - \frac{\varphi}{5}$.*

Proof. Let $m = \lfloor \frac{\varphi(T)}{5} \rfloor$. Suppose $s(T) \geq \lfloor \frac{n}{2} \rfloor + 2 - m$. We derive a contradiction by finding an independent set W with $\varphi(W) < 5m \leq \varphi(T)$. Let f be an optimal labeling of T, so that $|f| \geq \lfloor \frac{n}{2} \rfloor + 2 - m$. Let A denote the set of vertices receiving the first $\lfloor \frac{n}{2} \rfloor - m$ labels, W the set of vertices receiving the next $2m$ labels, and C the set of vertices receiving the last $\lceil \frac{n}{2} \rceil - m$ labels. Since $|f| \geq \lfloor \frac{n}{2} \rfloor + 2 - m$, each of A, W, B induces an independent set. This also implies that $\mu(T - W) = 0$ or 1.

Since a vertex in W has f-label at most $\lfloor \frac{n}{2} \rfloor + m$ and $|f| \geq \lfloor \frac{n}{2} \rfloor + 2 - m$, vertices in $N(W) \cap A$ must receive labels in the interval $[1, 2m - 2]$. So, $|N(W) \cap A| \leq 2m - 1$. Similarly, one can show that $|N(W) \cap B| \leq 2m - 1$. Now, $\varphi(W) = \frac{1}{2}\mu(T - W) + \frac{1}{2}|W| + |N(W)| \leq \frac{1}{2} + \frac{1}{2}(2m) + 4m - 2 < 5m$, a contradiction. This completes the proof. ■

For the rest of the paper, we develop bounds on $s(T)$ by bounding $\varphi(T)$. For the most part, we will be focusing on finding the correct order of magnitude of $\varphi(T)$ in terms of the order n of T and the maximum degree d of T.

4 Separation for trees of maximum degree d; lower bounds

In this section, we derive lower bounds on the separation for trees T with maximum degree d, and in the next section we show that these bounds are asymptotically tight when d is an absolute constant and when $n^q < d < \frac{n}{12}$ for any fixed constant $q \in (0,1)$, where $n = |V(T)|$.

By Theorem 3.2, to find a good lower bound on $s(T)$, it suffices to find a good upper bound on $\varphi(T)$. We accomplish this in two stages. In the first stage we use a variant of the usual inorder numbering of trees to first find a set M for which $\mu(T - M)$ and $|M|$ are small. In the second stage, we use this set M to carefully construct our independent set W with small $\varphi(W)$. Before we introduce our numbering algorithm, we need some notation.

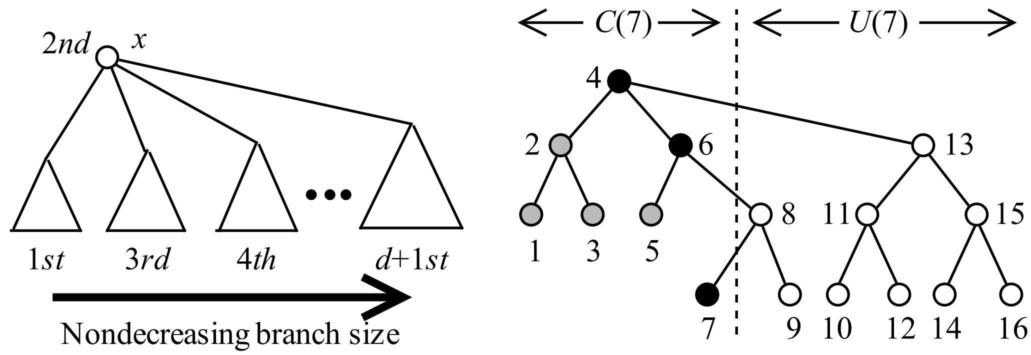
Let T be a tree rooted at r. For each vertex v in T let T_v denote the subtree of T rooted at v and let $n(v)$ denote $|V(T_v)|$. For $v \in V(T) - \{r\}$ let v^- denote the parent of v, i.e., the neighbor of v on the r, v-path in T. A neighbor of v other than v^- is a *child* of v. For any child x of v, we call T_x a *branch below* v. Order the children $v_1, v_2, \ldots, v_c$ of each vertex v so that $n(v_1) \leq n(v_2) \leq \ldots \leq n(v_c)$.

We now number the vertices of T from 1 to n as follows: we proceed recursively by traversing the lightest branch below r, then r, then the remaining branches below r in nondecreasing order of size, provided there are at least two branches below r. If there is only one such branch below r, then r is traversed first, and then the branch below r. As the tree is traversed, the labels 1 through $n = |V(T)|$ are assigned to the vertices in the order visited. Below is the formal algorithm. See Figure 1 for an illustration of the labeling.

Procedure Inorder(T, v)**:**
Input: a tree T rooted at v
Output: a vertex labeling $l : V(T) \to [1, n]$ (similar to the usual inorder numbering)
1. Let $v_1, v_2, \ldots, v_c$ be the children of v in nondecreasing order of branch size $n(v_1) \leq n(v_2) \leq \ldots \leq n(v_c)$
2. If $c = 0$ (i.e., v is a leaf) then
    $l(v) \leftarrow$ least integer from $[1, n]$ not already assigned as a label
  If $c = 1$ then
    $l(v) \leftarrow$ least integer from $[1, n]$ not already assigned as a label
    Apply Inorder(T_{v_1}, v_1)
  If $c \geq 2$ then
    Apply Inorder(T_{v_1}, v_1)
    $l(v) \leftarrow$ least integer from $[1, n]$ not already assigned as a label
    For $i = 2$ to c, apply Inorder(T_{v_i}, v_i)
3. If all labels in $[1, n]$ have been assigned, then halt.

To analyze this labeling, we use the following notation (see Figure 1 for an illustration). Let the two partite sets of T be R and B (red and blue). For each i with $1 \leq i \leq n(T)$, let $C(i)$ be the set of vertices labeled 1 through i. Let $C(0) = \emptyset$. Let $U(i) = V(T) - C(i)$. Let $M(i)$ consist of those vertices in $C(i)$ having at least one neighbor in $U(i)$, and let $L(i) = C(i) - M(i)$. We call $C(i), L(i), M(i)$ and $U(i)$ the *labeled, fully labeled, mixed,* and *unlabeled* vertices of T (respectively) at the i'th step of the procedure. We drop the index i when the context is clear.

For each subset S of $V(T)$, let $\mu^*(S) = |S \cap R| - |S \cap B|$. For each $i = 1, \ldots, n$, we have $|\mu^*(C(i)) - \mu^*(C(i-1))| = 1$. Since $\mu^*(C(0)) = 0$, there exists an i such that $\mu^*(C(i)) =$



$$L(7) = \{1, 2, 3, 5\}, M(7) = \{4, 6, 7\}, U = \{8, \ldots, 16\}.$$

Figure 1: Inorder labeling of a tree

$\lfloor \frac{\mu^*(V(T))}{2} \rfloor$. For the rest of the paper we fix i to be this value, and let $L = L(i), U = U(i), M = M(i)$ and still refer to these sets as fully labeled, unlabeled, and mixed vertices.

We will now analyze the structure of L, M, and U. Let M_1 be the set of mixed vertices having at least one unlabeled child and M_2 the set of mixed vertices v for which the parent v^- of v is the only unlabeled neighbor of v. Then $M = M_1 \cup M_2$. Let $x_1, x_2, \ldots, x_p$ be the mixed vertices, in nondecreasing order of distance from the root r.

Lemma 4.1 *(a) There is no edge xy in $T - M$ with $x \in L$ and $y \in U$.*

(b) Let y be any vertex in T. Then at most one branch under y can contain a mixed vertex.

(c) All the mixed vertices lie on a path P from the root r to x_p.

(d) For $i = 1, \ldots, p-1$, if $x_i \in M_2$ then $x_{i+1} \in M_1$.

Proof. (a) This is clear from the definitions of L and U.
(b) Suppose otherwise that y_1, y_2 are children of y such that T_{y_1} contains a mixed vertex x_r and T_{y_2} contains a mixed vertex x_s. Assume also that y_1 appears before y_2 in the ordering of the children of y. In our algorithm Inorder, by the time we label vertices in T_{y_2}, all of $V(T_{y_1})$ and y should have been labeled. So, x_r is already fully labeled, a contradiction.
(c) This follows from part (b) immediately.
(d) Let P be the path from r to x_p given in (c). For each vertex $v \in V(P) - x_p$, let v^+ denote its child on P. Suppose that $x_i, x_{i+1} \in M_2$. Then $x_i^+ \in L$ and $x_{i+1}^- \in U$. As we move along P from x_i^+ to x_{i+1}^- we must encounter a vertex z such that $z \in L$ and $z^+ \in U$. Such z would be a mixed vertex, contradicting x_i and x_{i+1} being consecutive mixed vertices on P. ■

We have completed the first stage. We now go to the second stage of constructing our independent set W. As we traverse the path P of Lemma 4.1(c) from r to x_p, we encounter the mixed vertices in the order $x_1, \ldots, x_p$. Select a distinguished integer q, $1 \leq q \leq p$, based on some criteria to be described later. We build W as a disjoint union of independent sets W_1 and W_2, where W_1 is derived from the segment $x_1, x_2, \ldots, x_q$ of mixed vertices while W_2 is derived from the segment $x_{q+1}, x_{q+2}, \ldots, x_p$.

To get W_1, start with the initialization $W_1 = \{x_q\}$. Now we treat the x_i, $i \le q$, in decreasing order of i, by greedily including x_i in W_1 if doing so preserves the independence of the current W_1. Otherwise, we instead include in W_1 the unlabeled neighbors of x_i. Below is the formal algorithm. Recall that for any vertex v on the path P, v^- denotes the parent of v in T. As in the proof of Lemma 4.1(d), we let v^+ denote the child of v on P.

1. (Initialization) $W_1 = \{x_q\}$, $i \leftarrow q-1$.
2. If $i \ge 1$, then
   a) If $x_i^+ \notin W_1$, then $W_1 \leftarrow W_1 \cup \{x_i\}$.
   b) If $x_i^+ \in W_1$, then $W_1 \leftarrow W_1 \cup \{\text{unlabeled neighbors of } x_i\}$.
   c) $i \leftarrow i-1$.
3. If $i = 0$, halt. Otherwise, go to step 2.

We construct W_2 similarly, except that we treat the x_i in increasing order of i.

1. (Initialization) $W_2 = \emptyset$, $i \leftarrow q+1$.
2. If $i \le p$, then
   a) If $x_i^- \notin W_2$, then $W_2 \leftarrow W_2 \cup \{x_i\}$.
   b) If $x_i^- \in W_2$, then $W_2 \leftarrow W_2 \cup \{\text{unlabeled neighbors of } x_i\}$.
   c) $i \leftarrow i+1$.
3. If $i = p+1$, halt. Otherwise, go to step 2.

Finally let $W = W_1 \cup W_2$. Thus, W is obtained from M by retaining certain (possibly all) vertices in M, and replacing the remaining vertices in M by their unlabeled neighbors.

Lemma 4.2 *(a) There is no edge xy in $T - W$ with $x \in L \cup (M - W)$ and $y \in U - W$.*
(b) We have $\mu(T - W) \le |W| + 1$ and $s(T) \ge \frac{n}{2} - \varphi(W) \ge \frac{n}{2} - \frac{1}{2} - |W \cup N(W)|$.

Proof. (a) Suppose such an edge xy exists. By Lemma 4.1 (a), there is no edge between L and U. So we must have $x \in M - W$. But by our construction of W, all unlabeled neighbors of x are included in W, and so x has no neighbor in $U - W$, contradicting $y \in U - W$.

(b) Recall that for each subset S of $V(T)$, $\mu^*(S) = |S \cap R| - |S \cap B|$. And, for our choice of i, we have $\mu^*(C(i)) = \lfloor \mu^*(V(T))/2 \rfloor$, where $C(i) = L \cup M$. Since $V(T) = L \cup M \cup U$, it follows that $\mu^*(L \cup M)$ and $\mu^*(U)$ differ by at most 1. Thus $\mu^*((L \cup M) - W)$ and $\mu^*(U - W)$ differ by at most $|W|+1$. By (a) there is no edge in $T - W$ between $(L \cup M) - W$ and $U - W$. Thus, by switching the red vertices with the blue vertices in $U - W$ if necessary, we obtain a bipartition of $T - W$ with discrepancy at most $|W|+1$. Now, $\varphi(T) \le \varphi(W) \le \frac{1}{2}(|W|+1) + \frac{1}{2}|W| + |N(W)| \le \frac{1}{2} + |W \cup N(W)|$. By Theorem 3.2, we have $s(T) \ge \frac{n}{2} - \varphi(T) \ge \frac{n}{2} - \frac{1}{2} - |W \cup N(W)|$. ■

Next we establish an upper bound on $|W \cup N(W)|$, which together with lemma 4.2 will give us lower bounds on $s(T)$. For each $x_i \in M$, let d_i be the number of unlabeled children of x_i, and let $f_i = d_i + 1$. Note that if $x_i \in M_2$, then $d_i = 0$, and so $f_i = 1$.

Lemma 4.3 *(a) For each $1 \le i \le p-1$, we have $n(x_i) \ge f_i \cdot n(x_{i+1})$. Thus, $n \ge f_1 \cdot f_2 \cdots f_p$.*
(b) $n \ge (f_1 \cdot f_2 \cdots f_q)(|W_2 \cup N(W_2)| - 1)$.

Proof. (a) If $x_i \in M_2$ then $f_i = 1$, so the claim follows trivially from $T_{x_{i+1}} \subseteq T_{x_i}$. Suppose then that $x_i \in M_1$. We consider two cases.

Case 1: x_i^+ is labeled.

Recall that the the procedure $Inorder(T, x_i)$ labels the branches below x_i in order of non-decreasing size, and all vertices of a branch must be labeled before the labeling of the next branch can begin. Since the branch $T_{x_i^+}$ contains mixed vertices (e.g. x_{i+1}), the labeling of $T_{x_i^+}$ has not been completed. Hence for each of the d_i unlabeled children y of x_i we have $|T_{x_i^+}| \leq |T_y|$. It follows that $n(x_i) \geq (d_i+1)n(x_i^+) \geq (d_i+1)n(x_{i+1}) = f_i \cdot n(x_{i+1})$.

Case 2: x_i^+ is unlabeled.

Note that some branch B under x_i^+ contains mixed vertices (e.g. x_{i+1}). Since some vertex in B has been labeled but x_i^+ has not, B must be the lightest branch under x_i^+, and x_i^+ has at least one other branch B' in which the labeling has not started. By our design, $|B'| \geq |B|$. Hence, $n(x_i^+) \geq |B| + |B'| \geq 2|B| \geq 2n(x_{i+1})$. Similarly, the fact that $T_{x_i^+}$ contains mixed vertices suggests that we have not finished labeling $T_{x_i^+}$, which implies that each of the branches under the other $d_i - 1$ unlabeled children of x_i is at least as heavy as $T_{x_i^+}$. So,

$$n(x_i) \geq d_i n(x_i^+) \geq 2n(x_{i+1})d_i \geq n(x_{i+1})(d_i+1) = n(x_{i+1})f_i.$$

It follows by induction that $n \geq f_1 \cdot f_2 \cdots f_p$.

(b) Note $T_{x_{q+1}} \supseteq (W_2 \cup N(W_2)) - x_{q+1}^-$. The claim follows from (a) by induction. ■

Next we develop an optimization lemma which we will use in conjunction with Lemma 4.3 to bound $|W \cup N(W)|$. For simplicity, we will be somewhat generous in our estimates.

Lemma 4.4 *Let D, N be real numbers such that $2 \leq D \leq N$. Let t be an arbitrary positive integer. Let $y_1, y_2, \ldots, y_t$ be real numbers satisfying $2 \leq y_i \leq D$ and $\prod_{i=1}^t y_i \leq N$. Then $\sum_{i=1}^t y_i \leq 2D \log_D N$.*

Proof. Among all multisets satisfying the constraints, pick $\{y_1, \ldots, y_m\}$ such that $\sum_i^m y_i$ is maximum and subject to that m is minimum. It suffices to prove the claims for this multiset. Suppose for some $i \neq j$ that $2 < y_i \leq y_j < D$. If $y_i y_j \leq 2D$ then replace y_i, y_j by 2, $\frac{y_i y_j}{2}$, and otherwise replace y_i, y_j by D, $\frac{y_i y_j}{D}$. Either way, one can check that the new multiset satisfies the constraints, but $\sum y_i$ will be larger than before, a contradiction. So, we may assume that among the y_i values at most one is strictly between 2 and D.

Suppose first that $D < 4$. Since each $y_i \geq 2$ we have $2^m \leq \prod_i^m y_i \leq N$. So, $m \leq \log N$. Thus, $\sum y_i \leq D \log N \leq 2D \log_D N$. Next, suppose $D \geq 4$. If there are two 2's among the y_i's, then replacing two by a single 4 yields a smaller multiset with the same product and sum as before, contradicting our choice of $\{y_1, \ldots, y_m\}$. So at most one y_i equals 2. By our earlier discussion, at most one y_i is strictly between 2 and D. Thus, we have $4D^{m-2} \leq \prod_i^m y_i \leq N$. Thus, $m - 2 \leq \log_D \frac{N}{4} \leq \log_D N$ and $m \leq \log_D N + 2$. If $N \geq D^2$ or $m \leq 2$, then we have $m \leq 2\log_D N$ and $\sum y_i \leq 2D \log_D N$, and we are done. So, we may assume $N < D^2$ and

$m \geq 3$. By our discussion, at least one y_i, say y_m, is D. Now, we have $\prod_{i=1}^{m-1} y_i \leq \frac{N}{D} < D$ and $\sum_{i=1}^{m-1} y_i \leq \prod_{i=1}^{m-1} y_i < D$. Thus, $\sum_{i=1}^{m} y_i \leq D + D \leq 2D \log_D N$. ■

Lemma 4.3 yields the following bound on $|W|$ independent of our choice of q.

Lemma 4.5 *Suppose $\Delta(T) = d$, where $d \geq 1$. Then $|W| \leq 4(d+1)\log_{d+1} n$.*

Proof. For each $x_i \in M_1$, we have $f_i = d_i + 1 \geq 2$ and $f_i \leq d+1$. Also, by Lemma 4.3, $\Pi_{x_i \in M_1} f_i \leq n$. By Lemma 4.4, with $D = d+1, N = n$, we have $\sum_{x_i \in M_1} f_i \leq 2(d+1)\log_{d+1} n$.

By Lemma 4.1 (d), $|M_2| \leq |M_1| + 1$. Since for each $x_i \in M_2$, $f_i = 1$, we have $\sum_{x_i \in M_2} f_i = |M_2| \leq |M_1| + 1 \leq 1 + \frac{1}{2}\sum_{x_i \in M_1} f_i$. So, $\sum_{x_i \in M} f_i \leq \frac{3}{2}(\sum_{x_i \in M_1} f_i) + 1 \leq 4(d+1)\log_{d+1} n$. Finally, note that in forming W we include for each i either x_i or its unlabeled neighbors, so $|W| \leq \sum_{x_i \in M} f_i \leq 4(d+1)\log_{d+1} n$. ■

We now define the distinguished integer q on which the construction above of W_1 and W_2 was based. Setting $k = \frac{n}{d}$, we let

$$q = min\{j : d_j \geq \lfloor\sqrt{k}\rfloor \ or \ \prod_{i \leq j} f_i \geq k \ or \ j = p\}.$$

We now estimate $|W \cup N(W)|$.

Lemma 4.6 *Suppose $\Delta(T) = d$, where $d \geq 1$ and $k = \frac{n}{d} \geq 4$. We have*

(a) $|W_1| \leq 1 + f_1 + f_2 + \ldots + f_{q-1} \leq 8\sqrt{k} + 1$.
(b) $|W_2 \cup N(W_2)| \leq (1 + o(1))\frac{n}{\sqrt{k}} = (1 + o(1))\sqrt{nd}$.
(c) $|W \cup N(W)| \leq (9 + o(1))\frac{n}{\sqrt{k}} = (17 + o(1))\sqrt{nd}$.
(d) $|W \cup N(W)| \leq 4(d+1)^2 \log_{d+1} n$.

Proof. (a) In the first inequality the term 1 accounts for x_q, while the summand f_i is at least as large as the number of unlabeled neighbors of x_i. Hence the first inequality follows. Consider now the second inequality. Let $X = \{i \leq q-1 : x_i \in M_1\}$ and $Y = \{i \leq q-1 : x_i \in M_2\}$. By our choice of q, $d_i \leq \lfloor\sqrt{k}\rfloor - 1$ for each $1 \leq i \leq q-1$ and $\prod_{i=1}^{q-1} f_i \leq k$. Hence for each $i \in X$, $2 \leq f_i \leq \sqrt{k}$ and $\prod_{i \in X} f_i \leq k$. By Lemma 4.4, with $D = \sqrt{k}$ and $N = k$, we have $\sum_{i \in X} f_i \leq 2\sqrt{k}\log_{\sqrt{k}} k = 4\sqrt{k}$. Now since $|Y| \leq |X| + 1$, by Lemma 4.1(d) and $f_i = 1$ for $i \in Y$, we get $\sum_{i \in Y} f_i = |Y| \leq 4\sqrt{k} + 1$. It follows that $\sum_{i=1}^{q-1} f_i \leq 8\sqrt{k} + 1$, proving (a).

(b) We consider cases, based on the defining property of q.
Case 1: $q = p$.
Since $|W_2| = 0$ in this case, (b) follows trivially.

Case 2: $d_q \geq \sqrt{k}$.
Recalling again that the branches of x_q are labeled in nondecreasing order of size and that the branch $T_{x_q^+}$ contains mixed vertices (e.g., x_{q+1}), we find as before that $|T_{x_q^+}| \leq |T_y|$ for any unlabeled child y of x_q. As there are d_q unlabeled such children, we get

$$n \geq (d_q + 1) \cdot |T_{x_q^+}| \geq (\lfloor\sqrt{k}\rfloor + 1) \cdot |T_{x_q^+}| \geq \sqrt{k} \cdot |T_{x_q^+}|.$$

Since all but at most one vertex of $W_2 \cup N(W_2)$ are contained in $T_{x_q^+}$, this vertex being x_q in case $x_{q+1} = x_q^+$, we have $|W_2 \cup N(W_2)| \leq |T_{x_q^+}| + 1 \leq \frac{n}{\sqrt{k}} + 1$ and the claim follows.

Case 3: $\prod_{i=1}^{q} f_i \geq k$. Applying Lemma 4.3 (b) we get $n \geq (|W_2 \cup N(W_2)| - 1) \prod_{i=1}^{q} f_i \geq k(|W_2 \cup N(W_2)| - 1)$. Thus $|W_2 \cup N(W_2)| \leq 1 + \frac{n}{k} \leq (1 + o(1)) \frac{n}{\sqrt{k}}$, as required.

(c) Applying (a) and (b) of this lemma, we have $|W \cup N(W)| \leq |W_1 \cup N(W_1)| + |W_2 \cup N(W_2)| \leq |W_1| + d|W_1| + (1 + o(1)) \frac{n}{\sqrt{k}} \leq 8\sqrt{k} + 1 + \frac{n}{k}(8\sqrt{k} + 1) + (1 + o(1)) \frac{n}{\sqrt{k}} \leq (17 + o(1)) \frac{n}{\sqrt{k}}$.

(d) By Lemma 4.5, $|W| \leq 4(d+1) \log_{d+1} n$. Thus, we have $|N(W) \cup W| \leq (d+1)|W| \leq 4(d+1)^2 \log_{d+1} n$. ■

Lemma 4.6 and Lemma 4.2 together imply our main result below.

Theorem 4.7 *Let T be an n-vertex tree with maximum degree d, where $1 \leq d \leq \frac{n}{4}$. We have*
(a) $s(T) \geq \frac{n}{2} - (17 + o(1))(\sqrt{nd}) = \frac{n}{2} - \Omega(\sqrt{nd})$, and
(b) $s(T) \geq \frac{n}{2} - 4(d+1)^2 \log_{d+1} n = \frac{n}{2} - \Omega(d^2 \log_d n)$.

5 Extremal tree constructions with maximum degree d

In this section we show that the lower bounds of Theorem 4.7 are best possible, up to constant factors in the $\Omega(\sqrt{nd})$ and $\Omega(d^2 \log_d n)$ terms, for suitable ranges on the maximum degree d. Toward that goal, we construct trees T with $\varphi(T) = \Omega(\sqrt{nd})$ or $\Omega(d^2 \log_d n)$. Using Theorem 3.2, we then get upper bounds for $s(T)$ which asymptotically match the lower bounds of Theorem 4.7. Since we are only interested in asymptotics, we will be very generous with constant factors. We start with a lemma that will be useful when we analyze discrepancy.

Lemma 5.1 *Let T be a rooted tree. Let F be a subgraph of T and v a vertex in F. Let $F_1, F_2, \ldots, F_p$ be the components of $F - v$ that contain a child of v in T. Then $\mu(F) - \mu(F - v) \leq 1 + \sum_{i=1}^{p} 2\mu(F_i)$. Also, $\mu(F) - \mu(F - v) \leq 2|V(T_v)|$, where T_v is the subtree of T rooted at v.*

Proof. Each F_i, being a tree, has a unique bipartition. Take a bipartition (A, B) of $F - v$ with discrepancy $\mu(F - v)$ and color vertices in A red and vertices in B blue. If the parent of v is in F we may assume that it is colored blue. Now, color v red. Note that $(A \cup v, B)$ may not be a bipartition of F since v may have red neighbors (which can only be children of v). To amend this, we switch red vertices with blue vertices in each F_i that contains a red neighbor of v; such a switch changes the overall #red vertices − #blue vertices count in such an F_i by at most $2\mu(F_i)$. The final red and blue sets form a bipartition of F with discrepancy at most $\mu(F - v) + 1 + \sum_{i=1}^{p} 2\mu(F_i)$.

For the second statement, note that $1 + \sum_{i=1}^{p} 2\mu(F_i) \leq 2|V(T_v)|$. ■

The next lemma will be used to extend constructions that work only for specific values of n and d to all values of n, and d in a certain range in term of n.

Lemma 5.2 *Let T^* be a tree and T a tree obtained from T^* by attaching a path P to T^* at a vertex $v \in V(T^*)$. Then $\varphi(T) \geq \varphi(T^*) - \frac{1}{2}$.*

Proof. Let W be an independent set of T with $\varphi(W) = \varphi(T)$, where $\varphi(W)$ is defined relative to T. Let $W_1 = W \cap V(T^*)$ and $W_2 = W \cap (V(P - v))$. Then W_1 and W_2 partition W. Observe that in any bipartition (A, B) of $P - v - W_2$, we have $||A| - |B|| \leq |W_2| + 1$. Hence, $\mu(T - W) \geq \mu(T^* - W_1) - |W_2| - 1$. Now, we have

$$\begin{aligned} \varphi(T) &= \varphi(W) = \frac{1}{2}\mu(T - W) + \frac{1}{2}|W| + |N_T(W)| \geq \frac{1}{2}[\mu(T^* - W_1) - |W_2| - 1] \\ &+ \frac{1}{2}(|W_1| + |W_2|) + |N_T(W)| = \frac{1}{2}\mu(T^* - W_1) + \frac{1}{2}|W_1| + |N_T(W)| - \frac{1}{2} \\ &\geq \frac{1}{2}\mu(T^* - W_1) + \frac{1}{2}|W_1| + |N_{T^*}(W_1)| - \frac{1}{2} \geq \varphi(T^*) - \frac{1}{2}. \end{aligned}$$

■

Now, we are ready for our constructions. We will first construct trees for specific n and d. Then we will use Lemma 5.2 to extend our constructions. We need some further notation. Let T be a tree with root r. For each integer $i \geq 0$, let L_i denote the set of vertices at distance i from r. Given a list of positive integers $d_1, d_2, \ldots, d_h$. Let $T(d_1, d_2, \ldots, d_h)$ be the $(h+1)$-level tree rooted at r in which for each $i = 1, \ldots, h$ each vertex in L_{i-1} has d_i children in L_i. When $d_1 = d_2 = \cdots = d_h = d$, we use T_h^d to denote $T(d_1, \ldots, d_h)$, commonly known as a *symmetric d-ary tree of height h*. Let $n = |V(T_h^d)|$. Note that $\mu(T_h^d) = n(1 - \frac{2}{d+1})$ when h is odd and $\mu(T_h^d) = (n-1)(1 - \frac{2}{d+1}) + 1$ when h is even. So, always $n(1 - \frac{2}{d+1}) \leq \mu(T_h^d) \leq n(1 - \frac{2}{d+1}) + 1$.

The following lemma, in combination with Theorem 3.3, will be used to show that the lower bound in Theorem 4.7(a) is best possible, up to the constant factor implied in the $\Omega(\sqrt{nd})$ term, when d is in the range $n^{\frac{1}{3}} \leq d \leq \frac{n}{3}$.

Lemma 5.3 *Let $m, d \geq 3$ be odd positive integers. Let $T = T(m, d, m)$.*
(a) Let W be an independent set in T. If $\mu(T - W) \leq \frac{1}{3}md$, then $|W \bigcup N(W)| \geq \frac{1}{6}md$.
(b) $\varphi(T) \geq \frac{1}{12}md$.

Proof. (a) Let r denote the root. Suppose the vertices of W are $x_1, \ldots, x_p$ in nondecreasing order of level. Initially let $F = T$. Then we remove $x_1, \ldots, x_p$ in order from F; updating F and $\mu(F)$ at each step. We consider two cases.

Case 1: $x_1 = r$.

Note that after one step, $F = T - x_1 = T - r$, which consists of m copies of $T(d, m)$. Since m is odd, $\mu(F) = \mu(T(d, m)) = md + 1 - d \geq \frac{2}{3}md$. Since W is independent, the other vertices in $W - x_1$ lie in $L_2 \cup L_3$. Suppose W has a vertices in L_2 and b vertices in L_3. When we remove a vertex x_i in $W \cap L_2$, by Lemma 5.1, we can decrease $\mu(F)$ by at most $2m + 1$. When we remove a vertex x_i in $W \cap L_3$, we can decrease $\mu(F)$ by at most one. Since $\mu(T - x_1) \geq \frac{2}{3}md$ while $\mu(T - W) \leq \frac{1}{3}md$, we must have $(2m + 1)a + b \geq \frac{2}{3}md - \frac{1}{3}md = \frac{1}{3}md$. Now, we have $|W \cup N(W)| = (m + 2)a + 2b \geq \frac{1}{6}md$.

Case 2: $x_1 \neq r$.

If $|W \cap L_1| \geq \frac{1}{3}m$ then already $|W \cap N(W)| \geq \frac{1}{3}md \geq \frac{1}{6}md$ and we are done. So suppose otherwise. For each $x_i \in W \cap L_1$ the removal of x_i decreases $\mu(F)$ by at most $2\mu(T(d,m)) \leq 2md$. Note however that $\mu(T) = m + m^2 d - 1 - md$. Hence, $\mu(T - W \cap L_1) \geq m^2 d + m - 1 - md - (\frac{1}{3}m)2md > \frac{2}{3}md$ (with a lot of room to spare). As in Case 1 (with $T - W \cap L_1$ playing the role of $F = T - x_1$), the contribution to $|W \cup N(W)|$ from vertices in $W \cap (L_2 \cup L_3)$ must be at least $\frac{1}{6}md$.

(b) It suffices to prove that for each independent set W, $\varphi(W) \geq \frac{1}{12}md$. If $\mu(T - W) \geq \frac{1}{3}md$, then certainly $\varphi(W) \geq \frac{1}{2}\mu(T - W) \geq \frac{1}{6}md \geq \frac{1}{12}md$. So, suppose $\mu(T - W) \leq \frac{1}{3}md$. Then by part (a), we have $|W| + |N(W)| \geq \frac{1}{6}md$. So, $\varphi(W) \geq \frac{1}{2}|W| + |N(W)| \geq \frac{1}{12}md$. ■

Proposition 5.4 *Let $n \geq 48$ be an integer. Let $d \geq 4$ be an integer such that $n^{\frac{1}{3}} < d \leq \frac{1}{12}n$. There exists a tree on n vertices with maximum degree d such that $s(T) \leq \frac{n}{2} - c\sqrt{nd}$ for some absolute constant c.*

Proof. First assume d is even so that $d-1$ is odd. Let m be the largest odd integer such that $M = 1 + m + m(d-1) + m^2(d-1) \leq n$. It is easy to check since $d > n^{\frac{1}{3}}$ that $m \leq d-1$. Also, $m > \frac{1}{2}\sqrt{\frac{n}{d}}$, and since $d \leq \frac{n}{12}$ we have $m \geq 3$. Let T be obtained from $T^* = T(m, d-1, m)$ by attaching a path P of length $n - M$ to a leaf of T^*. Note that T^* has M vertices while T has n vertices and max degree d.

By Lemma 5.2 and Lemma 5.3, $\varphi(T) \geq \varphi(T^*) - \frac{1}{2} \geq \frac{1}{12}md - \frac{1}{2} \geq \frac{1}{24}\sqrt{nd} - \frac{1}{2}$. By Theorem 3.3, $s(T) \leq \frac{1}{2}n - \frac{1}{120}\sqrt{nd} + \frac{5}{2}$.

If d is odd, we let $T^* = T(m, d-2, m)$, where m is the largest odd integer such that $|V(T(m, d-2, m)| < n$. We obtain T by attaching path of length $n - |V(T^*)|$ to T^* at a vertex of degree $d-1$. ■

The next lemma and the proposition following it will show that the lower bound in Theorem 4.7(b) is best possible, up to the constant factor implied in the $\Omega(d^2 \log_d n)$ term, when d is in the range $n^q \leq d \leq n^{1/3}$, where $q > 0$ is any fixed constant.

Lemma 5.5 *Let $d \geq 3$ be an odd integer. Let T be a symmetric d-ary tree of height $h \geq 3$ and order $n = |V(T)|$.*

(a) Let W be an independent set in T. If $\mu(T - W) \leq \frac{1}{6d}n$, then $|W \cup N(W)| \geq \frac{1}{12}d^2$.

(b) $\varphi(T) \geq \frac{1}{24}d^2$.

Proof. (a) Clearly, it suffices to prove that $|W| \geq \frac{d}{12}$. Let r denote the root of T. Suppose first that $r \in W$. Note that $T - r$ consists of d copies of T^d_{h-1}, each of which has the same discrepancy $\mu(T^d_{h-1}) \geq \frac{n-1}{d}(1 - \frac{2}{d+1}) \geq \frac{n}{3d}$. Since there are an odd number of these copies, we get $\mu(T - r) = \mu(T^d_{h-1}) \geq \frac{n}{3d}$. Since W is an independent set, if $x \in W - r$, then $x \in L_j$ for some $j \geq 2$. By Lemma 5.1, for any subgraph F of T containing x, since $|V(T_x)| \leq \frac{n}{d^2}$, we have $\mu(F - x) \geq \mu(F) - \frac{2n}{d^2}$. Since $\mu(T - r) \geq \frac{n}{3d}$ while $\mu(T - W) \leq \frac{n}{6d}$, there must be at least $\frac{d}{12}$ such x's. So $|W| \geq \frac{d}{12}$.

Suppose instead that $r \notin W$. Then for each $x \in W$, $x \in L_j$ for some $j \geq 1$. By Lemma 5.1, for any subgraph F of T that contains x, we have $\mu(F - x) \geq \mu(F) - \frac{2n}{d}$. Since $\mu(T) \geq (1 - \frac{2}{d+1})n$ while $\mu(T - W) \leq \frac{n}{6d}$, we must have $|W| \geq [(1 - \frac{2}{d+1})n - \frac{n}{6d}]/\frac{2n}{d} \geq \frac{d}{12}$.

(b) It suffices to prove that $\varphi(W) \geq \frac{d^2}{24}$ for each independent set W of T. Note that since $h \geq 3$, we have $n \geq d^3$. If $\mu(T - W) \geq \frac{n}{6d}$, then $\varphi(W) \geq \frac{1}{2}\mu(T - W) \geq \frac{n}{12d} \geq \frac{d^2}{24}$. Otherwise, $\mu(T - W) \leq \frac{n}{6d}$. By (a), $|W| + |N(W)| \geq \frac{d^2}{12}$. Hence, $\varphi(W) \geq \frac{1}{2}|W| + |N(W)| \geq \frac{d^2}{24}$. ■

Proposition 5.6 *Let $n \geq 64$ be an integer. Let $d \geq 4$ be an integer such that $n^q < d \leq n^{\frac{1}{3}}$, where $q < \frac{1}{3}$ is a fixed positive number. Then there exists a tree on n vertices with maximum degree d such that $s(T) \leq \frac{n}{2} - c'd^2 \log_d n$ for some absolute constant c'.*

Proof. First assume d is even so that $d - 1$ is odd. Let h be the largest integer such that $D = 1 + (d-1) + (d-1)^2 + \cdots + (d-1)^h \leq n$. It is easy to check that $h \geq \lfloor \log_d n \rfloor$. Since $d \leq n^{\frac{1}{3}}$, this yields $h \geq 3$. Let $T^* = T_h^{d-1}$ and T be obtained from T^* by attaching a path P of length $n - D$ to a leaf of T^*. Then T is an n-vertex tree with maximum degree d.

By Lemma 5.2 and Lemma 5.5, $\varphi(T) \geq \frac{1}{16}d^2 - \frac{1}{2}$. Thus, by Theorem 3.3 we have $s(T) \leq \frac{1}{2}n - \frac{1}{80}d^2 + \frac{21}{10}$. Since $\log_d n \leq \frac{1}{q}$, we have $s(T) \leq \frac{n}{2} - (\frac{q}{80})d^2 \log_d n + \frac{21}{10}$.

If d is odd, we let h be the largest integer such that $|V(T_h^{d-2})| < n$. Let $T^* = T_h^{d-2}$. We obtain T by adding a path of length $n - |V(T^*)|$ to T^* at a vertex of degree $d - 1$. ■

Next, we show that Theorem 4.7(b) is best possible, up to the constant factor implied in the $\Omega(d^2 \log_d n)$ term, when d is an absolute constant. In what follows, $n(H)$ denotes the number of vertices in H.

Lemma 5.7 *Let $d \geq 3$ be an odd integer. Let T be a symmetric d-ary tree of height $h \geq 3$ and order $n = |V(T)|$.*

(a) Let W be an independent set of T. If $\mu(T - W) \leq \frac{1}{2}\sqrt{n}$, then $|W| \geq \lfloor \frac{h}{2} \rfloor \geq \frac{1}{2}\log_d n - 1$.

(b) $\varphi(T) \geq \frac{1}{4}d(h-1) \geq \frac{1}{4}d(\log_d n - 2)$.

Proof. (a) Let $\beta = 1 - \frac{2}{d+1}$. For any $p \geq 1$, by earlier discussions, we have $\beta \cdot n(T_p^d) \leq \mu(T_p^d) \leq \beta \cdot n(T_p^d) + 1$. Let r denote the root of T. Suppose the vertices of W are $x_1, x_2, \ldots, x_p$ in nondecreasing order of level. We use induction to prove for each $i = 1, \ldots, \lfloor \frac{h}{2} \rfloor - 1$ that $\mu(T - \{x_1, \ldots, x_i\}) \geq \frac{\beta n}{d^i} - 2d^i - 1$.

For the basis step, let $i = 1$. If $x_1 = r$, then $T - x_1$ consists of d copies of T_{h-1}^d each having discrepancy $\mu(T_{h-1}^d) \geq \beta \cdot n(T_{h-1}^d) = \beta\frac{n-1}{d}$. Since d is odd, we have $\mu(T - x_1) = \mu(T_{h-1}^d) \geq \beta(\frac{n-1}{d}) = \frac{\beta n}{d} - \frac{\beta}{d} \geq \frac{\beta n}{d} - 2d - 1$. So the claim holds. If $x_1 \neq r$, then $x_1 \in L_j$ for some $j \geq 1$. Each of the d subtrees under x_1 has discrepancy at most $\beta\frac{n}{d^{j+1}} + 1 \leq \beta\frac{n}{d^2} + 1$. By Lemma 5.1, $\mu(T - x_1) \geq \mu(T) - 2d(\beta\frac{n}{d^2} + 1) - 1$. Also, $\mu(T) \geq \beta n$. Thus, we have $\mu(T - x_1) \geq \beta n - 2d(\beta\frac{n}{d^2} + 1) - 1 \geq (1 - \frac{2}{d})\beta n - 2d - 1 \geq \frac{\beta n}{d} - (2d + 1)$, since $d \geq 3$. So the claim holds.

For the induction step, let $i > 1$. Suppose first that $x_i \in L_0 \cup L_1 \ldots \cup L_{i-1}$. Note that $T' = T - L_0 \cup L_1 \cup \ldots \cup L_{i-1}$ consists of d^i copies of T_{h-i}^d each with the same discrepancy

$\mu(T^d_{h-i})$. Since d is odd, we have $\mu(T') = \mu(T^d_{h-i})$. Note that $n(T^d_{h-i}) \geq \frac{n-2d^{i-1}}{d^i} \geq \frac{n}{d^i} - 1$. Hence, $\mu(T') = \mu(T^d_{h-i}) \geq \beta \cdot n(T^d_{h-i}) \geq \beta(\frac{n}{d^i} - 1) \geq \frac{\beta n}{d^i} - 1$. Note that $T - \{x_1, \ldots, x_i\}$ can be obtained from T' by adding at most $|L_0 \cup L_1 \cup \ldots \cup L_{i-1}| \leq 2d^{i-1}$ vertices. It follows that $\mu(T - \{x_1, \ldots, x_i\}) \geq \beta n - 1 - 2d^{i-1} \geq \beta n - 2d^i - 1$. So the claim holds.

Suppose next that $x_i \notin L_0 \cup L_1 \cup \ldots \cup L_{i-1}$. Then $x_i \in L_j$ for some $j \geq i$. In this case, each branch below x_i has discrepancy at most $\beta\frac{n}{d^{j+1}} + 1 \leq \beta\frac{n}{d^{i+1}} + 1$. By Lemma 5.1, for any subgraph F of G containing x_i, we have $\mu(F - x_i) \geq \mu(F) - [2d(\beta\frac{n}{d^{i+1}} + 1) + 1] = \mu(F) - \frac{2\beta n}{d^i} - 2d - 1$. By induction hypothesis, $\mu(T - \{x_1, \ldots, x_{i-1}\}) \geq \frac{\beta n}{d^{i-1}} - 2d^{i-1} - 1$. So $\mu(T - \{x_1, \ldots, x_i\}) \geq (\frac{\beta n}{d^{i-1}} - 2d^{i-1} - 1) - \frac{2\beta n}{d^i} - 2d - 1 \geq \frac{\beta n}{d^i} - 2d^i - 1$. This completes the induction step, so the claim holds.

Note that $\beta = 1 - \frac{2}{d+1} \geq \frac{1}{2}$ and $n \geq 9$ since $h \geq 3$. We have for each $i \leq \lfloor \frac{h}{2} \rfloor - 1$, $\mu(T - \{x_1, \ldots, x_i\}) \geq \frac{\beta n}{d^i} - 2d^i - 1 \geq \frac{n}{2d^i} - \sqrt{n} \geq \frac{n}{2\sqrt{n/d}} - \sqrt{n} \geq \frac{1}{2}\sqrt{n}$. Since $\mu(T - W) < \frac{1}{2}\sqrt{n}$, we must have $|W| \geq \lfloor \frac{h}{2} \rfloor \geq \frac{1}{2}\log_d n - 1$.

(b) Let W be any independent set of T. If $\mu(T - W) \geq \frac{1}{2}\sqrt{n}$, then $\varphi(W) \geq \frac{1}{2}\mu(T - W) \geq \frac{1}{4}\sqrt{n} \geq \frac{1}{4}d^{\frac{h}{2}} \geq \frac{1}{4}d(3)^{\frac{h}{2}-1} \geq \frac{1}{4}dh \geq \frac{1}{4}d(\log_d n - 1)$. If $\mu(T - W) < \frac{1}{2}\sqrt{n}$, then by (a), $|W| + |N(W)| \geq d\lfloor \frac{h}{2} \rfloor \geq \frac{1}{2}d(h-1)$. Hence $\varphi(W) \geq \frac{1}{2}|W| + |N(W)| \geq \frac{1}{4}d(h-1)$. Since this holds for all W, $\varphi(T) \geq \frac{1}{4}d(h-1) \geq \frac{1}{4}d(\log_d n - 2)$. ∎

Proposition 5.8 *Let $d \geq 4$ be a fixed positive integer. Let $n \geq 1 + (d-1) + (d-1)^2 + (d-1)^3$ be an integer. There exists a tree on n vertices with maximum degree d such that $s(T) \leq \frac{n}{2} - c''d\log_d n$, for some absolute constant c''.*

Proof. First assume d is even so that $d-1$ is odd. Let h be the largest integer such that $D = 1 + (d-1) + (d-1)^2 + \cdots + (d-1)^h \leq n$. Note that $h \geq \lfloor \log_d n \rfloor \geq \log_d n - 1$. Let T^* be the complete $(d-1)$-ary tree of height h and let T be obtained from T^* by attaching path P of length $n - D$ to a leaf of T^*. Then T has n vertices and maximum degree d. Then by Lemma 5.2 and Lemma 5.7, we have $\varphi(T) \geq \varphi(T^*) - \frac{1}{2} \geq \frac{1}{4}d(h-1) - \frac{1}{2} \geq \frac{1}{4}d(\log_d n - 2) - \frac{1}{2}$. By Theorem 3.3, $s(T) \leq \frac{1}{2}n + \frac{21}{10} + \frac{d}{10} - \frac{1}{20}d\log_d n$.

If d is odd, let h be the largest integer such that $|V(T^{d-2}_h)| < n$. Let $T^* = T^{d-2}_h$. We obtain T by adding a path of length $n - |V(T^*)|$ to T^* at a vertex of degree $d-1$. ∎

We summarize our results below.

Proposition 5.9 *Let n be an integer tending to infinity. Let $d \geq 4$ be an integer. Let $g(n,d) = \min\{s(T) : T$ is a tree with n vertices and maximum degree $d\}$. There exist absolute constants $c_1, c_2, c_3, c_4, c_5, c_6$ such that*

(a) If $n^{\frac{1}{3}} < d \leq \frac{n}{12}$, then $\frac{n}{2} - c_1\sqrt{nd} \leq g(n,d) \leq \frac{n}{2} - c_2\sqrt{nd}$.

(b) If $n^q \leq d \leq n^{\frac{1}{3}}$, where $0 < q < \frac{1}{3}$ is fixed, then $\frac{n}{2} - c_3d^2\log_d n \leq g(n,d) \leq \frac{n}{2} - c_4d^2\log_d n$.

(c) If $d \geq 4$ is an absolute constant, then $\frac{n}{2} - c_5\log_d n \leq g(n,d) \leq \frac{n}{2} - c_6\log_d n$.

Finally, we focus on the symmetric d-ary tree T^d_h. By Proposition 5.5 and Proposition 5.7 $\varphi(T^d_h) \geq \frac{1}{24}d^2$ and $\varphi(T^d_h) \geq \frac{1}{4}d(h-1) \geq \frac{1}{8}dh$. Thus, in particular, we have $\varphi(T^d_h) \geq \frac{1}{48}(d^2 + dh)$.

By Theorem 3.3, we have $s(T_h^d) \leq \frac{n}{2}+2-\frac{1}{240}(d^2+dh)$. We show next that this is asymptotically tight. Our bounds improve the estimates $\frac{n}{2} - O(d^2h) \leq s(T_h^d) \leq \frac{n}{2} - O(h)$ obtained in [1].

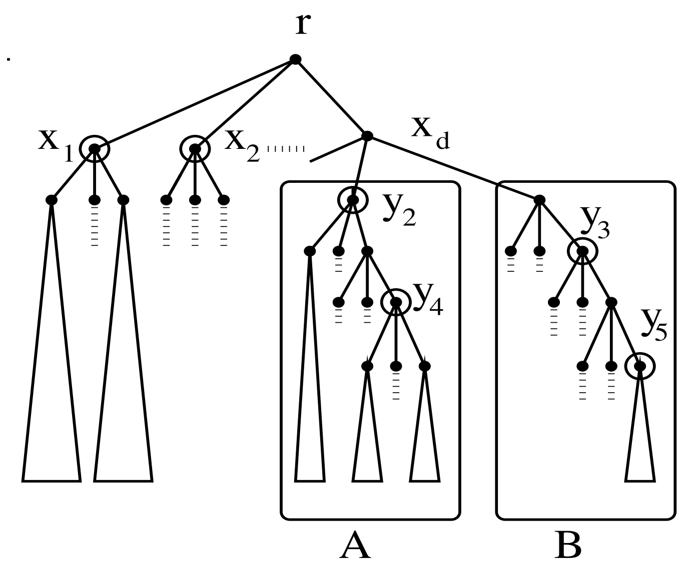


Figure 2: The symmetric d-ary tree of height h.

Proposition 5.10 *For all integers $h \geq 3$ and odd integers $d \geq 3$, we have*

$$\frac{n}{2} - 3(d^2+dh) \leq s(T_h^d) \leq \frac{n}{2} + 2 - \frac{1}{240}(d^2+dh).$$

Proof. It remains to prove the lower bound. By Theorem 3.2, it suffices to find an independent set S with $\varphi(S) \leq 3(d^2+dh)$. We draw $T = T_h^d$ in the plane in the natural noncrossing fashion where the root r is at the top. Let $x_1, \ldots, x_d$ denote r's children from left to right. As before, for each i, let L_i be the set of vertices in T at distance i from r. Let (X, Y) denote the unique bipartition of T, where $|Y| \geq |X|$. Observe that Y contains L_h, the set of leaves of T.

Suppose $d = 2k+1$. Let $S_0 = \{x_1, \ldots, x_{k+1}\}$. Note that there are d^2 copies of T_{h-2}^d rooted in L_2. After the deletion of S_0, $(k+1)d = \frac{d(d+1)}{2}$ of these become components by themselves. If we flip the first (from the left) $\frac{d^2-1}{2}$ of these T_{h-2}^d-components (interchanging X-vertices with Y-vertices in them), we obtain a bipartition (X', Y') of $T - S_0$ with $\mu(T_{h-2}^d) - d - 1 \leq \mu(T - S_0) = |Y'| - |X'| \leq \mu(T_{h-2}^d) + d + 1$.

Now, there are d branches under x_d, each being a copy of T_{h-2}^d. Let A and B denote two of these branches. Note that the roots of A and B are in L_2. Let P be a path of length $h-2$ in A that starts at A's root and moves down the levels such that each vertex is the rightmost child of the previous vertex. Define the path Q similarly for B. Let y_2 be the root of A, which is the only element in $V(P) \cap L_2$. Let y_3 be the only vertex in $V(Q) \cap L_3$. Let y_4 be the only vertex in $V(P) \cap L_4$. Let y_5 be the only vertex in $V(Q) \cap L_5$. We continue like this, alternating between P and Q as we move from one level to the next, obtaining $y_2, \ldots, y_{h-1}$ in that order. Here, we start our indices at 2 to be consistent with the level number and we stop at level $h-1$. Note that the subtree rooted at any y_i is a copy of T_{h-i}^d (See Figure 2).

Sequentially, delete $y_2, \ldots, y_{h-1}$, increasing $|Y'| - |X'|$ by at most $h-2$. When we delete y_i, the copy of T^d_{h-i} rooted at y_i breaks into d copies of T^d_{h-i-1}, at which point we flip the first $\frac{d-1}{2}$ of these copies, interchanging X'-vertices with Y'-vertices. Such a flip reduces $|Y'| - |X'|$ by $\frac{d-1}{2} \cdot 2\mu(T^d_{h-i-1}) = (d-1)\mu(T^d_{h-1-i})$.

Hence, after doing the flipping for each $i = 2, \ldots, h-1$, $|Y'| - |X'|$ is further reduced by $p = \sum_{i=2}^{h-1}(d-1)\mu(T^d_{h-1-i})$. Recall that $(1-\frac{2}{d+1})n(T^d_q) \leq \mu(T^d_q) \leq (1-\frac{2}{d+1})n(T^d_q) + 1$. Also, $n(T^d_q) = 1 + d + d^2 + \cdots + d^q = \frac{d^{q+1}-1}{d-1}$. So, $\mu(T^d_q) = (1-\frac{2}{d+1})\frac{d^{q+1}-1}{d-1} + \epsilon_q$, for some $0 \leq \epsilon_q \leq 1$. Hence, $p = \sum_{i=2}^{h-1}(d-1)\mu(T^d_{h-1-i}) = \sum_{i=2}^{h-1}(d-1)[(1-\frac{2}{d+1})\frac{d^{h-i}-1}{d-1} + \epsilon_{h-1-i}] = (1-\frac{2}{d+1})(n(T^d_{h-2})-1) - (1-\frac{2}{d+1})(h-2) + (d-1)\sum_{i=2}^{h-1}\epsilon_{h-1-i}$. Since $\mu(T^d_{h-2})$ is within 1 from $(1-\frac{2}{d+1})n(T^d_{h-2})$, it is easy to see that $|p - \mu(T^d_{h-2})| \leq dh$.

Recall that before removing y_i's, $\mu(T^d_{h-2}) - d - 1 \leq |Y'| - |X'| \leq \mu(T^d_{h-2}) + d + 1$, that the removals change $|Y'| - |X'|$ by at most $h-2$, and the flips reduce $|Y'| - |X'|$ by p. For the new X', Y', we have $||Y'| - |X'|| \leq d + 1 + h - 2 + dh \leq 2dh$. Let $S = S_0 \cup \{y_2, \ldots, y_{h-1}\}$. (In Figure 2, vertices in S are circled.) We have argued that $\mu(T - S) \leq 2dh$. Observe also that S is an independent set in T with $|S| \leq d + h$. We have $\varphi(S) = \frac{1}{2}|S| + \frac{1}{2}\mu(T-S) + |N(S)| \leq \frac{1}{2}(d+h) + \frac{1}{2} \cdot 2dh + d(d+h) \leq 3(d^2 + dh)$, completing the proof. ∎

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