# Bounding Mean Orders of Sub-k-Trees of k-Trees

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#### Abstract

For a k-tree T, we prove that the maximum local mean order is attained in a k-clique of degree 1 and that it is not more than twice the global mean order. We also bound the global mean order if T has no k-cliques of degree 2 and prove that for large order, the k-star attains the minimum global mean order. These results solve the remaining problems of Stephens and Oellermann [J. Graph Theory 88 (2018), 61–79] concerning the mean order of sub-k-trees of k-trees.

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## 1 Introduction

In [10] and [11] Jamison considered the mean number of nodes in subtrees of a given tree. He showed that for trees of order n, the average number of nodes in a subtree of T is at least (n + 2)/3, with this minimum achieved if and only if T is a path. He also showed that the average number of nodes in a subtree containing a root is at least (n + 1)/2 and always exceeds the average over all unrooted subtrees. The mean subtree order in trees was further investigated, e.g. in [3, 7, 14, 20, 22], as well as extensions to arbitrary graphs [1, 4–6] and the mean order of the connected induced subgraphs of a graph [8, 9, 17–19].

In [16], Stephens and Oellermann extended the study to k-trees and families of sub-k-trees. A k-tree is a generalization of a tree that has the following recursive construction.

**Definition 1** (k-tree). Let k be a fixed positive integer.

1. The complete graph  $K_k$  is a k-tree.

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- 2. If T is a k-tree, then so is the graph obtained from T by joining a new vertex to all vertices of some k-clique of T.
- 3. There are no other k-trees.

Note that for k = 1 we have the standard recursive construction of trees. A sub-k-tree of a k-tree T is a subgraph that is itself a k-tree. Let S(T) denote the collection of all sub-k-trees of T and let N(T) := |S(T)| be the number of sub-k-trees. We denote by  $R(T) = \sum_{X \in S(T)} |X|$  the total number of vertices in all sub-k-trees (where for a graph G the notation |G| is used throughout to mean the number of vertices in G). The global mean (sub-k-tree) order is

$$\mu(T) = \frac{R(T)}{N(T)}.$$

For an arbitrary k-clique C of T, let S(T; C) denote the collection of sub-k-trees containing C and let N(T; C) := |S(T; C)|. The local clique number is  $R(T; C) = \sum_{X \in S(T;C)} |X|$  and the local mean (sub-k-tree) order is

$$\mu(T;C) = \frac{R(T;C)}{N(T;C)}.$$

The degree of C is the number of (k+1)-cliques that contain C.

Stephens and Oellermann concluded their study of the mean order of sub-k-trees of k-trees with several open questions. Our main contribution here is to answer three of them.

It was conjectured by Jamison in [10] and proven by Vince and Wang in [20] that for trees of order n without vertices of degree 2—called *series-reduced* trees—the global mean subtree order is between  $\frac{n}{2}$  and  $\frac{3n}{4}$ . For k-trees we provide similar asymptotically sharp bounds, answering [16, Problem 6].

**Theorem 2.** For every k-tree T without k-cliques of degree 2, the global mean sub-k-tree order satisfies

$$\frac{n+k}{2} - o_n(1) < \mu(T) < \frac{3n+k-3}{4}.$$

These bounds are asymptotically sharp. In particular, for large k,  $\frac{3n}{4}$  is not an upper bound. For large n, the k-star is the unique extremal k-tree for the lower bound.

Wagner and Wang proved in [21] that the maximum local mean subtree order occurs at a leaf or a vertex of degree 2. We prove an analogous result for k-trees, answering [16, Problem 4]. In contrast to the result for trees, it turns out that for  $k \ge 2$ , the maximum can only occur at a k-clique of degree 1, unless T is a k-tree of order k + 2.

**Theorem 3.** Suppose that  $k \ge 2$ . For a k-tree T of order  $n \ne k+2$ , if a k-clique C maximizes  $\mu(T; C)$ , then C must be a k-clique of degree 1. For n = k+2, every k-clique C satisfies  $\mu(T; C) = k + 1$ .

Lastly, Jamison [10] conjectured that for a given tree T and any vertex v, the local mean order is at most twice the global mean order of all subtrees in T. Wagner and Wang [21] proved that this is true. Answering [16, Problem 2] affirmatively, we show

**Theorem 4.** The local mean order of the sub-k-trees containing a fixed k-clique C is less than twice the global mean order of all sub-k-trees of T.

### 1.1 Related Results

A total of six questions were posed in [16]. Problems 1 and 3 were solved by Luo and Xu [13]. Regarding the first problem, Jamison [10] showed that for any tree T and any vertex v of T, the local mean order of subtrees containing v is an upper bound on the global mean order of subtrees of T. Stephens and Oellermann asked about a generalization to k-trees, to which Luo and Xu showed:

**Theorem 5** ([13]). For any k-tree T of order n with a k-clique C, we have  $\mu(T; C) \ge \mu(T)$ with equality if and only if  $T \cong K_k$ .

For the third problem, it was shown in [10] that paths have the smallest global mean subtree order. For k-trees we have:

**Theorem 6** ([13]). For any k-tree T of order n, we have

$$\mu(T) \geqslant \frac{\binom{n-k+2}{3}}{\binom{n-k+1}{2} + (n-k)k + 1} + k$$

with equality if and only if T is a path-type k-tree.

Very recently, Li, Ma, Dong, and Jin [12] gave a partial proof of Theorem 3, showing that the maximum local mean order always occurs at a k-clique of degree 1 or 2, thus also solving [16, Problem 4]. They did this by combining the fact that the 1-characteristic trees of adjacent k-cliques can be obtained from each other by a partial Kelmans operation [12, Lem. 4.6], an inequality between local orders of neighboring vertices after performing a partial Kelmans operation [12, Thm. 3.3], as well as [16, Lem. 11] and [21, Thm. 3.2]. Theorem 3 also solves Problem 5.4 from [12], asking whether the maximum local mean order can ever occur at a k-clique of degree 2, but not at a k-clique of degree 1.

**Outline:** In Section 2, we go over definitions and notation. Theorems 2, 3, 4 are proven in Sections 3, 4, 5 respectively. We additionally address [16, Problem 5], which is a more general question asking what one can say about the local mean order of sub-k-trees containing a fixed r-clique for  $1 \leq r \leq k$ . We give a possible direction and partial results in the concluding section.

## 2 Notation and Definitions

The global mean sub-k-tree order  $\mu(T)$  and the local mean sub-k-tree order  $\mu(T; C)$  are defined in the introduction. The local mean order always counts the k vertices from C and it sometimes will be more convenient to work with the average number of additional vertices in a (uniform random) sub-k-tree of T containing C, in which case we use the notation  $\mu^{\bullet}(T; C) = \mu(T; C) - k$ . Moreover, the number of sub-k-trees not containing C

will be denoted by  $\overline{N}(T;C) = N(T) - N(T;C)$  and the total number of vertices in the sub-k-trees that do not contain C will be denoted by  $\overline{R}(T;C) = R(T) - R(T;C)$ .

A k-leaf or simplicial vertex is a vertex belonging to exactly one (k + 1)-clique of T, i.e., a vertex of degree k. A simplicial k-clique is a k-clique containing a k-leaf. Note that a k-clique of degree 1 is not necessarily simplicial. A major k-clique is a k-clique with degree at least 3. Two k-cliques are adjacent if they share a (k - 1)-clique.

The stem of a k-tree T is the k-tree obtained by deleting all k-leaves from T.

Subclasses of trees generalize to subclasses of k-trees. We will reference two in particular: paths generalize to *path-type k-trees* that are either isomorphic to  $K_k$  or  $K_{k+1}$  or have precisely two k-leaves. Note that for every  $n \ge k + 4$  and  $k \ge 2$ , there are multiple non-isomorphic path-type k-trees of order n.

A k-star is either  $K_k$  or  $K_{k+1}$ , or it is the unique k-tree with n - k simplicial vertices when  $n \ge k+2$ .

Furthermore, the combination of a k-star and a k-path is called a k-broom: take a k-path of a certain length and add some simplicial vertices to a simplicial k-clique of the k-path.



Figure 1: Examples of a 3-path, 3-star and 2-broom.

For a given k-clique C in T, it is often useful to decompose T into C and the sub-k-trees that result from deleting C. Let  $B_1, B_2, \ldots, B_d$  be the (k + 1)-cliques that contain C, and let  $v_i$  be the vertex of  $B_i \setminus C$ . Moreover, let  $C_{i,1}, \ldots, C_{i,k}$  be the k-subcliques of  $B_i$ other than C. The k-tree T can be *decomposed* into C and k-trees  $T_{1,1}, \ldots, T_{d,k}$ , rooted at  $C_{1,1}, \ldots, C_{d,k}$  respectively, that are pairwise disjoint except for the vertices of the cliques  $C_{i,j}$ .

In a 1-tree, any two vertices are connected by a unique path. This fact generalizes to k-trees through the construction of the 1-characteristic tree of a k-tree T [13,16]. For a k-clique C in T, a perfect elimination ordering of T to C is an ordering  $v_1, v_2, \ldots, v_{n-k}$  of its vertices other than  $V(C) = \{c_1, \ldots, c_k\}$  such that each vertex  $v_i$  is simplicial in the k-tree spanned by C and  $v_j, 1 \leq j \leq i$ . In [16] it is shown that for any  $v \notin C$ , there is a unique sequence of vertices that along with C induce a path-type k-tree P(C, v) and that form a perfect elimination ordering of P(C, v) to C. It is also proven that T can be written as  $\bigcup P(C, v)$  where the union is taken over all k-leaves  $v \in V$ . Each k-tree P(C, v) has an associated 1-tree P'(C, v) where the vertices consist of a single vertex representing the entire clique C, along with the remaining non-C vertices of P(C, v). The edges are consecutive pairs from the perfect elimination ordering. Taking  $\bigcup P'(C, v)$  over all k-leaves v gives us what is called the 1-characteristic tree of T, which we will denote  $T'_C$ . See Figure 2 for an example.



Figure 2: A 2-tree (left) with 2-clique  $C = \{c_1, c_2\}$  and the 1-characteristic tree (right).



Figure 3: Series-reduced trees with minimum mean subtree order for  $6 \leq n \leq 10$ .

## 3 Excluding *k*-cliques of degree 2

In this section, we prove

**Theorem 2.** For every k-tree T without k-cliques of degree 2, the global mean sub-k-tree order satisfies

$$\frac{n+k}{2} - o_n(1) < \mu(T) < \frac{3n+k-3}{4}.$$

These bounds are asymptotically sharp. In particular, for large k,  $\frac{3n}{4}$  is not an upper bound. For large n, the k-star is the unique extremal k-tree for the lower bound.

## 3.1 The lower bound

Among series-reduced trees of order n, for  $4 \leq n \leq 8$  the star attains the maximum mean subtree order, but for  $n \geq 11$  it attains the minimum mean subtree order. It can be derived from [7, Lem. 12] and an adapted version of [7, Cor. 11] (with 2 replaced by any  $\varepsilon > 0$ , at the cost of replacing 30 by  $n_{\varepsilon}$ ) that this is indeed the case for n sufficiently large.<sup>1</sup> In [2], it is shown that for  $6 \leq n \leq 10$ , the series-reduced trees attaining the minimum mean subtree order are those presented in Figure 3, and for  $n \geq 11$ ,  $S_n$  is always the unique extremal graph.

In this subsection, we will prove that the above extremal statement generalizes to k-trees without a k-clique of degree 2.

First, we prove the following lemma, which states that every k-tree contains a (k+1)-clique C that plays the role of a centroid in a tree (a vertex or edge whose removal splits the tree into components of size at most  $\frac{n}{2}$ ). Figure 4 is an example of a 2-tree demonstrating why we must take a (k + 1)-clique and not a k-clique.

**Lemma 7.** Any k-tree T (of order  $n \ge k+1$ ) has a (k+1)-clique C such that the order of all components of  $T \setminus C$  is at most  $\left\lceil \frac{n-(k+1)}{2} \right\rceil$ .

<sup>&</sup>lt;sup>1</sup>We thank John Haslegrave for this remark.

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Figure 4: 2-tree with a centroid 3-clique but no centroid 2-clique.

Proof. Suppose for contradiction that such a (k + 1)-clique does not exist. Consider the (k + 1)-clique C for which the largest component of  $T \setminus C$  has minimum order over all choices of C. By assumption, the largest component of  $T \setminus C$  has order  $n_0 > \left\lceil \frac{n - (k+1)}{2} \right\rceil$ , and by the construction of a k-tree, there exist vertices  $u \in C$  and v in the largest component  $T_0$  of  $T \setminus C$  such that u has no neighbor in  $T_0$  and  $v \cup (C \setminus u)$  forms a (k + 1)-clique C'. Now  $T \setminus C'$  has components whose sizes are bounded by max  $\{n - n_0 - k, n_0 - 1\} < n_0$ , which gives a contradiction. Hence C satisfies the stated property.

The following lemma and its proof are similar to [15, Lemma 5.1].

**Lemma 8.** For any k-tree T without k-cliques of degree 2, there is a k-clique C' for which  $\mu(T;C') - \mu(T) \leq \frac{n^3}{2^{(n-k)/4+1}} = o_n(1).$ 

*Proof.* Take C as in Lemma 7. Let its vertices be  $\{u_1, u_2, \ldots, u_{k+1}\}$ .

For every component of  $T \setminus C$ , there is a unique vertex  $u_i, 1 \leq i \leq k+1$ , such that the component together with  $C \setminus u_i$  forms a k-tree. Now we consider two cases that are handled analogously.

**Case 1:** There is some  $u_i$  such that the union of components that form a k-tree when adding  $C' = C \setminus u_i$  has order at least  $\frac{n-k}{2}$ .

In this case, we consider the  $r \leq n-k$  components of  $T \setminus C'$  and for every  $1 \leq j \leq r$ , we let  $T_j$  be the union of such a component and C'.

We then apply the following claim:

**Claim 9.** Let C' be a k-clique in a k-tree T of order n with no k-cliques of degree 2. Then T has at least  $\frac{n-k+1}{2}$  simplicial vertices that are not in C'.

*Proof.* Consider the 1-characteristic tree  $T'_{C'}$ , whose order is n-k+1. For every  $u \in T \setminus C'$ , either all the k-cliques containing u have degree 1, in which case u has degree 1 in  $T'_{C'}$ , or (at least) one of them has degree at least 3 and so does u in  $T'_{C'}$ . Thus  $T'_{C'}$  is series-reduced and thus has at least  $\frac{n-k+1}{2} + 1$  leaves. The latter implies that T has at least  $\frac{n-k+1}{2}$  simplicial vertices that are not in C'.

By the choice of C, for every  $1 \leq j \leq r$ , there are at least  $\lfloor \frac{n-k+1}{2} \rfloor$  vertices that do not belong to  $T_j$ . By Claim 9, among them are at least  $\frac{n-k}{4}$  simplicial vertices of T. Observe that given any sub-k-tree of T containing C', we can map it to its sub-k-tree intersection

with  $T_j$ . If two elements of S(T; C') differ only in some subset of k-leaves of  $\bigcup_{h\neq j} T_h$ , then they map to the same element of  $S(T_j; C')$ . Thus, each element of  $S(T_j; C')$  is mapped to at least  $2^{\frac{n-k}{4}}$  times, and  $N(T; C') \ge 2^{\frac{n-k}{4}} N(T_j; C')$ .

Using the perfect elimination ordering, every sub-k-tree S in  $T_j$  not containing C' can be extended in a minimal way into a sub-k-tree containing C'. Furthermore, by considering the 1-characteristic tree  $T'_{C'}$  of C', it is clear that there are no more than  $|T_j| - k \leq \left\lceil \frac{n-(k+1)}{2} \right\rceil \leq \frac{n}{2}$  k-trees that extend to the same tree. Here we have used Lemma 7 again. Thus, if we define a map from  $\overline{S}(T_j; C')$  to  $S(T_j; C')$  using the minimal extension, every element of  $S(T_j; C')$  is mapped to at most  $\frac{n}{2}$  times.

Putting the previous two observations together, we have that the number of sub-k-trees containing C' is  $N(T;C') \ge 2^{\frac{n-k}{4}} N(T_j;C') \ge \frac{1}{n} 2^{\frac{n-k}{4}+1} \overline{N}(T_j;C')$ .

By summing over all j, we obtain that

$$rN(T;C') \ge \frac{1}{n} 2^{\frac{n-k}{4}+1} \sum_{j=1}^{r} \overline{N}(T_j;C') = \frac{1}{n} 2^{\frac{n-k}{4}+1} \overline{N}(T;C').$$

Since  $r \leq n$ , we have that  $N(T;C') \geq \frac{1}{n^2} 2^{\frac{n-k}{4}+1} \overline{N}(T;C')$ . This implies that  $\frac{\mu(T)}{\mu(T;C')} \geq 1 - \frac{n^2}{2^{\frac{n-k}{4}+1}}$ . The result follows now from  $\mu(T;C') \leq n$ .

**Case 2:** For every  $u_i$  the union of components in  $T \setminus C$  that form a k-tree when adding  $C \setminus u_i$  has order smaller than  $\frac{n-k}{2}$ .

Let  $T_i$ ,  $1 \leq i \leq k+1$ , be the k-trees obtained above when adding  $C \setminus u_i$ . By Claim 9, for each *i* there are at least  $\frac{n-k}{4}$  k-leaves not belonging to  $T_i$ . Thus, the same computations apply and in particular we have that  $N(T; C') \geq \frac{1}{n^2} 2^{\frac{n-k}{4}+1} \overline{N}(T; C')$  as before. Now for  $C' = C \setminus u_1$ , we conclude by inclusion monotonicity [13, Thm. 33] that  $\mu(T; C') - \mu(T) \leq \mu(T; C) - \mu(T) \leq \frac{n^3}{2^{(n-k)/4+1}}$ .

Proof of Theorem 2, lower bound. Take a k-clique C' which satisfies Lemma 8. Let  $T'_{C'}$  be the 1-characteristic tree of T with respect to C'. By [13, Thm. 33] and [7, Lem. 12], we conclude that  $\mu(T; C') = \mu(T'_{C'}; C') + k - 1 \ge \frac{n+k}{2} + \frac{i-1}{10}$ , where i is the number of internal vertices in  $T'_{C'}$ . By Lemma 8, we conclude.

For sharpness, observe that if T is not a k-star, we have  $i \ge 2$  and the lower bound inequality is strict. When T is a k-star, it contains no k-cliques of degree 2 provided that n > k + 2. As computed in [16] (page 64),  $\mu(T) = \frac{R(T)}{N(T)} = \frac{(n+k)2^{n-k-1}}{2^{n-k}+(n-k)k} = \frac{n+k}{2} - o_n(1)$ .  $\Box$ 

#### 3.2 The upper bound

In this subsection, we generalize to k-trees the statement that a series-reduced tree has average subtree order at most  $\frac{3n}{4}$  by giving a lower bound for the number of k-leaves and proving that k-leaves belong to at most half of the sub-k-trees. This idea was also used in [7]. Note that the upper bound is slightly larger than  $\frac{3n}{4}$  for larger k, which intuitively can be explained by the fact that the smallest sub-k-tree already has k vertices, and more precisely the vertices in the base k-clique will all be major vertices.

Proof of Theorem 2, upper bound. Our upper bound will come from the observation that  $\mu(T) = \sum_{v \in T} p(v)$  where p(v) is the fraction of sub-k-trees containing v. We will specifically consider when v is a k-leaf and bound the corresponding terms in the summation.

We first prove that the 1-characteristic tree  $T'_C$  of a k-tree T without k-cliques of degree 2 is a series-reduced tree, for any k-clique C of T. Indeed, given a k-clique C, there is either exactly one vertex adjacent to C or at least 3. As such, the degree of C in  $T'_C$  is not 2. For any other vertex  $v \in T \setminus C$ , either it is a leaf or some vertex w was added to a k-clique C', where v is the latest vertex of C'. In the latter case, note that v was added to some k-clique of the form  $C' \cup \{u\} \setminus \{v\}$ . This implies that u and w are adjacent to all of C', and since T has no k-cliques of degree 2, there must be at least another vertex w' with this property. Now v is adjacent to w, w', and some earlier vertex, so its degree in  $T'_C$  is at least 3.

Thus  $T'_C$  has at least  $\frac{n-k+1}{2} + 1$  leaves, which implies that T contains at least this many k-leaves (here one must also observe that if C has degree 1 in  $T'_C$ , some vertex of C is simplicial in T).

Now fix a k-leaf v. Since  $n \ge k+2$ , there is a vertex u (different from v) such that  $N(v) \cup \{u\}$  spans a  $K_{k+1}$ . Define a function f on sub-k-trees containing v such that  $f(C') = (C' \setminus \{v\}) \cup \{u\}$  for a k-clique C' and  $f(T') = T' \setminus v$  otherwise. We can check that f maps k-cliques to k-cliques and is in fact an injection from sub-k-trees containing v to sub-k-trees not containing v. Indeed, because v is a k-leaf,  $C' \cup \{u\}$  is not a (k+1)-clique and thus not a sub-k-tree. Hence there does not exist a (k+1)-clique C''  $\{v\} \cup \{v\} = (C' \setminus \{v\}) \cup \{u\}$ .

This implies that every k-leaf belongs to at most half of the sub-k-trees in T. Remembering that there are at least  $\frac{n-k+3}{2}$  k-leaves, the global mean order of T is then

$$\mu(T) = \sum_{v \text{ non-k-leaf}} p(v) + \sum_{v \text{ k-leaf}} p(v) \leqslant n - \frac{1}{2} \cdot \frac{n - k + 3}{2} = \frac{3n + k - 3}{4}$$

For sharpness, let n = 2s + 3 - k for an integer s. We construct T by first constructing a caterpillar T' which consists of a path-type k-tree  $P_s^{k+1}$  on vertices  $v_1, v_2, \ldots, v_s$ , for which every k + 1 consecutive vertices form a clique, and adding a k-leaf connected to every k consecutive vertices. To obtain T, we extend T' by adding two k-leaves, which are connected to  $\{v_1, \ldots, v_k\}$  and  $\{v_{s-k+1}, \ldots, v_s\}$  respectively. Note that T has a "stem" of s vertices and the number of k-leaves is  $\ell + 2 = (s - k + 1) + 2 = s - k + 3$ .

This k-tree T has the property that none of the k-cliques has degree 2: if a k-clique contains one of the k-leaves, its degree is 1, since every k-leaf only belongs to one (k + 1)-clique. Otherwise, a k-clique consists entirely of vertices of the stem. If they are consecutive vertices  $v_i, v_{i+1}, \ldots, v_{i+k-1}$ , the degree of the clique is 3: the clique can be extended to a (k + 1)-clique by adding  $v_{i-1}, v_{i+k}$ , or the additional k-leaf that is adjacent to it. If the k-clique consists of stem vertices that are non-consecutive, then it must be a subset of a clique of k + 1 consecutive vertices  $v_i, v_{i+1}, \ldots, v_{i+k}$  (otherwise its first and last vertex would not be adjacent). This only extends to one (k + 1)-clique (by adding the missing vertex), so the degree is 1.

For every  $1 \leq i \leq s - k$ , there are *i* sub-*k*-trees of the stem each of order s + 1 - i. Each of these can be extended by adding any subset of the  $\ell + 1 - i$  neighboring *k*-leaves, or even one or two more if some of the end-vertices of the stem are involved. Now we can compute that

$$N(T) = (k(n-k) + 1 - \ell) + 2^{\ell+2} + 2\sum_{i=2}^{\ell} 2^i + \sum_{i=3}^{s-k+1} (i-2) \cdot 2^{\ell+1-i}$$
  
~ 9 \cdot 2^{\ell}.

The first expression  $k(n-k) + 1 - \ell$  counts the number of simplicial k-cliques different from the ones consisting of k consecutive vertices in the stem.  $2^{\ell+2}$  is the number of sub-k-trees containing the whole stem. The third term counts the number of sub-k-trees containing  $v_1$  or  $v_s$  but not both and at least k vertices of the stem. The last summation counts the sub-k-trees containing at least k vertices of the stem and none of  $v_1$  and  $v_s$ . We can also compute R(T) by summing the total size of the respective sub-k-trees.

$$\begin{split} R(T) &= (k(n-k)+1-\ell)k + 2^{\ell+2} \left(s + \frac{\ell+2}{2}\right) + 2\sum_{i=2}^{\ell} 2^i \left(k+i-2+\frac{i}{2}\right) \\ &+ \sum_{i=3}^{s-k+1} (i-2) \cdot 2^{\ell+1-i} \left(s+1-i + \frac{\ell+1-i}{2}\right) \\ &\sim 2^{\ell+2} \left(s + \frac{\ell+2}{2}\right) + 2^{\ell+2} (k-2) + 3 \cdot 2^{\ell+1} (\ell-1) + 2^{\ell} \left(s+1 + \frac{\ell+1}{2}\right) - 15 \cdot 2^{\ell-1} \\ &= \left(5s + \frac{17}{2}\ell + 4k - 16\right) 2^{\ell} \\ &= \left(\frac{27}{4}n + \frac{9}{4}k - \frac{111}{4}\right) 2^{\ell}. \end{split}$$

Finally, we conclude that  $\mu(T) = \frac{R(T)}{N(T)} \sim \frac{3}{4}n + \frac{1}{4}k - \frac{37}{12}$ , which is only  $\frac{7}{3}$  away from the upper bound. These computations have also been verified in https://github.com/StijnCambie/AvSubOrder\_ktree/blob/main/M\_comb\_ktree.mw.

## 4 The maximum local mean order

In this section, we prove

**Theorem 3.** Suppose that  $k \ge 2$ . For a k-tree T of order  $n \ne k+2$ , if a k-clique C maximizes  $\mu(T; C)$ , then C must be a k-clique of degree 1. For n = k+2, every k-clique C satisfies  $\mu(T; C) = k + 1$ .

We consider the k-clique in a k-tree T for which the local mean order is greatest. Our aim is to show that its degree cannot be too large, specifically at most 2. To do so,



Figure 5: Sketch of k-trees with mean sub-k-tree order roughly  $\frac{n}{2}$  and  $\frac{3n}{4}$  for k = 3.

we prove that if a k-clique C has degree at least 2, then there is a neighboring k-clique whose local mean order is not smaller, with strict inequality when C has degree at least 3. From this, it already follows that any k-clique attaining the maximum has degree at most 2. Moreover, in the case where the maximum is attained at a k-clique of degree 2, we will show that one can always move along maximizing k-cliques without doubling back, which means that one always ends up in at least one k-clique with degree 1 in which the maximum is attained.

The proof requires some technical inequalities, which we prove first. We start with a generalization of [21, Lemma 2.1] to the k-tree case as follows.

**Lemma 10.** For a sub-k-tree T and a k-clique C, we have

$$R(T;C) \leqslant \frac{N(T;C)^2 + (2k-1)N(T;C)}{2}.$$

Equality holds if and only if T is a path-type k-tree and C is a simplicial k-clique.

*Proof.* The statement is clearly true when T = C, so assume |T| > k. Observe that every sub-k-tree T' of T containing C has a vertex v (not belonging to C) which is simplicial within T' (consider a perfect elimination order where C is taken as the base k-clique). This implies that  $T' \setminus v$  is a sub-k-tree containing C as well.

If there exists a sub-k-tree containing C of order  $\ell > k$ , then the above implies that there must also exist a sub-k-tree of order  $\ell - 1$  containing C. Thus, if we list the sub-k-trees in S(T; C) from smallest to largest order, we see that

$$R(T;C) \leq k + (k+1) + \dots + (k+N(T;C)-1) = \frac{1}{2}(N(T;C)^2 + (2k-1)N(T;C))$$

as desired.

The equality case is clear, since every sub-k-tree  $T' \neq C$  of T must have exactly one k-leaf not belonging to C, and equality is attained when T is a path-type k-tree.

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Using the previous lemma, we can now bound the local mean order in terms of the number of sub-k-trees.

**Lemma 11.** For a k-tree T and one of its k-cliques C, we have

$$k + \frac{\log_2 N(T;C)}{2} \leqslant \mu(T;C) \leqslant \frac{N(T;C) + (2k-1)}{2}.$$

The minimum occurs if and only if T is a k-star and C its base k-clique. The maximum is attained exactly when T is a path-type k-tree and C is simplicial.

*Proof.* The upper bound follows immediately from Lemma 10 by dividing both sides of the inequality by N(T; C). The equality cases are the same.

By [16, Thm. 12] we have  $\mu(T; C) \ge \frac{|T|+k}{2}$ . Since a sub-k-tree is determined by its vertices, we also have

$$N(T;C) \leqslant 2^{|T|-k}.\tag{1}$$

Combining these two inequalities, we get  $\mu(T; C) \ge \frac{\log_2 N(T; C)}{2} + k$ .

To attain the lower bound, equality must hold for (1). This is the case if and only if T is a k-star and C its base k-clique. Indeed, for a k-star of order n with base clique C, we have  $N(T;C) = 2^{n-k}$  and  $\mu(T;C) = \frac{n+k}{2}$ . In the other direction, every vertex together with C needs to form a k-tree and thus a (k + 1)-clique, which is possible only for a k-star.  $\Box$ 

We will also make use of the following elementary inequality, which can be considered as the opposite statement of the inequality between the arithmetic mean and geometric mean (AM-GM).

**Lemma 12.** Let  $x_1, x_2, \ldots, x_n \in \mathbb{R}_{\geq 1}$ , and let  $P = \prod_i x_i$ . Then  $\sum_i x_i \leq P + (n-1)$ . Furthermore, equality is attained if and only if  $x_i = P$  for some i and  $x_j = 1$  for all  $j \neq i$ .

*Proof.* This can be proven in multiple ways. The most elementary way is to observe that if  $x_i, x_j > 1$ , then  $x_i x_j + 1 > x_i + x_j$  since  $(x_i - 1)(x_j - 1) > 0$ . Repeating this with pairs of elements which are strictly larger than 1 gives the result. Alternatively, one could consider the variables  $\alpha_i = \log(x_i) \ge 0$ . Since their sum is the fixed constant  $\log P$  and the exponential function is convex, as a corollary of Karamata's inequality  $\sum_i \exp(\alpha_i)$  is maximized when all except one are equal to 0.

We are now ready to prove Theorem 3. Recall that T can be decomposed into C and k-trees  $T_{1,1}, \ldots, T_{d,k}$  rooted at  $C_{1,1}, \ldots, C_{d,k}$  respectively that are pairwise disjoint except for the vertices of the cliques  $C_{i,j}$ . Let  $B_i$  denote the (k + 1)-clique that contains C as well as  $C_{i,1}, \ldots, C_{i,k}$ , and let  $v_i$  be the vertex of  $B_i \setminus C$ . Finally, set  $N_{i,j} = N(T_{i,j}; C_{i,j})$  and  $\mu_{i,j}^{\bullet} = \mu^{\bullet}(T_{i,j}; C_{i,j})$ .

*Proof of Theorem 3.* We first observe that

$$N(T;C) = \prod_{i=1}^{d} \left( 1 + \prod_{j=1}^{k} N_{i,j} \right).$$
(2)

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This is because a sub-k-tree S of T containing C is specified as follows: given  $1 \leq i \leq d$ , choose the sub-k-tree intersection of S with  $T_{i,1}, \ldots, T_{i,k}$ . There are  $\prod_{j=1}^{k} N_{i,j}$  ways to do this if  $v_i \in S$  and one if  $v_i \notin S$ . We do this independently for each *i*, resulting in the product above.

Next, we would like to express the local mean order at C in terms of the quantities  $N_{i,j}$ and  $\mu_{i,j}^{\bullet}$ : it is given by

$$\mu^{\bullet}(T;C) = \sum_{i=1}^{d} \frac{1 + \sum_{j=1}^{k} \mu_{i,j}^{\bullet}}{1 + \prod_{j=1}^{k} N_{i,j}^{-1}}.$$
(3)

To see this, note that we can interpret  $\mu(T; C)$  as the expected size of a random sub-k-tree chosen from S(T; C), which can then be written as the sum of the expected sizes of the intersection with each component  $T_{i,j}$  in the decomposition. We have that  $\frac{1}{1+\prod_{i=1}^{k} N_{i,i}^{-1}} =$ 

 $\frac{\prod_{j=1}^{k} N_{i,j}}{1+\prod_{j=1}^{k} N_{i,j}}$  is the probability that a randomly chosen sub-k-tree of T that contains C also contains  $v_i$  (by the same reasoning that gave us (2)). Once  $v_i$  is included, it adds 1 to the number of vertices, and an average total of  $\sum_{j=1}^{k} \mu_{i,j}^{\bullet}$  is added from the extensions in  $T_{i,1}, \ldots, T_{i,k}$ .

Without loss of generality, we can assume that  $N_{1,1} = \min_{i,j} N_{i,j}$ . We want to compare  $\mu^{\bullet}(T; C)$  to  $\mu^{\bullet}(T; C_{1,1})$  and prove that  $\mu^{\bullet}(T; C_{1,1}) \ge \mu^{\bullet}(T; C)$  provided that  $d \ge 2$ , with strict inequality if d > 2. Observe that this will be enough to prove our claim: no clique with degree greater than 2 can attain the maximum local mean order, and starting from any clique, we may repeatedly apply the inequality above to obtain a sequence of neighboring cliques whose local mean orders are weakly increasing and the last of which is a degree-1 k-clique. (More precisely, for the first step replacing C with  $C' := C_{1,1}$  and considering the decomposition  $\{C'_{i,j}\}$  and  $\{T'_{i,j}\}$  with respect to C', the clique adjacent to C' with equal or larger  $\mu^{\bullet}$  cannot be the original clique C as C will not correspond to  $\min_{i,j} N'_{i,j}$ . So in repeatedly applying the inequality, we will obtain a sequence of distinct cliques which must terminate but can only terminate once we have reached a clique of degree 1.)

Let us first express  $\mu^{\bullet}(T; C_{1,1})$  in terms of the  $N_{i,j}$  and  $\mu^{\bullet}_{i,j}$  as well. First, we have

$$N(T; C_{1,1}) = N_{1,1} + \prod_{j=1}^{k} N_{1,j} \prod_{i=2}^{d} \left( 1 + \prod_{j=1}^{k} N_{i,j} \right).$$

The reasoning is similar to (2): there are  $N_{1,1}$  sub-k-trees that contain  $C_{1,1}$ , but not the full (k + 1)-clique  $B_1$ , and the remaining product counts sub-k-trees containing  $B_1$ . We also have

$$\mu^{\bullet}(T;C_{1,1}) = \frac{N_{1,1}\mu_{1,1}^{\bullet}}{N(T;C_{1,1})} + \left(1 - \frac{N_{1,1}}{N(T;C_{1,1})}\right) \left(1 + \sum_{j=1}^{k} \mu_{1,j}^{\bullet} + \sum_{i=2}^{d} \frac{1 + \sum_{j=1}^{k} \mu_{i,j}^{\bullet}}{1 + \prod_{j=1}^{k} N_{i,j}^{-1}}\right),$$

using the fact that  $\frac{N_{1,1}}{N(T;C_{1,1})}$  is the probability that a random sub-k-tree containing  $C_{1,1}$  does not contain  $B_1$ . Let us now take the difference  $\mu^{\bullet}(T;C_{1,1}) - \mu^{\bullet}(T;C)$ : we have, after

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some manipulations,

$$\begin{split} \mu^{\bullet}(T;C_{1,1}) - \mu^{\bullet}(T;C) &= \frac{N_{1,1}}{N(T;C_{1,1})} \left( \mu^{\bullet}_{1,1} - \mu^{\bullet}(T;C) \right) \\ &+ \left( 1 - \frac{N_{1,1}}{N(T;C_{1,1})} \right) \left( 1 + \sum_{j=1}^{k} \mu^{\bullet}_{1,j} - \frac{1 + \sum_{j=1}^{k} \mu^{\bullet}_{1,j}}{1 + \prod_{j=1}^{k} N_{i,j}^{-1}} \right) \\ &= \frac{N_{1,1}}{N(T;C_{1,1})} \left( \mu^{\bullet}_{1,1} - \mu^{\bullet}(T;C) \right) \\ &+ \left( 1 - \frac{N_{1,1}}{N(T;C_{1,1})} \right) \left( \frac{1 + \sum_{j=1}^{k} \mu^{\bullet}_{1,j}}{1 + \prod_{j=1}^{k} N_{1,j}} \right). \end{split}$$

Now let  $F := \frac{1 + \sum_{j=1}^{k} \mu_{1,j}^{\bullet}}{1 + \prod_{j=1}^{k} N_{1,j}}$ . We want to show that  $\mu^{\bullet}(T; C_{1,1}) - \mu^{\bullet}(T; C) \ge 0$ , i.e., that

$$\frac{N_{1,1}}{N(T;C_{1,1})}\mu_{1,1}^{\bullet} + F \ge \frac{N_{1,1}}{N(T;C_{1,1})}\left(\mu^{\bullet}(T;C) + F\right).$$

Equivalently,

$$\mu_{1,1}^{\bullet} + \frac{N(T; C_{1,1})}{N_{1,1}} \cdot F \ge \mu^{\bullet}(T; C) + F.$$
(4)

Using the previous computations, we know that

$$\frac{N(T;C_{1,1})}{N_{1,1}} = 1 + \prod_{j=2}^{k} N_{1,j} \prod_{i=2}^{d} \left( 1 + \prod_{j=1}^{k} N_{i,j} \right).$$

So the left-hand side of (4) is equal to

$$\mu_{1,1}^{\bullet} + F + \frac{\prod_{j=2}^{k} N_{1,j}}{1 + \prod_{j=1}^{k} N_{1,j}} \left( 1 + \sum_{j=1}^{k} \mu_{1,j}^{\bullet} \right) \prod_{i=2}^{d} \left( 1 + \prod_{j=1}^{k} N_{i,j} \right).$$

We can subtract F from both sides and use (3) to replace  $\mu^{\bullet}(T; C)$ . Taking into account that  $\mu_{1,1}^{\bullet} \ge 0$ , it is sufficient to prove

$$\frac{\prod_{j=2}^{k} N_{1,j}}{1+\prod_{j=1}^{k} N_{1,j}} \left(1+\sum_{j=1}^{k} \mu_{1,j}^{\bullet}\right) \prod_{i=2}^{d} \left(1+\prod_{j=1}^{k} N_{i,j}\right) \geqslant \sum_{i=1}^{d} \frac{1+\sum_{j=1}^{k} \mu_{i,j}^{\bullet}}{1+\prod_{j=1}^{k} N_{i,j}^{-1}}.$$
 (5)

We first prove (5) for d = 2, in which case it can be rewritten as

$$\frac{\prod_{j=1}^{k} N_{1,j}}{N_{1,1}(1+\prod_{j=1}^{k} N_{1,j})} \left(1+\sum_{j=1}^{k} \mu_{1,j}^{\bullet}\right) \left(1-N_{1,1}+\prod_{j=1}^{k} N_{2,j}\right) \\ \geqslant \frac{\prod_{j=1}^{k} N_{2,j}}{1+\prod_{j=1}^{k} N_{2,j}} \left(1+\sum_{j=1}^{k} \mu_{2,j}^{\bullet}\right).$$

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Write  $\prod_{j=1}^{k} N_{1,j} = N_{1,1}^{k-1} y$  and  $\prod_{j=1}^{k} N_{2,j} = N_{1,1}^{k-1} z$  where  $y, z \ge N_{1,1}$ . By Lemma 11, we have  $\mu_{1,j}^{\bullet} \ge \frac{1}{2} \log_2 N_{1,j}$  and  $\mu_{2,j}^{\bullet} \le \frac{1}{2} (N_{2,j} - 1)$ . Applying Lemma 12 to the numbers  $\frac{N_{2,j}}{N_{1,1}}$ ,  $1 \le j \le k$ , gives us that  $\sum_{j=1}^{k} N_{2,j} \le (k-1)N_{1,1} + z$ . Hence we find that it suffices to prove that

$$\frac{y\left(1-N_{1,1}+N_{1,1}^{k-1}z\right)}{N_{1,1}\left(1+N_{1,1}^{k-1}y\right)}\left(1+\frac{(k-1)\log_2 N_{1,1}+\log_2 y}{2}\right)$$
$$\geqslant \frac{z}{1+N_{1,1}^{k-1}z}\left(1+\frac{(k-1)N_{1,1}+z-k}{2}\right).$$

We note that the left-hand side is strictly increasing in y and the right-hand side is independent of y, which implies that it is sufficient to prove the equality when  $y = N_{1,1}$ . That is, we want to prove that for every  $z \ge y \ge 1$ 

$$\frac{1 - y + y^{k-1}z}{1 + y^k} \left( 1 + \frac{k}{2}\log_2 y \right) \ge \frac{z}{1 + y^{k-1}z} \left( 1 + \frac{(k-1)y + z - k}{2} \right).$$
(6)

If  $y = N_{1,1} = 1$ , (6) reduces to  $\frac{z}{2} \ge \frac{z}{2}$ .

If  $y = N_{1,1} \ge 2$ ,  $z \ge y$  and  $k \ge 2$  imply that  $2 + (k-1)y + z - k \le kz$ . Together with  $\log_2 y \ge 1$ , we conclude that it is sufficient to prove that

$$\frac{1 - y + y^{k-1}z}{1 + y^k} \frac{k+2}{2} \ge \frac{z}{1 + y^{k-1}z} \frac{kz}{2}$$

which is equivalent to

$$(1 - y + y^{k-1}z)(k+2)(1 + y^{k-1}z) \ge (1 + y^k)kz^2.$$

For k = 2, the difference between the two sides is an increasing function in y, and for y = 2 it reduces to  $3z^2 - 2 \ge 0$ , which holds.

For  $k \ge 3$ , the inequality is immediate, using that  $y^{2(k-1)}z^2 \ge (1.5y^k+1)z^2 \ge y^kz+y^kz^2+z^2$  (remember that  $z \ge y \ge 2$ ).

Once (5) has been verified for d = 2, we can apply induction to prove it for  $d \ge 3$ . Let  $C = \frac{\prod_{j=2}^{k} N_{1,j}}{1+\prod_{j=1}^{k} N_{1,j}} \left(1+\sum_{j=1}^{k} \mu_{1,j}^{\bullet}\right)$ ,  $g_i = 1+\prod_{j=1}^{k} N_{i,j}$  and  $f_i = \frac{1+\sum_{j=1}^{k} \mu_{i,j}^{\bullet}}{1+\prod_{j=1}^{k} N_{i,j}^{-1}}$ . We can then rewrite (5) as

$$C\prod_{i=2}^{d}g_i \geqslant \sum_{i=1}^{d}f_i$$

By the induction hypothesis, we have

$$\frac{C}{g_m} \prod_{i=2}^d g_i \geqslant \left(\sum_{i=1}^d f_i\right) - f_m$$

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for every  $2 \leq m \leq d$ . Summing over m, we obtain that

$$C \prod_{i=2}^{d} g_i \left( \sum_{m=2}^{d} \frac{1}{g_m} \right) \ge f_1 + (d-2) \sum_{i=1}^{d} f_i.$$

Since we have  $g_m \ge 2$  for every m, the conclusion now follows as

$$\sum_{m=2}^{d} \frac{1}{g_m} \leqslant \frac{(d-1)}{2} \leqslant d-2,$$

and since  $f_1 > 0$ , inequality (5) is even strict in the case that d > 2.

We conclude that if C has degree  $d \ge 2$ , then  $\mu^{\bullet}(T; C) \le \mu^{\bullet}(T; C_{1,1})$ . Equality can only be attained when d = 2. Looking back over the proof of (5), we also see that for equality to hold, all  $N_{i,j}$  except for  $N_{2,2}$  (up to renaming) must be equal to 1, and due to Lemma 11,  $T_{2,2}$  has to be a path-type k-tree.

For  $n \ge k+3$ , we compute that in a path-type k-tree T the maximum among the degree-1 k-cliques is attained by a central one, which implies that no degree-2 k-cliques can be extremal. Let  $B_1$  be the unique (k + 1)-clique containing C, and assume that  $T \setminus B_1$  contains components of size a and b. Thus a + b = n - (k + 1). Then  $\mu(T;C) = \frac{k+(a+1)(b+1)\frac{n+k}{2}}{(a+1)(b+1)+1} = \frac{n+k}{2} - \frac{n-k}{2((a+1)(b+1)+1)}$ , and this is maximized if and only if  $|a-b| \le 1$ . The latter can also be derived from considering the 1-characteristic tree. This is illustrated in Figure 6 below. We emphasize that the maximizing k-clique of degree 1 is not simplicial. When  $n \le k+2$ , every k-clique has the same local mean sub-k-tree order, and so the (unique) degree-2 k-clique when n = k+2 is the only case where equality can occur at a k-clique with degree 2. This concludes the proof of Theorem 3.



Figure 6: 2-path for which the maximum local mean is attained in a non-simplicial clique C, with its 1-characteristic tree  $T'_C$ .

## 5 Bounding local mean order by global mean order

In this section, we prove

**Theorem 4.** The local mean order of the sub-k-trees containing a fixed k-clique C is less than twice the global mean order of all sub-k-trees of T.

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As before, given a k-tree T and a k-clique C in T, we utilize the decomposition of T into C and k-trees  $T_{1,1}, \ldots, T_{d,k}$  rooted at  $C_{1,1}, \ldots, C_{d,k}$ . Set  $N_{i,j} = N(T_{i,j}; C_{i,j})$ ,  $\overline{N}_{i,j} = \overline{N}(T_{i,j}; C_{i,j}), \ \mu_{i,j} = \mu(T_{i,j}; C_{i,j}), \ \mu_{i,j} = \overline{\mu}(T_{i,j}; C_{i,j}), \ \mu_{i,j} = \mu^{\bullet}(T_{i,j}; C_{i,j})$  and  $R_{i,j} = R(T_{i,j}; C_{i,j}), \ \overline{R}_{i,j} = \overline{R}(T_{i,j}; C_{i,j}).$ 

Since a sub-k-tree not containing C needs to be a sub-k-tree of some k-tree  $T_{i,i}$ , we have

$$\overline{N}(T;C) = \sum_{i=1}^{d} \sum_{j=1}^{k} (N_{i,j} + \overline{N}_{i,j})$$

and

$$\overline{R}(T;C) = \sum_{i=1}^{d} \sum_{j=1}^{k} (R_{i,j} + \overline{R}_{i,j}).$$

Following the proof for trees, we show

**Lemma 13.** For any k-tree T and k-clique  $C \in T$ ,

$$R(T;C) > \overline{N}(T;C).$$

*Proof.* Assume to the contrary that there exists a minimum counterexample T. Since the statement is true when T = C, we have |T| > k and we can consider the decomposition as before.

Note that if  $N_{i,j} = 1$ , we have that  $\overline{N}_{i,j} = 0$ , and otherwise we have  $\overline{N}_{i,j} \leq R_{i,j} = \mu_{i,j}N_{i,j} = (k + \mu_{i,j}^{\bullet})N_{i,j}$ . We can rewrite  $R(T; C) - \overline{N}(T; C)$  as

$$N(T;C) \left(k + \mu^{\bullet}(T;C)\right) - \overline{N}(T;C).$$

Thus it suffices to show that

$$N(T;C)(k+\mu^{\bullet}(T;C)) - \sum_{i=1}^{d} \sum_{j=1}^{k} N_{i,j} - \sum_{\substack{i=1\\N_{i,j}>1}}^{d} \sum_{j=1}^{k} (k+\mu_{i,j}^{\bullet}) N_{i,j}$$

is nonnegative. Expanding using (2) and (3) gives an expression that is increasing in  $\mu_{i,j}^{\bullet}$  for each i, j, and so it suffices to prove that this expression is nonnegative when each of these is 0.

Let f be a function on the positive integers defined by  $f(x) = \begin{cases} 1 & \text{if } x = 1, \\ 1 + kx & \text{if } x > 1. \end{cases}$ We now want to prove that

We now want to prove that

$$\left(k + \sum_{i=1}^{d} \frac{1}{1 + \prod_{j=1}^{k} N_{i,j}^{-1}}\right) N(T;C) \ge \sum_{i=1}^{d} \sum_{j=1}^{k} f(N_{i,j}).$$
(7)

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When d = 1, this becomes  $k + (k+1) \prod_{j=1}^{k} N_{1,j} \ge \sum_{j=1}^{k} f(N_{1,j})$ . When increasing a value  $N_{1,j}$  which is at least equal to 2, the left-hand side increases more than the right-hand side. As such, it is sufficient to consider the case where a of the terms  $N_{1,j}$  equal 2, while the other k - a terms equal 1. In this case, the desired inequality holds since  $k + (k+1)2^a > k + 2ak$  for every integer  $0 \le a \le k$ .

Next, we consider the case  $d \ge 2$ . In this case, when  $N_{i,j}$  increases by 1, the left-hand side of (7) increases by at least 2k and the right-hand side by at most 2k. When all  $N_{i,j}$  are equal to 1, the conclusion follows from  $\left(k + \frac{d}{2}\right) 2^d > k2^d > dk$ .

We now bound the local mean order by the global mean order.

Proof of Theorem 4. Let T be a k-tree and C a k-clique in T. We want to prove that

$$\mu(T;C) < 2\mu(T).$$

We proceed by induction on the number of vertices in T. Note first that the inequality is trivial if  $|T| \leq 2k$ : since the mean is taken over sub-k-trees, which have at least k vertices each, we have  $\mu(T) \geq k$ . On the other hand, we clearly have  $\mu(T; C) \leq |T|$ , and both inequalities hold with equality only if |T| = k.

We thus proceed to the induction step, and assume that |T| > 2k. We have two cases with respect to C.

Case 1: C is simplicial.

Let v be a k-leaf in C, let C' denote the clique adjacent to C, and let  $T' = T - \{v\}$ . Moreover, let  $N, \overline{N}, R$ , and  $\overline{R}$  denote  $N(T'; C'), \overline{N}(T; C'), R(T'; C')$  and  $\overline{R}(T'; C')$ , respectively. We have

$$\mu(T;C) = \frac{N+R+k}{N+1}$$

and

$$\mu(T) = \frac{2R + R + N + k^2}{2N + \overline{N} + k}.$$

We want to prove that

$$(2N + \overline{N} + k)(2\mu(T) - \mu(T;C)) > 0,$$

which is equivalent to

$$2R + 2\overline{R} + 2k^2 - 2k - \frac{(N+R+k)(\overline{N}+k-2)}{N+1} > 0.$$

By the induction hypothesis, we have

$$2\frac{R+\overline{R}}{N+\overline{N}} = 2\mu(T') > \mu(T';C') = \frac{R}{N},$$

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so it is sufficient to prove that

$$\frac{R(N+\overline{N})}{N} + 2k^2 - 2k - \frac{(N+R+k)(\overline{N}+k-2)}{N+1} > 0.$$

Multiplying by  $\frac{N+1}{N}$ , this is seen to be equivalent to

$$R - \overline{N} + 2k^2 - 3k + 2 - \frac{(k-3)R + k\overline{N} - k^2}{N} + \frac{\overline{N}R}{N^2} > 0.$$

This can be broken up into three terms as follows:

$$\frac{(N^2 - kN + 3N + \overline{N})(R - \overline{N})}{N^2} + \left(\frac{\overline{N}}{N} - k\right)^2 + \left((k - 1)(k - 2) + \frac{k^2}{N} + \frac{3\overline{N}}{N}\right) > 0.$$

Note here that the second term is trivially nonnegative, and the last term trivially positive. Since  $|T'| \ge 2k$ , we have N > k (one gets at least k + 1 sub-k-trees containing C' by successively adding vertices); hence  $N^2 - kN + 3N + \overline{N} > 0$ . Thus the first term is positive by Lemma 13, completing the induction step in this case. **Case 2:** C is not simplicial.

By Theorem 3, we only need to consider the case where C has degree 1. Let v be the unique common neighbor of C, and let  $C_i$ ,  $1 \leq i \leq k$ , be the other k-cliques in the (k+1)-clique spanned by  $C \cup \{v\}$ .

Let  $T_i, 1 \leq i \leq k$ , be the sub-k-trees rooted at  $C_i$  (pairwise disjoint except for the vertices of the cliques  $C_i$ ). Let  $N_i = N(T_i; C_i), \ \overline{N}_i = \overline{N}(T_i; C_i), \ R_i = R(T_i; C_i), \ \overline{R}_i = \overline{R}(T_i; C_i), \ \mu_i = \mu(T_i; C_i)$  and  $\mu_i^{\bullet} = \mu^{\bullet}(T_i; C_i)$ . We can assume without loss of generality that  $N_1 \geq N_2 \geq \cdots \geq N_j > 1 = N_{j+1} = \cdots = N_k$ , where  $j \geq 2$  since C is not simplicial.

We can now express the local and global mean in a similar way to Case 1. Here  $N(T; C) = \prod_{i=1}^{k} N_i + 1$ , and all the sub-k-trees counted here, except for C, contain v. We have

$$\mu(T;C) = \frac{\prod_{i=1}^{k} N_i (1 + \sum_{i=1}^{k} \mu_i^{\bullet})}{\prod_{i=1}^{k} N_i + 1} + k,$$
  
$$\mu(T) = \frac{\prod_{i=1}^{k} N_i (1 + \sum_{i=1}^{k} \mu_i^{\bullet} + k) + \sum_{i=1}^{k} (R_i + \overline{R}_i) + k}{\prod_{i=1}^{k} N_i + \sum_{i=1}^{k} (N_i + \overline{N}_i) + 1}$$

In the remainder of this section, we will omit the bounds in products and sums if they are over the entire range from 1 to k:  $\sum N_i$  and  $\prod N_i$  mean  $\sum_{i=1}^k N_i$  and  $\prod_{i=1}^k N_i$  respectively. Then  $(\prod N_i + \sum (N_i + \overline{N}_i) + 1) (2\mu(T) - \mu(T; C))$  equals

$$(\prod N_i)(1+\sum \mu_i^{\bullet}+k)+k+2\sum (R_i+\overline{R}_i)-k\sum (N_i+\overline{N}_i)-\frac{(\prod N_i)(1+\sum \mu_i^{\bullet})\sum (N_i+N_i)}{\prod N_i+1}.$$

$$(8)$$

We want to show that this expression is positive. By induction, we know that  $2(R_i + \overline{R}_i) > (k + \mu_i^{\bullet})(N_i + \overline{N}_i)$ , thus  $2(R_i + \overline{R}_i) - k(N_i + \overline{N}_i) > \mu_i^{\bullet}(N_i + \overline{N}_i)$ . It follows that (8) is greater than

$$(\prod N_i)(1+\sum \mu_i^{\bullet}+k)+k+\sum \mu_i^{\bullet}(N_i+\overline{N}_i)-\frac{(\prod N_i)(1+\sum \mu_i^{\bullet})\sum (N_i+\overline{N}_i)}{\prod N_i+1}.$$

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Multiplying by  $\frac{\prod N_i+1}{\prod N_i}$  and observing that this factor is greater than 1, we find that (8) is indeed positive if we can prove that

$$(\prod N_i + 1)(1 + \sum \mu_i^{\bullet} + k) + k + \sum \mu_i^{\bullet}(N_i + \overline{N}_i) \ge (1 + \sum \mu_i^{\bullet}) \sum (N_i + \overline{N}_i).$$
(9)

In particular, a potential counterexample would have to satisfy

$$\frac{(1+\sum\mu_i^{\bullet})\sum(N_i+\overline{N}_i)}{\prod N_i+1} > 1 + \sum\mu_i^{\bullet} + k.$$

$$(10)$$

To simplify proving eq. (9), we first note that it is sufficient to consider the case where k = j. Once  $N_i, \mu_i^{\bullet}$  and  $\overline{N}_i$  are fixed for  $1 \leq i \leq j$ , the terms that are dependent on k are  $(\prod_{i \leq j} N_i + 1)k + k$  on the left, and  $(1 + \sum_{i \leq j} \mu_i^{\bullet})(k - j)$  on the right. The latter since if  $N_i = 1$ , then  $T_i$  only consists of  $C_i$ , and thus  $\overline{N}_i = \mu_i^{\bullet} = 0$ . Now since  $\prod_{i \leq j} N_i + 1 \geq 1 + \sum_{i \leq j} N_i > 1 + \sum_{i \leq j} \mu_i^{\bullet}$ , the increase of the left side is larger than the increase on the right side. Here  $\prod_{i \leq j} N_i \geq \sum_{i \leq j} N_i$  is true since the product of  $j \geq 2$  numbers, each greater than or equal to 2, is at least equal the sum of the same j numbers. Moreover,  $N_i > \mu_i^{\bullet}$  follows from Lemma 11.

So from now on, we can assume that j = k and all  $N_i$  are at least equal to 2.

By lemma 13,  $\overline{N}_i \leq R_i = \mu_i N_i = (k + \mu_i^{\bullet}) N_i$ . Since (9) is a linear inequality in each  $\overline{N}_i$  and the coefficient on the right-hand side is always greater than the coefficient on the left-hand side, we can reduce eq. (9) to a sufficient inequality that is only dependent on k,  $N_i$  and  $\mu_i^{\bullet}$  for  $1 \leq i \leq k$  by taking  $\overline{N}_i = (k + \mu_i^{\bullet}) N_i$ . This will be assumed in the following. If now all the parameters in (9) are fixed except for one  $\mu_i^{\bullet}$ , we have a linear inequality in  $\mu_i^{\bullet}$ : the quadratic terms stemming from  $\mu_i^{\bullet} \overline{N}_i$  are equal on both sides and cancel. As such, it is sufficient to prove the inequality for the extremal values of  $\mu_i^{\bullet}$ . Here we use the trivial inequality  $\mu_i^{\bullet} \geq 0$  as well as the upper bound  $\mu_i^{\bullet} \leq \frac{N_i-1}{2}$ , which is taken from lemma 11. So if (9) can be proven in the case where  $\overline{N}_i = (k + \mu_i^{\bullet})N_i$  and  $\mu_i^{\bullet} \in \{0, \frac{N_i-1}{2}\}$  for all i with  $1 \leq i \leq k$ , we are done.

For  $2 \leq k \leq 5$ , this is achieved by exhaustively checking all  $2^k$  cases that result (using symmetry, there are actually only k + 1 cases to consider). See the detailed verifications in https://github.com/StijnCambie/AvSubOrder\_ktree. So for the rest of the proof, we assume that  $k \geq 6$ , and we will use the slightly weaker bound  $\mu_i^{\bullet} \leq \frac{N_i}{2}$  instead of  $\mu_i^{\bullet} \leq \frac{N_i-1}{2}$  for  $1 \leq i \leq k$  in a few cases.

We distinguish two further cases, depending on the value of  $\mu_1^{\bullet}$ . In these cases, we will use the following two inequalities.

Claim 14. Let  $k \ge 6$  and  $N_1 \ge N_2 \ge \ldots \ge N_k \ge 2$ . Then

$$\prod_{i=2}^{k} N_i \ge 3 \sum_{2 \leqslant i \leqslant k} N_i, \tag{11}$$

$$\frac{5}{3}\left(\prod_{i=1}^{k} N_i + 1\right) \geqslant \left(\sum_{2 \leqslant i \leqslant k} N_i - 2\right) \sum_{1 \leqslant i \leqslant k} N_i.$$

$$(12)$$

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*Proof.* The first inequality, eq. (11), is true if all the  $N_i$  are equal to 2, since  $2^{k-1} > 6(k-1)$  for every  $k \ge 6$ . Increasing some  $N_i$  by 1 increases the product by at least  $2^{k-2}$ , while the sum increases by only 3. So the inequality holds by a straightforward inductive argument. Next, we prove eq. (12). When all  $N_i$  are equal to 2, it becomes  $\frac{5}{3}(2^k+1) \ge 4(k-2)k$ . This is easily checked for  $k \in \{6,7\}$ , and for  $k \ge 8$ , the stronger inequality  $2^k \ge 4k^2$  can be shown by induction.

Now observe that the difference between the left- and right-hand sides is increasing with respect to  $N_1$ , since  $\prod_{i\geq 2} N_i > \sum_{i\geq 2} N_i$  by the first inequality. It is also increasing in the other  $N_i$ 's; for example, we can see this is true for  $N_2$  since

$$\frac{5}{3}\prod_{i\neq 2}N_i \ge 5\sum_{i\neq 2}N_i > 2\sum_{1\leqslant i\leqslant k}N_i > \left(\sum_{2\leqslant i\leqslant k}N_i - 2\right) + \sum_{1\leqslant i\leqslant k}N_i.$$

In the first step, we have applied eq. (11) but replacing  $N_1$  with  $N_2$ . Again, we may conclude using induction.

**Claim 15.** Given  $\mu_1^{\bullet} = \frac{N_1}{2}$ , it is sufficient to consider the case where  $\mu_i^{\bullet} = \frac{N_i}{2}$  for all  $1 \leq i \leq k$ .

*Proof.* Starting from any counterexample to (9), we can iteratively change  $\mu_i^{\bullet}$  (considered as variables) for  $1 \leq i \leq k$  based on the worst case of the linearization (to 0 if the coefficient on the left-hand side is greater and to  $\frac{N_i}{2}$  if the coefficient on the right-hand side is greater) to obtain further counterexamples.

To show that it suffices to consider  $\mu_i^{\bullet} = \frac{N_i}{2}$  for every  $1 \leq i \leq k$ , we prove that, given  $\mu_1^{\bullet} = \frac{N_1}{2}$ , the coefficient of  $\mu_2^{\bullet}$  on the left-hand side in eq. (9) is not greater than the coefficient on the right-hand side. This then implies that  $\mu_2^{\bullet} = \frac{N_2}{2}$  is indeed the worst case. For  $3 \leq i \leq k$ , we can argue in the same fashion.

Assume for sake of contradiction that the coefficient on the left-hand side is greater. Recall that  $\overline{N}_2 = (k + \mu_2^{\bullet})N_2$ . After subtracting  $\mu_2^{\bullet}(N_2 + \overline{N}_2)$  from both sides, the coefficient of  $\mu_2^{\bullet}$  on the left is  $\prod N_i + 1$ , while on the right it is  $\sum_{i \neq 2} (N_i + \overline{N}_i) + (1 + \sum_{i \neq 2} \mu_i^{\bullet})N_2$ . Thus we must have

$$\prod N_i + 1 > \sum_{i \neq 2} (N_i + \overline{N}_i) + (1 + \sum_{i \neq 2} \mu_i^{\bullet}) N_2 \ge \sum_{i \neq 2} (N_i + \overline{N}_i) + (1 + \mu_1^{\bullet}) N_2.$$

Using that

$$(1+\mu_1^{\bullet})N_2 = \left(1+\frac{N_1}{2}\right)N_2 \ge \left(1+\frac{N_2}{2}\right)N_2 \ge (1+\mu_2^{\bullet})N_2 = N_2 + \overline{N}_2 - kN_2$$

(recall here that we are assuming without loss of generality that  $N_1 \ge N_2 \ge \cdots \ge N_k$ ), this implies that  $\prod N_i + 1 \ge \sum (N_i + \overline{N}_i) - kN_2$ . Adding  $kN_2$  to both sides and multiplying both sides by  $1 + \sum \mu_i^{\bullet}$  results in

$$\left(\prod N_i + 1 + kN_2\right)\left(1 + \sum \mu_i^{\bullet}\right) \ge \left(1 + \sum \mu_i^{\bullet}\right)\sum \left(N_i + \overline{N}_i\right) > \left(1 + \sum \mu_i^{\bullet} + k\right)\left(\prod N_i + 1\right).$$

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In the second inequality, we applied (10) which we may do since we began with the assumption that we have a counterexample to (9). After simplification, we get that  $N_2(1 + \sum \mu_i^{\bullet}) > \prod N_i$ , and thus

$$\sum_{i \neq 2} N_i > 1 + \frac{1}{2} \sum N_i \ge 1 + \sum \mu_i^{\bullet} > \prod_{i \neq 2} N_i.$$

Since  $k \ge 6$ , this is a clear contradiction to eq. (11).

Having proven Claim 15, we are left with two cases to consider:  $\mu_i^{\bullet} = \frac{N_i}{2}$  for all  $1 \leq i \leq k$ , or  $\mu_1^{\bullet} = 0$ . It is easy to conclude in the former case, except when k = 6 and at least 5 values  $N_i$  are equal to 2, which has to be handled separately. See https://github.com/StijnCambie/AvSubOrder\_ktree/blob/main/2M-mu\_j\_large\_case1.mw for details. The final remaining case is when  $\mu_1^{\bullet} = 0$ . We obtain two new inequalities by multiplying eq. (12) with  $\frac{k+1}{2}$  and eq. (11) with  $(1 + \sum \mu_i^{\bullet})\frac{N_1}{6}$ , and use that  $N_1 = \max\{N_i\}$  and  $\mu_i^{\bullet} \leq \frac{N_i-1}{2}$ .

$$\frac{5(k+1)}{6} (\prod N_i + 1) \ge \frac{k+1}{2} \left( \sum_{2 \le i \le k} N_i - 2 \right) \sum_{1 \le i \le k} N_i \ge (1 + \sum \mu_i^{\bullet}) \sum_{1 \le i \le k} (1+k) N_i,$$
(13)

$$\frac{\prod N_i}{6} (1 + \sum \mu_i^{\bullet}) \ge (1 + \sum \mu_i^{\bullet}) \frac{N_1}{2} \sum_{2 \le i \le k} N_i \ge (1 + \sum \mu_i^{\bullet}) \sum_{2 \le i \le k} N_i \mu_i^{\bullet}.$$
(14)

Summing these two inequalities together, we have that eq. (9) holds as a corollary of

$$\left(\prod N_i + 1\right)\left(1 + \sum \mu_i^{\bullet} + k\right) \ge \left(1 + \sum \mu_i^{\bullet}\right) \sum \left(N_i\left(1 + k + \mu_i^{\bullet}\right)\right).$$

We remark that by considering a suitable k-broom, one can show that theorem 4 is sharp, as was also the case for trees.

## 6 Conclusion

This paper together with [13, Thm. 18 & 20] answers all of the open questions from [16] except for one, which was stated as rather general and open-ended:

**Problem 16.** For a given *r*-clique R,  $1 \le r < k$ , what is the (local) mean order of all sub-*k*-trees containing R?

One natural version of this question is to consider the local mean sub-k-tree order over sub-k-trees that contain a fixed vertex. In this direction, we prove the following result, which can be considered as another monotonicity result related to [13, Thm. 23].

**Theorem 17.** Let T be a k-tree,  $k \ge 2$ , C a k-clique of T, and v a vertex in C. Then  $\mu(T; v) < \mu(T; C)$ .

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 $\diamond$ 

Proof. The statement is trivially true if  $|T| \leq k + 1$ . So assume that T with  $|T| \geq k + 2$ is a minimum counterexample to the statement. Recalling the decomposition into trees  $T_{i,j}$  used earlier, note that all sub-k-trees containing v and not C are part of  $T_{i,j}$  for some i, j. Without loss of generality, we can assume that  $\mu(T_{1,1}; v) = \max_{i,j} \mu(T_{i,j}; v)$ . It suffices to prove that  $\mu(T_{1,1}; v) < \mu(T; C)$ . Taking into account (3), it is sufficient to consider the case where C is a simplicial k-clique of T. Let u be the simplicial vertex of  $B_1$ . Let  $T' = T \setminus \{u\}$  and  $C' = B_1 \setminus \{u\}$ .

Claim 18. We have  $\mu(T'; C') < \mu(T; C)$ .

*Proof.* Let R = R(T'; C') and N = N(T'; C'). We now need to prove that  $\mu(T; C) = \frac{2R+N+k}{2N+1} > \frac{R}{N} = \mu(T'; C')$ , which is equivalent to  $N + k > \frac{R}{N}$ . The latter is immediate since  $N \ge |T'| - (k-1)$  and  $\frac{R}{N} = \mu(T'; C') \le |T'|$ .

Since the sub-k-trees containing v are exactly those that contain C, or sub-k-trees of T' containing C', or k-cliques within  $B_1$  different from C, we conclude that  $\mu(T; v) < \mu(T; C)$ .

Luo and Xu [13, Ques. 35] also asked if for a given order, a k-tree attaining the largest global mean sub-k-tree order is necessarily a caterpillar-type k-tree. In contrast with the questions in [16], this question is still open for trees. We prove that the local version (proven in [3, Thm. 3]), which states that for fixed order, the maximum is attained by a broom, is also true for the generalization of k-trees. This is almost immediate by observations from [16].

**Proposition 19.** If a k-tree T of order n and k-clique C of T attain the maximum possible value of  $\mu(T; C)$ , then T has to be a k-broom with C being one of its simplicial k-cliques.

Proof. Let  $T'_C$  be the characteristic 1-tree of T with respect to C. Then by [16, Lem. 11]  $\mu(T; C) = \mu(T'_C; C) + k - 1$ . Since  $T'_C$  is a tree on n - (k - 1) vertices, by [3, Thm. 3], the maximum local mean subtree order is attained by a broom B. Since there is a k-broom T with C being a simplicial k-clique for which  $T'_C \cong B$  with C as root, this maximum can be attained. Reversely, if  $\mu(T'_C; C)$  is maximized, then  $T'_C$  is a broom where C is its root (and thus simplicial).

As such, we conclude that the k-tree variants of many results on the average subtree order for trees are now also proven. The analogue of [10, Ques. (7.5)] can be considered as the only question among them where the answer is slightly different for k-trees: in contrast with the case of trees (k = 1), the maximum local mean sub-k-tree order cannot occur in a k-clique with degree 2 when  $k \ge 2$  (with one small exception).

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