

On the quartet distance given partial information

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Abstract

Let T be an arbitrary phylogenetic tree with n leaves. It is well-known that the average quartet distance between two assignments of taxa to the leaves of T is $\frac{2}{3}\binom{n}{4}$. However, a longstanding conjecture of Bandelt and Dress asserts that $(\frac{2}{3} + o(1))\binom{n}{4}$ is also the *maximum* quartet distance between two assignments. While Alon, Naves, and Sudakov have shown this indeed holds for caterpillar trees, the general case of the conjecture is still unresolved. A natural extension is when partial information is given: the two assignments are known to coincide on a given subset of taxa. The partial information setting is biologically relevant as the location of some taxa (species) in the phylogenetic tree may be known, and for other taxa it might not be known. What can we then say about the average and maximum quartet distance in this more general setting? Surprisingly, even determining the *average* quartet distance becomes a nontrivial task in the partial information setting and determining the maximum quartet distance is even more challenging, as these turn out to be dependent of the structure of T . In this paper we prove nontrivial asymptotic bounds that are sometimes tight for the average quartet distance in the partial information setting. We also show that the Bandelt and Dress conjecture does not generally hold under the partial information setting. Specifically, we prove that there are cases where the average and maximum quartet distance substantially differ.

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1 Introduction

Phylogenetic tree reconstruction is a central problem in computational biology. An important concept in this area are undirected phylogenetic trees, where the taxa (species) are mapped bijectively to the leaves of the tree and the tree-structure represents the evolutionary relationship among the taxa. More formally, a phylogenetic tree T of order n is an undirected tree with n leaves where each internal vertex is incident with three edges. For a taxa set $[n] = \{1, \dots, n\}$, a bijection between $[n]$

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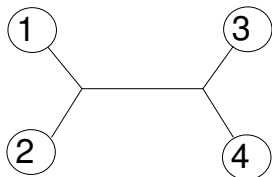


Figure 1: The quartet tree [12|34].

and the leaves of T forms a *labeled* phylogenetic tree. Hereafter, when we refer to trees or labeled trees we always mean phylogenetic trees or labeled phylogenetic trees, respectively.

The smallest labeled tree is a *quartet*, a tree with four leaves. A quartet with leaves labeled $\{a, b, c, d\}$ is denoted by $[ab|cd]$ when there is an edge in the tree separating the pair $\{a, b\}$ from the pair $\{c, d\}$, as shown in Figure 1. Observe that there are precisely three possible labeled quartets on a given set of four taxa $\{a, b, c, d\}$: either $[ab|cd]$ or $[ac|bd]$ or $[ad|bc]$. A labeled tree of order n therefore contains the information of exactly $\binom{n}{4}$ quartets.

Significant research effort has been devoted to phylogenetic tree reconstruction from quartets, a field denoted as *quartet-based reconstruction* (see e.g. [5, 11, 12, 14, 20]). Here, several (or even all $\binom{n}{4}$) quartets are constructed, normally using some *quartet oracle* [7, 8, 10]. These quartets are combined together into the big tree on the full taxa set. The problem of deciding whether there exists a tree compatible¹ to all the quartets in a given set, is NP-complete [18]. Moreover, the ideal case in which all quartets are compatible with a single tree, is very rare. This raises the problem of finding a tree maximizing the number of compatible quartets - *maximum quartet compatibility* (MQC) [15]. As MQC is NP-hard, several approximation algorithms have been designed for it [4, 13, 16, 17], but the best approximation to the general problem is still obtained by a naive “random tree” with expected approximation ratio of $\frac{1}{3}$.

Related to the problem of compatibility is the concept of *quartet distance* [9, 19]. This notion quantifies the similarity of two different labeled trees of order n , or even two identical trees with different labellings, by counting how many quartets are compatible with both of them. More formally, if T_1 and T_2 are two labeled trees of order n , let $qd(T_1, T_2)$ denote the difference between $\binom{n}{4}$ and the number of quartets compatible with both T_1 and T_2 . Several questions immediately arise. Here are some notable ones: How large can $qd(T_1, T_2)$ possibly be? How large could it be if T_1 and T_2 have the same tree structure? In the latter case, how large could it be if we know that some subset of taxa are pinned to their leaves in both trees? What can be said about (the random variable) $qd(T_1, T_2)$ if T_1 and T_2 are the same tree, and a subset of taxa are pinned to their leaves in both trees, while the unpinned taxa are placed randomly in the remaining leaves in both trees?

Somewhat surprisingly, already for the first question, the answer is significantly smaller than

¹The notion of compatibility, which is central in phylogeny, is formally defined in Section 2.

$\binom{n}{4}$, namely, one can never obtain total incompatibility. Bandelt and Dress [3] showed that the maximum is always strictly smaller than $\frac{14}{15}\binom{n}{4}$ for $n \geq 6$. They also conjectured that the ratio between the maximum quartet distance and $\binom{n}{4}$ converges to $\frac{2}{3}$ as n tends to infinity.

Conjecture 1.1 (Bandelt and Dress). *The maximum quartet distance between two labeled trees of order n is $(\frac{2}{3} + o(1))\binom{n}{4}$.*

As the lower bound of $\frac{2}{3}\binom{n}{4}$ can be easily obtained by the random labeling argument (there are also highly explicit constructions achieving this lower bound [6]), Conjecture 1.1 implies, perhaps surprisingly, that the average distance between two random trees is asymptotically the same as the maximum distance. Alon, Snir, and Yuster [2] improved the upper bound on the maximum quartet distance proving it is asymptotically smaller than $\frac{9}{10}\binom{n}{4}$. Alon, Naves, and Sudakov [1] further improved the upper bound to at most $(0.69 + o(1))\binom{n}{4}$. In fact, for the particular important case where both T_1 and T_2 are the *caterpillar tree* they established the validity of Conjecture 1.1. We stress that even if T_1 and T_2 are assumed to be different labellings of the *same* tree, nothing better than the lower bound ratio $\frac{2}{3} + o(1)$ and the upper bound $0.69 + o(1)$ is known.

We note that the random labeling which achieves the $\frac{2}{3}$ ratio is the natural approach one takes when no information on the tree or its labeling is given. In fact, even if the tree structure is known, but no information on the labeling is given, the natural approach is still random labeling. However, a more likely scenario is that *some information* is known. Our contribution here is for this more general case. We consider here the case where the tree structure is known and some subset of taxa are known to be at certain leaves. It is reasonable to expect that the more information given, the random labeling approach of the remaining taxa will achieve a better ratio, approaching 0 when almost full information is given. However, quantifying this ratio, while straightforward in the “no information” setting, becomes difficult in the partial information setting. Likewise, it is reasonable to expect that the more information given, the maximum possible distance will achieve a better ratio. Quantifying this ratio is not only difficult, but it is also not clear what should be the “right conjecture”. In fact, in some cases, it is provably not true that the average distance is asymptotically the same as the maximum distance, as conjectured by Bandelt and Dress in the no information setting.

In the next section we formalize the aforementioned problems and results whereas in the later sections we prove our main claims.

2 Problems definitions and statements of main results

For a tree T , the set of leaves of T is denoted by $\mathcal{L}(T)$. For $A \subseteq \mathcal{L}(T)$, the topological subtree $T|_A$ is the tree obtained by removing the leaves $\mathcal{L}(T) \setminus A$, the paths leading exclusively to them, and contracting vertices with degree two.

Recall that an isomorphism \simeq between two graphs where some of the vertices of the graphs are labeled and some are not is a bijective function between the vertices which preserves adjacencies

and non-adjacencies and a labeled vertex in the first tree is mapped to a labeled vertex in the other tree having the same label, while a non-labeled vertex in the first tree is mapped to a non-labeled vertex in the other tree. For two labeled trees T and T' , we say that T *satisfies* T' if $\mathcal{L}(T') \subseteq \mathcal{L}(T)$ and $T|_{\mathcal{L}(T')} \simeq T'$, namely the topological subtree of T induced by $\mathcal{L}(T')$ is isomorphic to T' .

If T' is a quartet, we say that T' is *compatible* with T if T satisfies T' . Observe that if T is a labeled tree of order n , then it contains precisely $\binom{n}{4}$ compatible quartets, each one corresponding to the labeled topological subtree obtained by considering four taxa. Let, therefore $\mathcal{Q}(T)$ denote the quartet set consisting of all compatible quartets of the labeled tree T . Now, given two labeled trees T_1 and T_2 of order n , (that is, both are labeled with the taxa set $[n]$) let $qd(T_1, T_2) = \binom{n}{4} - |\mathcal{Q}(T_1) \cap \mathcal{Q}(T_2)|$. We call $qd(T_1, T_2)$ the *quartet distance* between T_1 and T_2 . We mention here that Colonijs and Schulze observed that if $qd(T_1, T_2) = 0$ then T_1 and T_2 are isomorphic (see [15]). Of course, it may be that T_1 and T_2 have the same tree-structure (i.e. they are isomorphic as unlabeled trees) but $qd(T_1, T_2) > 0$, for example $qd([ab|cd], [ac|bd]) = \binom{4}{4} - 0 = 1$.

Let \mathcal{T}_n denote the set of all labeled trees of order n . Consider the equivalence relation on \mathcal{T}_n where two elements are equivalent if they have the same tree structure. Hence, we can represent an equivalence class by T , where T is an unlabeled tree of order n . For example, if $n = 4$ then there is only one equivalence class (an unlabeled quartet) consisting of the three possible quartets on $\{1, 2, 3, 4\}$. Let X_n be the random variable corresponding to $qd(T_1, T_2)$ where T_1 and T_2 are uniformly drawn (say, with replacement) from \mathcal{T}_n . By linearity of expectation we have that $\mathbb{E}[X_n] = \frac{2}{3} \binom{n}{4}$. Similarly, for an unlabeled tree T of order n , let X_T be the random variable corresponding to $qd(T_1, T_2)$ where T_1 and T_2 are uniformly drawn random labellings of T (one can view this as sampling from \mathcal{T}_n conditioned on a given tree structure). Again, linearity of expectation gives $\mathbb{E}[X_T] = \frac{2}{3} \binom{n}{4}$. Let M_n be the maximum possible value that X_n can attain, or stated otherwise, just the maximum possible quartet distance between two elements of \mathcal{T}_n . Similarly, let M_T be the maximum possible value that X_T can attain, or stated otherwise, the maximum possible quartet distance between two labellings of T . Notice that $M_n \geq M_T$ for every tree T of order n .

Using the notations X_n, X_T, M_n, M_T we can now reformulate the aforementioned results and conjecture from the introduction. Bandelt and Dress conjectured that $M_n = (1 + o(1)) \frac{2}{3} \binom{n}{4} = (1 + o(1)) \mathbb{E}[X_n]$ which, if true, implies that $M_T = (1 + o(1)) \frac{2}{3} \binom{n}{4} = (1 + o(1)) \mathbb{E}[X_T]$ for every tree T of order n . The result of [1] proves that $M_n \leq (0.69 + o(1)) \binom{n}{4}$. The *caterpillar* CAT_n of order $n \geq 4$ is the tree having only two internal vertices x, y adjacent to two leaves each. We call the four edges connecting x to its two adjacent leaves and y to its two adjacent leaves *endpoint edges*. So, a quartet is a caterpillar of order 4 where every edge except the central edge is an endpoint edge and every tree of order 5 is isomorphic to CAT_5 , but already for $n = 6$ not every tree is a caterpillar. The result of [1] also proves that $M_{\text{CAT}_n} = (1 + o(1)) \frac{2}{3} \binom{n}{4}$ so at least for caterpillars, the Bandelt and Dress conjecture holds.

We are now ready to state our generalization for X_T and M_T to the partial information setting. Let T be an unlabeled tree of order n and let $S \subseteq \mathcal{L}(T)$ be a subset of leaves. An *S-labeling* (also called a partial labeling if S is clear from the context) is a labeling of S with the taxa set

$[k]$ where $k = |S|$. We think of a partial labeling as if some information is given to us: we are told which leaf is assigned with a taxa from $[k]$ but we have no information about the assignment of the remaining $n - k$ taxa to the remaining $n - k$ leaves. As we are concerned with asymptotic behavior, we set $k = \alpha n$ where $\alpha \in [0, 1]$ is a fixed rational and always assume that n is such that αn is an integer. We let $T(S)$ denote the tree T with its S -labeling. A *completion* of $T(S)$ is a full labeling of $T(S)$ with the remaining $n - k$ taxa assigned to the remaining set of leaves $\mathcal{L}(T) \setminus S$. Let $X_{T(S)}$ be the random variable corresponding to $qd(T_1, T_2)$ where T_1 and T_2 are independently and randomly chosen completions of $T(S)$. Notice that it is more convenient and equivalent to view T_1 as some fixed completion and only consider T_2 as randomly chosen from all $(n - k)!$ possible completions. Let $M_{T(S)}$ be the maximum possible quartet distance between two completions of $T(S)$ (again, it may be more convenient and equivalent to fix one completion and consider the maximum quartet distance between the fixed completion and the other completions). Notice that $X_T = X_{T(\emptyset)}$, $M_T = M_{T(\emptyset)}$ and $X_{T(\mathcal{L}(T))} = M_{T(\mathcal{L}(T))} = 0$.

The definitions of $X_{T(S)}$ and $M_{T(S)}$ as generalizations of the well-studied “no-information” variants X_T and M_T give rise to several intriguing questions from which naturally stand out the following, where we assume that $\alpha \in [0, 1]$ is fixed, T is an unlabeled tree of order n , and $S \subset \mathcal{L}(T)$ has $|S| = \alpha n$.

Definition 2.1.

$$\begin{aligned} \text{minexp}(T, \alpha) &= \min_S \mathbb{E}[X_{T(S)}] \\ \text{minexp}(n, \alpha) &= \min_T \text{minexp}(T, \alpha) \\ \text{maxexp}(T, \alpha) &= \max_S \mathbb{E}[X_{T(S)}] \\ \text{maxexp}(n, \alpha) &= \max_T \text{maxexp}(T, \alpha) \\ \text{maxqd}(T, \alpha) &= \max_S M_{T(S)} \\ \text{maxqd}(n, \alpha) &= \max_T \text{maxqd}(T, \alpha) \end{aligned}$$

Hence, assuming an α fraction of the taxa are bound to fixed locations, $\text{minexp}(T, \alpha)$ (resp. $\text{maxexp}(T, \alpha)$) asks for the smallest (resp. largest) expectation of the quartet distance of two labellings of T , and $\text{minexp}(n, \alpha)$ (resp. $\text{maxexp}(n, \alpha)$) asks for the smallest (resp. largest) expectation of the quartet distance of two labellings of any tree of order n . Likewise, $\text{maxqd}(T, \alpha)$ asks for the largest quartet distance of two labellings of T and $\text{maxqd}(n, \alpha)$ asks for the largest quartet distance of two labellings of any tree of order n .

When $\alpha = 1$, all of these parameters are zero. On the other hand, when $\alpha = 0$ all the first four parameters are (trivially) $\frac{2}{3} \binom{n}{4}$ and the fifth parameter amounts to M_T . But when $0 < \alpha < 1$ all the first four parameters (moreover the fifth and sixth) become nontrivial to determine.

As there are exponentially many non-isomorphic trees of order n , it seems hopeless to obtain

a “closed” formula for $\text{minexp}(T, \alpha)$, $\text{maxexp}(T, \alpha)$, and $\text{maxqd}(T, \alpha)$ for each possible T . Hence, the main combinatorial challenge is to either determine or at least find nontrivial bounds for $\text{minexp}(n, \alpha)$, $\text{maxexp}(n, \alpha)$ and $\text{maxqd}(n, \alpha)$.

We next state our main results which concern $\text{minexp}(n, \alpha)$, $\text{maxexp}(n, \alpha)$. We mention that the constants in the forthcoming theorems are (quite obviously) polynomials of degree 4 in α . For clarity of exposition we will therefore state our results also for the median case $\alpha = \frac{1}{2}$. Our first result concerns $\text{minexp}(n, \alpha)$ which is asymptotically determined.

Theorem 2.2.

$$\text{minexp}(n, \alpha) = \left(\frac{2}{3}(1 - \alpha)^4 + \frac{8}{3}\alpha(1 - \alpha)^3 \right) \binom{n}{4} (1 + o(1)).$$

In particular,

$$\text{minexp}(n, \frac{1}{2}) = \frac{5}{24} \binom{n}{4} (1 + o(1)).$$

The method used in the proof of Theorem 2.2, which suffices to asymptotically determine $\text{minexp}(n, \alpha)$ can also be used to supply a relatively simple upper bound of $\frac{5}{8} \binom{n}{4} (1 + o(1))$ for $\text{maxexp}(n, \frac{1}{2})$ and, more generally, $\left(\frac{2}{3} - \frac{2\alpha^4}{3} \right) \binom{n}{4} + o(n^4)$ for $\text{maxexp}(n, \alpha)$ (see Section 4). However as we next prove, this upper bound is not tight and one can always do significantly better. Furthermore, the lower bound we obtain for $\text{maxexp}(n, \alpha)$, is quite close to it. The proof of our upper bound requires using linear and non-linear optimization.

Theorem 2.3.

$$\begin{aligned} & \left(\frac{2}{3} - \frac{653\alpha^4 + 414\alpha^3 + 33\alpha^2}{1650} \right) \binom{n}{4} + o(n^4) \\ & \geq \text{maxexp}(n, \alpha) \geq \\ & \left(\frac{2}{3} - \frac{10\alpha^4 + 32\alpha^3 + 12\alpha^2}{81} \right) \binom{n}{4} + o(n^4). \end{aligned}$$

In particular,

$$0.606 \binom{n}{4} (1 + o(1)) \geq \text{maxexp}(n, \frac{1}{2}) \geq 0.572 \binom{n}{4} (1 + o(1)).$$

As for $\text{maxqd}(n, \alpha)$, the situation becomes even more involved bearing in mind that $\text{maxqd}(n, 0)$ is a longstanding conjecture. That being said, it is interesting to note that unlike the case $\alpha = 0$ where Conjecture 1.1 states that M_T and $\mathbb{E}[X_T]$ are asymptotically the same for every tree T of order n , this is provably not so in many cases of the partial information setting. Namely, there are cases of trees T and partial labellings $T(S)$ such that $\mathbb{E}[X_{T(S)}]$ is significantly smaller than $M_{T(S)}$, as the next theorem shows. Recall that a *split* in a tree T is an edge which is not incident to a leaf. Removing a split from T separates it to two subtrees, as if $e = uv$ is a split, then after removal there are two tree components T_u and T_v , where u is a non-leaf in one component and v is a non-leaf in the other. Both u and v have degree 2 in these components so they can be contracted

to an edge which we call the *join edge* of the split, and hence after contraction, the components T_u and T_v become proper (phylogenetic) trees. Note that a split can be identified with the partition $(\mathcal{L}(T_u), \mathcal{L}(T_v))$ of $\mathcal{L}(T)$.

Theorem 2.4. *Let $0 < \alpha < 1$. Let T be a tree of order n and let $T(S)$ be a partial labeling where $|S| = \alpha n$. Suppose there exists a split $e = uv$ such that $\mathcal{L}(T_u) = S$ and T_v is a caterpillar where the joint edge of T_v is an endpoint edge of the caterpillar. Then*

$$M_{T(S)} - \mathbb{E}[X_{T(S)}] = \Theta(n^4).$$

We note that there are many $T(S)$ which satisfy Theorem 2.4. In fact, let T_1 be any labeled tree of order αn and let $T_2 = CAT_{n(1-\alpha)}$ where T_2 is unlabeled. Split some edge of T_1 introducing a new vertex u and split some endpoint edge of T_2 introducing a new vertex v and connect u and v . The resulting $T(S)$ satisfies Theorem 2.4. We emphasize that Theorem 2.4 does not undermine the Badelt-Dress conjecture. In fact, the statement of the theorem is reminiscent of the fact that for the related measure of triplet distance for rooted trees, total incompatibility can be reached.

In Section 3 we develop a form for expressing $\mathbb{E}[X_{T(S)}]$ and use it to prove our result concerning the minimum expectation, namely Theorem 2.2. In Section 4 we prove our bounds for maximum expectation, namely Theorem 2.3. The proof uses the form developed in Section 3 but requires considerable more effort in order to exploit it for a good upper bound. In Section 5 we prove Theorem 2.4.

3 $\mathbb{E}[X_{T(S)}]$ and $minexp(n, \alpha)$

Given a partial labeling $T(S)$ with $|S| = k = \alpha n$, we express $\mathbb{E}[X_{T(S)}]$ using certain parameters of the tree involving pairs and triples of taxa from $[k]$. Although our approach gives an exact expression for $\mathbb{E}[X_{T(S)}]$ it is a nontrivial task to determine which tree structures and partial assignments thereof optimize that expression.

3.1 A formula for $\mathbb{E}[X_{T(S)}]$

Recall that T is a tree on n leaves, $S \subset \mathcal{L}(T)$ with $|S| = k = \alpha n$, the taxa in $[k]$ are bijectively assigned to S , and $T(S)$ denotes this partial labeling. The set of all $(n-k)!$ completions of $T(S)$ is viewed as a symmetric probability space. Let T_0 be an arbitrary fixed completion of $T(S)$. Then, $X_{T(S)} = qd(T_0, T^*)$ where T^* is a randomly chosen completion. We can then write $X_{T(S)}$ as the sum of $\binom{n}{4}$ indicator random variables, one for each quartet $q \in Q(T_0)$ and we denote this indicator variable by $X_T(q)$, where $X_T(q) = 0$ if q is satisfied by T^* . Indeed observe that

$$X_{T(S)} = qd(T_0, T^*) = \sum_{q \in Q(T_0)} X_T(q).$$

We can split these indicator variables into 5 types, according to the number of elements of $[k]$ that q contains. We say that an indicator variable $X_T(q)$ is of type i if q contains i elements of $[k]$. We next determine $\mathbb{E}[X_T(q)]$ for the various types.

Type-4 variables: In this case $X_T(q) \equiv 0$ since all four taxa of q are in the same position in both T^* and T_0 , so q is satisfied by T^* .

Type-0 variables: In this case $\mathbb{E}[X_T(q)] = \frac{2}{3}$ since each of the three possible quartets on the elements of q is equally likely to be in $\mathcal{Q}(T^*)$, so q is satisfied by T^* with probability $\frac{1}{3}$.

Type-1 variables: Suppose $q = [ax|yz]$ where $a \in [k]$. If we are given the set $P \subset \mathcal{L}(T) \setminus S$ of three leaves of T^* occupying $\{x, y, z\}$ (but not told which of them goes to each element of P) each of the three quartets $[ax|yz], [ay|xz], [az|xy]$ is equally likely in T^* . Hence, given P , q is satisfied by T^* with probability $\frac{1}{3}$. As this holds for any P , we have that $\mathbb{E}[X_T(q)] = \frac{2}{3}$.

Type-2 variables: Let $a, b \in [k]$ and consider the sum of all type-2 variables involving a, b , denoting it by $X_T(\{a, b\})$. Let $N_{a,b}$ be the number of pairs of leaves in $\mathcal{L}(T) \setminus S$ such that if we take two taxa x, y in $[n] \setminus [k]$ and assign x, y to the pair of leaves, then in the resulting quartet, a and b are not on the same side. Then $\binom{n-k}{2} - N_{a,b}$ is the number of pairs of leaves in $\mathcal{L}(T) \setminus S$ such that if we take two taxa x, y in $[n] \setminus [k]$ and assign x, y to the pair of leaves, then in the resulting quartet, a and b are on the same side. For convenience, let $p_{a,b} = N_{a,b} / \binom{n-k}{2}$ and so we can view $p_{a,b}$ as the probability that if we take a random pair of leaves in $\mathcal{L}(T) \setminus S$ and assign them to elements of $[n] \setminus [k]$, then in the resulting quartet, the pair a, b will not be on the same side.

Given a type-2 variable $X_T(q)$ with $q = [ax|by]$, the probability that q is not satisfied by T^* is $(1 - p_{a,b}) + p_{a,b}/2 = 1 - p_{a,b}/2$ since with probability $1 - p_{a,b}$ in the quartet induced by the taxa of q in T^* the pair a, b will be on the same side (and then q is surely not satisfied by T^*), and with probability $p_{a,b}$ they will not be on the same side and then q is satisfied by T^* with probability $\frac{1}{2}$, as the two quartets $[ax|by]$ and $[ay|bx]$ are equally likely. On the other hand, given a type-2 variable $X_T(q)$ with $q = [ab|xy]$, the probability that q is not satisfied by T^* is clearly $p_{a,b}$. Summing over all type-2 variables involving a, b , we have that

$$\mathbb{E}[X_T(\{a, b\})] = N_{a,b}(1 - p_{a,b}/2) + \left(\binom{n-k}{2} - N_{a,b}\right)p_{a,b} = \binom{n-k}{2}(2p_{a,b} - 1.5p_{a,b}^2).$$

Type-3 variables: Let $a, b, c \in [k]$ and consider the sum of all type-3 variables involving a, b, c , denoting it by $X_T(\{a, b, c\})$. Let $N_{ab|c}$ be the number of leaves in $\mathcal{L}(T) \setminus S$ such that if we assign that leaf a taxa x from $[n] \setminus [k]$ the resulting quartet on a, b, c, x is $[ab|cx]$. Similarly define $N_{ac|b}$ and $N_{bc|a}$. Observe that $N_{ab|c} + N_{ac|b} + N_{bc|a} = n - k$, so by dividing by $n - k$ we can define $p_{ab|c}$, $p_{ac|b}$ and $p_{bc|a}$ accordingly where $p_{ab|c} + p_{ac|b} + p_{bc|a} = 1$.

Given a type-3 variable $X_T(q)$ with $q = [ab|cx]$, the probability that q is not satisfied by T^* is $p_{ac|b} + p_{bc|a}$. Given a type-3 variable $X_T(q)$ with $q = [ac|bx]$, the probability that q is not satisfied by T^* is $p_{ab|c} + p_{bc|a}$. Given a type-3 variable $X_T(q)$ with $q = [bc|ax]$, the probability that q is not

satisfied by T^* is $p_{ab|c} + p_{ac|b}$. Summing over all type-3 variables involving a, b, c , we have that

$$\begin{aligned}\mathbb{E}[X_T(\{a, b, c\})] &= N_{ab|c}(p_{ac|b} + p_{bc|a}) + N_{ac|b}(p_{ab|c} + p_{bc|a}) + N_{bc|a}(p_{ab|c} + p_{ac|b}) \\ &= 2(n-k)(p_{ab|c}p_{ac|b} + p_{ab|c}p_{bc|a} + p_{ac|b}p_{bc|a}).\end{aligned}$$

We therefore obtain an exact expression for $\mathbb{E}[X_{T(S)}]$ expressed in terms of the various $p_{a,b}$ for unordered pairs $a, b \in [k]$ and the various $p_{ab|c}, p_{ac|b}, p_{bc|a}$ for unordered triples $a, b, c \in [k]$ which is:

$$\begin{aligned}\frac{2}{3}\binom{n-k}{4} + \frac{2}{3}k\binom{n-k}{3} + \sum_{a,b \in [k]} \binom{n-k}{2}(2p_{a,b} - 1.5p_{a,b}^2) + \\ \sum_{a,b,c \in [k]} 2(n-k)(p_{ab|c}p_{ac|b} + p_{ab|c}p_{bc|a} + p_{ac|b}p_{bc|a}).\end{aligned}\tag{1}$$

For $k = \alpha n$ we obtain

$$\begin{aligned}\mathbb{E}[X_{T(S)}] &= \left(\frac{2}{3}(1-\alpha)^4 + \frac{8}{3}\alpha(1-\alpha)^3\right)\binom{n}{4} \\ &+ (1-\alpha)^2\binom{n}{2} \sum_{a,b \in [k]} (2p_{a,b} - 1.5p_{a,b}^2) \\ &+ 2(1-\alpha)n \sum_{a,b,c \in [k]} (p_{ab|c}p_{ac|b} + p_{ab|c}p_{bc|a} + p_{ac|b}p_{bc|a}) + o(n^4).\end{aligned}\tag{2}$$

3.2 $\text{minexp}(n, \alpha)$

We determine $\text{minexp}(n, k/n)$ for every $k = 1, \dots, n-1$ and hence determine $\text{minexp}(n, \alpha)$ asymptotically for every $\alpha \in [0, 1]$ thereby proving Theorem 2.2. Our goal is to minimize (1) over all $T(S)$ with $|S| = k$. Clearly if $T(S)$ has the property that $p_{a,b} = 0$ for all $a, b \in [k]$ and if we could have that two out of the three $p_{ab|c}, p_{ac|b}, p_{bc|a}$ are zero for all triples $a, b, c \in [k]$, then we have minimized $\mathbb{E}[X_{T(S)}]$. Indeed, there are many cases where this can be attained. Recalling the notion of a split from Section 2, suppose that T is a tree of order n and there is a split $e = uv$ such that in the resulting trees T_u and T_v we have $|\mathcal{L}(T_u)| = k$ and $|\mathcal{L}(T_v)| = n-k$. One example of a tree T for which this holds for all $k = 1, \dots, n-1$ is CAT_n , but for a given k , one can construct many other trees with this property. Now, assume that $S = \mathcal{L}(T_u)$, so indeed $|S| = k$ and consider $T(S)$. It is immediate to verify that $T(S)$ has the property that $p_{a,b} = 0$ for all $a, b \in [k]$. Indeed, in any quartet of type-2 involving a, b , we have that a, b will be on the same side in any completion of $T(S)$. Furthermore, precisely two out of the three $p_{ab|c}, p_{ac|b}, p_{bc|a}$ are zero and the third equals 1 for all triples $a, b, c \in [k]$, as in any quartet of type-3 involving the three of them, it holds that in all completions either a, b are always on the same side (so $p_{ab|c} = 1$) or else a, c are on the same side (so $p_{ac|b} = 1$) or else b, c are on the same side (so $p_{bc|a} = 1$). Hence, we have that $T(S)$ is as

small as possible and obtain from (1) that

$$\text{minexp}(n, k/n) = \frac{2}{3} \binom{n-k}{4} + \frac{2}{3} k \binom{n-k}{3}.$$

Consequently, using (2) we obtain that

$$\text{minexp}(n, \alpha) = \left(\frac{2}{3} (1-\alpha)^4 + \frac{8}{3} \alpha (1-\alpha)^3 \right) \binom{n}{4} + o(n^4).$$

For $\alpha = \frac{1}{2}$ this gives

$$\text{minexp}(n, \frac{1}{2}) = \frac{5}{24} \binom{n}{4} (1 + o(1)).$$

This proves Theorem 2.2. □

4 $\text{maxexp}(n, \alpha)$

We can use (1) to obtain an upper bound for $\text{maxexp}(n, k/n)$ but, as we shall see, unlike the case of $\text{minexp}(n, k/n)$, this bound cannot be realized by a construction. Consider the expressions $r(a, b) = 2p_{a,b} - 1.5p_{a,b}^2$ and $r(a, b, c) = p_{ab|c}p_{ac|b} + p_{ab|c}p_{bc|a} + p_{ac|b}p_{bc|a}$. Recall that $r(a, b)$ is maximized when $p_{a,b} = \frac{2}{3}$ and $r(a, b, c)$ is maximized when $p_{ab|c} = p_{ac|b} = p_{bc|a} = \frac{1}{3}$. We therefore have that $r(a, b) \leq \frac{2}{3}$ and $r(a, b, c) \leq \frac{1}{3}$. Consequently, we obtain from (1) that

$$\text{maxexp}(n, k/n) \leq \frac{2}{3} \binom{n-k}{4} + \frac{2}{3} k \binom{n-k}{3} + \frac{2}{3} \binom{k}{2} \binom{n-k}{2} + \frac{2}{3} \binom{k}{3} (n-k).$$

Using (2) we obtain that

$$\text{maxexp}(n, \alpha) \leq \left(\frac{2}{3} - \frac{2\alpha^4}{3} \right) \binom{n}{4} + o(n^4)$$

which for $\alpha = \frac{1}{2}$ this gives

$$\text{maxexp}(n, \frac{1}{2}) \leq \frac{5}{8} \binom{n}{4} (1 + o(1)).$$

Unfortunately, it is impossible to *simultaneously* achieve $r(a, b) = \frac{2}{3}$ for all pairs a, b and $r(a, b, c) = \frac{1}{3}$ for all triples a, b, c . There is, however, a construction which does achieve these optimal bounds for many pairs and many triples, so we use this construction as our lower bound for $\text{maxexp}(n, \alpha)$.

4.1 Lower bound for $\text{maxexp}(n, \alpha)$

Take three copies of the caterpillar $CAT_{n/3+1}$, denoting them by C_1, C_2, C_3 . Denote the leaves of C_i ordered from left to right by $c_{i,0}, \dots, c_{i,n/3}$. Assign the taxa $\{1, \dots, \alpha n/3\}$ to the leaves

$c_{1,1}, \dots, c_{1,\alpha n/3}$. Assign the taxa $\{\alpha n/3 + 1, \dots, 2\alpha n/3\}$ to the leaves $c_{2,1}, \dots, c_{2,\alpha n/3}$. Assign the taxa $\{2\alpha n/3 + 1, \dots, \alpha n\}$ to the leaves $c_{3,1}, \dots, c_{3,\alpha n/3}$. Now create a tree H by identifying the $c_{i,0}$ for $i = 1, 2, 3$, so H is a “3-way caterpillar”. As αn of the leaves of H are assigned with the taxa set $[k] = [\alpha n]$, we denote this partial labeling by $H(S)$. We compute (1) for $H(S)$. The number of pairs a, b of elements of $[k]$ where a and b are in distinct C_i is $3(\alpha n/3)^2 = \alpha^2 n^2/3$ and for such pairs we indeed have $p_{a,b} = (2/3) + o(1)$ which, recall, makes $r(a, b)$ asymptotically reach its maximum value $2/3$. There are $3\binom{\alpha n/3}{2} = (1 + o(1))\alpha^2 n^2/6$ pairs a, b of elements of S where a and b are in the same C_i . For such pairs we have $p_{a,b} = (4/9) + o(1)$ as for a and b to be in different sides of a quartet we must choose an unlabeled leaf from C_i and another unlabeled leaf not from C_i . Hence, $r(a, b) = (16/27) + o(1)$ in this case. There are $\alpha^3 n^3/27$ triples $a, b, c \in S$ where each is in a distinct C_i and in this case we have $p_{ab|c} = p_{ac|b} = p_{bc|a} = (1/3) + o_n(1)$ so $r(a, b, c) = \frac{1}{3} + o(1)$ and asymptotically reaches its maximum value. There are $3\binom{\alpha n/3}{3} = (1 + o(1))\alpha^3 n^3/54$ triples $a, b, c \in S$ where all three are in the same C_i and in this case we have that $\{p_{ab|c}, p_{ac|b}, p_{bc|a}\} = \{0, (1/3) + o(1), (2/3) + o(1)\}$ (which variable gets which value depends on the order of a, b, c inside the C_i). Then, $r(a, b, c) = (2/9) + o(1)$ in this case. Finally, there are $2\alpha n\binom{\alpha n/3}{2} = (1 + o(1))\alpha^3 n^3/9$ triples $a, b, c \in S$ where one of them is in some C_i and the other two are in another C_i . Here it also holds that $\{p_{ab|c}, p_{ac|b}, p_{bc|a}\} = \{0, (1/3) + o(1), (2/3) + o(1)\}$ and again $r(a, b, c) = (2/9) + o(1)$. Plugging these values in (2) we obtain

$$\begin{aligned} \mathbb{E}[X_{H(S)}] &= \left(\frac{2}{3}(1-\alpha)^4 + \frac{8}{3}\alpha(1-\alpha)^3\right) \binom{n}{4} (1+o(1)) \\ &\quad + (1-\alpha)^2 \binom{n}{2} \left(\frac{2}{3} \cdot \frac{\alpha^2 n^2}{3} + \frac{16}{27} \cdot \frac{\alpha^2 n^2}{6}\right) (1+o(1)) \\ &\quad + 2(1-\alpha)n \left(\frac{1}{3} \cdot \frac{\alpha^3 n^3}{27} + \frac{2}{9} \cdot \frac{\alpha^3 n^3}{54} + \frac{2}{9} \cdot \frac{\alpha^3 n^3}{9}\right) (1+o(1)) \\ &= \binom{n}{4} \left(\frac{2}{3} - \frac{10\alpha^4 + 32\alpha^3 + 12\alpha^2}{81}\right) (1+o(1)) \end{aligned}$$

We therefore have

$$\max_{\text{exp}}(n, \alpha) \geq \binom{n}{4} \left(\frac{2}{3} - \frac{10\alpha^4 + 32\alpha^3 + 12\alpha^2}{81}\right) (1+o(1))$$

and in particular,

$$\max_{\text{exp}}\left(n, \frac{1}{2}\right) \geq \frac{371}{648} \binom{n}{4} (1+o(1)) \geq 0.572 \binom{n}{4} (1+o(1)).$$

4.2 Upper bound for $maxexp(n, \alpha)$

Consider the expressions

$$f(T(S)) = \sum_{a,b,c \in [k]} (p_{ab|c}p_{ac|b} + p_{ab|c}p_{bc|a} + p_{ac|b}p_{bc|a}) = \sum_{a,b,c \in [k]} r(a, b, c)$$

$$g(T(S)) = \sum_{a,b \in [k]} (2p_{a,b} - 1.5p_{a,b}^2) = \sum_{a,b \in [k]} r(a, b).$$

We first present our building block for upper-bounding these quantities.

Recall from Section 2 that for $A \subseteq \mathcal{L}(T)$, the topological subtree $T|_A$ is the tree obtained by removing the leaves $\mathcal{L}(T) \setminus A$, the paths leading exclusively to them, and contracting vertices with degree two. Now suppose we are given a partial labeling $T(S)$ where the leaves in S are labeled with the taxa set $[k]$. Suppose $2 \leq r \leq k$ is fixed and let $A \subseteq S$ be fixed with $|A| = r$. Consider $T|_A$ which is a labeled tree of order r where its r leaves are labeled by the taxa from $[k]$ assigned to A . Also observe that $T|_A$ has $2r - 3$ edges and denote the set of edges of $T|_A$ by F . We can partition the leaves in $\mathcal{L}(T) \setminus S$ (namely, the unlabeled leaves of $T(S)$) into $|F| = 2r - 3$ parts as follows. Recall that each $e \in F$ corresponds to some contracted path e^* of T . Now let $\ell \in \mathcal{L}(T) \setminus S$ and consider the path in T connecting ℓ to some arbitrary leaf of A . So, this path starts at ℓ and then hits for the first time some path e^* . Then we place ℓ in the set X_e . Notice that for every $\ell \in \mathcal{L}(T) \setminus S$, the set X_e in which it is placed is well-defined, and $\{X_e : e \in F\}$ is a partition of $\mathcal{L}(T) \setminus S$ (some parts may be empty).

Consider some triple $a, b, c \in A$ and the variable $p_{ab|c}$. We claim that we can determine $p_{ab|c}$ from the sizes of the X_e 's. Indeed, suppose x is some taxa assigned to some leaf $\ell \in \mathcal{L}(T) \setminus S$. Then $[ab|cx]$ is a quartet of T if and only if the following holds: $\ell \in X_e$ where the path from c to e in $T|_A$ does not use any edge of the path from a to b in $T|_A$. Thus, if $F(ab|c) \subset F$ is the union of all edges of F such that the path leading from c to each of them does not use any edge of the path from a to b in $T|_A$, then, denoting $x_e = |X_e|/(n - k)$ we have

$$p_{ab|c} = \frac{\sum_{e \in F(ab|c)} |X_e|}{|\mathcal{L}(T) \setminus S|} = \sum_{e \in F(ab|c)} x_e.$$

For our bound for $f(T(S))$ we will use $r = 5$. Indeed this is the largest r such that $T|_A$ is unique, as there is only one tree of order 5 which is the quintet, or, equivalently, CAT_5 . (For larger r we must consider all possible tree structures of order r and for each of them derive and solve an optimization problem; the gain is marginal compared with $r = 5$ and the size of the problems gets very large.) So, assume $A = \{a, b, c, d, e\}$ and that $T|_A$ is given in Figure 2 where we have labeled the edges of $F = \{e_1, \dots, e_7\}$.

In Table 1 we have listed the various variables and the corresponding expressions we obtain in this case. For shorthand, we defined $x_i = x_{e_i}$ so the variables are x_1, \dots, x_7 . Bearing in mind

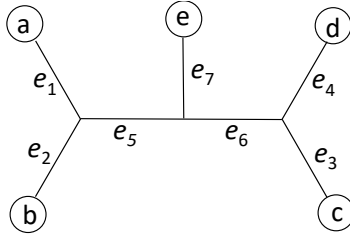


Figure 2: The quintet with $A = \{a, b, c, d, e\}$ and $F = \{e_1, \dots, e_7\}$.

variable	expression in terms of the x_i 's
$p_{ab c}, p_{ab d}, p_{ab e}$	$x_3 + x_4 + x_5 + x_6 + x_7$
$p_{cd a}, p_{cd b}, p_{cd e}$	$x_1 + x_2 + x_5 + x_6 + x_7$
$p_{ae c}, p_{ae d}, p_{be c}, p_{be d}$	$x_3 + x_4 + x_6$
$p_{ce a}, p_{ce b}, p_{de a}, p_{de b}$	$x_1 + x_2 + x_5$
$p_{bc a}, p_{bd a}, p_{be a}$	x_1
$p_{ac b}, p_{ad b}, p_{ae b}$	x_2
$p_{ad c}, p_{bd c}, p_{de c}$	x_3
$p_{ac d}, p_{bc d}, p_{ce d}$	x_4
$p_{ac e}, p_{ad e}, p_{bc e}, p_{bd e}$	x_7

Table 1: The variables whose values can be derived in terms of the x_i 's from the quintet of Figure 2. Variables having the same expression are grouped together.

that $x_1 + \dots + x_7 = 1$ we can now optimize the sum of the various expressions $r(u, v, w) = p_{uv|w}p_{uw|v} + p_{uw|w}p_{vw|u} + p_{uw|v}p_{vw|u}$ for $u, v, w \in A = \{a, b, c, d, e\}$. In other words, we maximize

$$r(A) = \sum_{u,v,w \in A} r(u, v, w) \quad \text{s.t.} \quad x_1 + x_2 + x_3 + x_4 + x_5 + x_6 + x_7 = 1.$$

From Table 1 this amounts to finding the global maximum of a quadratic polynomial in 6 variables x_1, \dots, x_6 and its maximum is attained when $x_1 = x_2 = x_3 = x_4 = \frac{7}{33}$, $x_5 = x_6 = 0$ and $x_7 = \frac{5}{33}$. In that point the maximum is $\frac{98}{33}$.

Returning now to $f(T(S))$ we observe that the number of $A \subset S$ with $|A| = 5$ is $\binom{k}{5}$ and each triple $\{a, b, c\} \subset S$ occurs in $\binom{k-3}{2}$ such A . As we have proved that $r(A) \leq \frac{98}{33}$ for each A , this implies that

$$f(T(S)) \leq \frac{98}{33} \frac{\binom{k}{5}}{\binom{k-3}{2}} = \frac{49}{990} k(k-1)(k-2).$$

We can use $T|_A$ of Figure 2 to upper bound $g(T(S))$ as well, but in this case, the values of the variables do not solely depend on the x_i 's. Indeed, consider the variable $p_{a,b}$ and recall that

variable	expression in terms of the x_i 's and d_i 's
$p_{a,b}$	$1 - (x_3 + x_4 + x_5 + x_6 + x_7)^2 - d_1 - d_2$
$p_{a,c}$	$1 - x_4^2 - x_2^2 - x_7^2 - d_5 - d_6 - d_1 - d_3$
$p_{a,d}$	$1 - x_3^2 - x_2^2 - x_7^2 - d_5 - d_6 - d_1 - d_4$
$p_{a,e}$	$1 - (x_3 + x_4 + x_6)^2 - x_2^2 - d_1 - d_5 - d_7$
$p_{b,c}$	$1 - x_1^2 - x_4^2 - x_7^2 - d_5 - d_6 - d_2 - d_3$
$p_{b,d}$	$1 - x_1^2 - x_3^2 - x_7^2 - d_5 - d_6 - d_2 - d_4$
$p_{b,e}$	$1 - (x_3 + x_4 + x_6)^2 - x_1^2 - d_2 - d_5 - d_7$
$p_{c,d}$	$1 - (x_1 + x_2 + x_5 + x_6 + x_7)^2 - d_3 - d_4$
$p_{c,e}$	$1 - (x_1 + x_2 + x_5)^2 - x_4^2 - d_3 - d_6 - d_7$
$p_{d,e}$	$1 - (x_1 + x_2 + x_5)^2 - x_3^2 - d_4 - d_6 - d_7$

Table 2: The variables of the form $p_{u,v}$ whose values, up to $o(1)$, can be derived in terms of the x_i 's and d_i 's from the quintet of Figure 2.

it corresponds to the probability that a randomly chosen pair of leaves in $\mathcal{L}(T) \setminus S$ forms together with a, b a quartet in which a and b are on different sides. So, $1 - p_{a,b}$ corresponds to a, b remaining on the same side, or stated otherwise, the probability that if we chose two leaves from $\mathcal{L}(T) \setminus S$, the path connecting them will not pass through the path connecting a and b . Thus, considering Figure 2, we have that $1 - p_{a,b} = (x_3 + x_4 + x_5 + x_6 + x_7)^2 + d_1 + d_2$ where d_i is the probability that a chosen pair of leaves from X_i will be connected with a path that does not intersect e_i^* . But observe that unlike the case for $f(T(S))$ and Table 1 where the expressions only involve the x_i 's, here the expressions involve the d_i 's as well, and the only thing we know about them is that $0 \leq d_i \leq x_i^2$. In Table 2 we have listed the various variables and the corresponding expressions we obtain in this case.

We can now optimize the sum of the various expressions $r(u, v) = 2p_{u,v} - 1.5p_{u,v}^2$ for $u, v \in A = \{a, b, c, d, e\}$. In other words, we wish to maximize

$$\sum_{u,v \in \{a,b,c,d,e\}} r(u, v) \quad \text{s.t.} \quad x_1 + x_2 + x_3 + x_4 + x_5 + x_6 + x_7 = 1, \quad 0 \leq d_i \leq x_i^2 \text{ for } i = 1, \dots, 7.$$

There is no simple analytic solution to this nonlinear optimization problem (notice that it involves the sum of polynomials of degree at most 4 and that it involves inequalities, as opposed to the case of $f(T(S))$ which required optimizing a single quadratic polynomial) and we can only solve it numerically using a nonlinear optimization algorithm, such as NLPsolve of Maple ². Using that method, we obtain that the maximum is (slightly less than) 6.6316 with $x_1 = x_4 = 0.08134$, $x_2 = x_3 = 0.39336$, $x_7 = 0.05059$, $x_5 = x_6 = 0$, $d_1 = d_4 = 0$, $d_2 = d_3 = 0.12914$, $d_5 = d_6 = d_7 = 0$.

²Maple code of our program available at <https://www.dropbox.com/s/va6dwf3yw773vyx/quartets-partial.zip?dl=0>

Compare this maximum to the one we can obtain from the trivial upper bound $r(u, v) \leq \frac{2}{3}$ which would give a bound of 6.666... (as there are 10 terms in the sum to maximize). So, while for the case of $f(T(S))$ we obtained a significant improvement (expressed analytically as a rational number), here the improvement is rather marginal (and we cannot express the bound analytically). In any case, we have

$$g(T(S)) \leq 6.6316 \frac{\binom{k}{5}}{\binom{k-2}{3}} = 0.33158k(k-1) .$$

Plugging our bounds for $f(T(S))$ and $g(T(S))$ in (2) we obtain that

$$\begin{aligned} \maxexp(n, \alpha) &\leq \left(\frac{2}{3}(1-\alpha)^4 + \frac{8}{3}\alpha(1-\alpha)^3 + 3.98\alpha^2(1-\alpha)^2 + \frac{392}{165}\alpha^3(1-\alpha) \right) \binom{n}{4} + o(n^4) \\ &= \left(\frac{2}{3} - \frac{653\alpha^4 + 414\alpha^3 + 33\alpha^2}{1650} \right) \binom{n}{4} + o(n^4) \end{aligned}$$

which for $\alpha = \frac{1}{2}$ gives

$$\maxexp(n, \frac{1}{2}) \leq 0.606 \binom{n}{4} (1 + o(1)) .$$

If one only uses the easier bound $g(T(S)) \leq k(k-1)/3$ then the constant 3.98 in the bound for $\maxexp(n, \alpha)$ can be replaced with 4 and the constant 0.606 in the bound for $\maxexp(n, \frac{1}{2})$ can be replaced with $\frac{267}{440} < 0.607$. We have thus completed the proof of Theorem 2.3. \square

5 $\mathbb{E}[X_{T(S)}]$ versus $M_{T(S)}$

In this section we prove Theorem 2.4. So we assume that T is a tree of order n with a split $e = uv$ such that $\mathcal{L}(T_u) = S$ and T_v is a caterpillar (where the join edge of T_v is an endpoint edge of the caterpillar) and our partial labeling is $T(S)$. Notice that $T(S)$ is a special case of the partial labellings that minimize $\mathbb{E}[X_{T(S)}]$ as proved in Subsection 3.2 (the special case is that T_v is a caterpillar and for minimizing $\mathbb{E}[X_{T(S)}]$ this is not required). In particular, by Theorem 2.2,

$$\mathbb{E}[X_{T(S)}] = \left(\frac{2}{3}(1-\alpha)^4 + \frac{8}{3}\alpha(1-\alpha)^3 \right) \binom{n}{4} (1 + o(1)) . \quad (3)$$

We proceed to lower-bound $M_{T(S)}$. Recall that the vertices of S are labeled with the taxa set $[k]$ where $k = \alpha n$. We construct two completions of $T(S)$, denoted by T_1 and T_2 as follows. Suppose that $\mathcal{L}(T_v) = \{\ell_1, \dots, \ell_{n-k}\}$ where leaf ℓ_j is closer to the split than leaf ℓ_{j+1} . A completion assigns the taxa set $\{k+1, \dots, n\}$ to $\mathcal{L}(T_v)$. In T_1 we assign taxa $k+j$ to leaf ℓ_j for $j = 1, \dots, n-k$. We next describe T_2 . For ease of exposition we separate the cases $\alpha > 1/3$ and $\alpha \leq 1/3$.

Consider first the case $\alpha > 1/3$. In T_2 we reverse the ordering with respect to T_1 and assign taxa $k+j$ to leaf $\ell_{n-k+1-j}$. We compute $qd(T_1, T_2)$. Quartets of type $i = 0, 2, 3, 4$ of T_1 are also quartets in T_2 where recall that a quartet is of type i if it contains i taxa from S . On the other

hand, each quartet of type 1 in T_1 is not a quartet of T_2 . Since assume that the quartet is of the form $[ax|yz]$ in T_1 . Then x is assigned to a leaf closer to the split than the leaves assigned to y and z . But in T_2 , the leaf assigned to z will be closer to the split than the leaves assigned to y and x . So, in T_2 the quartet would be $[az|yx]$. It follows that $qd(T_1, T_2)$ equals the number of quartets of type 1 hence

$$M_{T(S)} \geq qd(T_1, T_2) = \alpha n \binom{(1-\alpha)n}{3} = 4\alpha(1-\alpha)^3 \binom{n}{4} (1+o(1)). \quad (4)$$

Simple calculus shows that (4) minus (3) is $\Theta(n^4)$ for $\alpha > 1/3$.

When $\alpha \leq 1/3$ the aforementioned “reversal labeling” for T_2 produces inferior results than that of a random labeling. We now show how to obtain a more delicate labeling of T_2 which is a mixture of a random and a deterministic labeling. Let $1 - \alpha \geq \beta \geq 0$ be a parameter. We partition $\mathcal{L}(T_v)$ into three parts. The $\beta n/2$ leaves closest to the split are denoted B_1 , so $B_1 = \{\ell_1, \dots, \ell_{\beta n/2}\}$. The last $\beta n/2$ leaves furthest from the split are denoted $B_2 = \{\ell_{(1-\alpha-\beta/2)n+1}, \dots, \ell_{(1-\alpha)n}\}$. The remaining $(1 - \alpha - \beta)n$ leaves in $\mathcal{L}(T_v)$ (the middle leaves of the caterpillar) are denoted by C . Let $B = B_1 \cup B_2$ and observe that $|B| = \beta n$, $|C| = (1 - \alpha - \beta)n$ and $B \cup C = \mathcal{L}(T_v)$. The taxa assigned to C in T_1 are randomly permuted in T_2 , but stay inside C so that any label assigned in T_1 to a leaf of C is also assigned in T_2 to some leaf of C . The taxa assigned to B_1 in T_1 are now assigned to B_2 in T_2 and are also reversed. Similarly, the taxa assigned to B_2 in T_1 are now assigned to B_1 in T_2 and are also reversed. In particular, for $j = 1, \dots, \beta n/2$, taxa $k + j$ that was assigned in T_1 to $\ell_j \in B_1$ is now assigned in T_2 to $\ell_{(1-\alpha)n+1-j} \in B_2$ and taxa $n + 1 - j$ that was assigned in T_1 to $\ell_{(1-\alpha)n+1-j} \in B_2$ is now assigned in T_2 to $\ell_j \in B_1$.

Observe that now $qd(T_1, T_2)$ is a random variable as the taxa assigned to C in T_1 are randomly permuted in T_2 . We compute $\mathbb{E}[qd(T_1, T_2)]$ which (obviously) serves as a lower bound for $M_{T(S)}$. Once again, quartets of type $i = 4, 3, 2$ of T_1 are also quartets in T_2 so it remains to consider quartets of type 0 and type 1. We will designate such quartets by words of the form $\{S, B, C\}^4$ where a word of the form $W_1 W_2 W_3 W_4$ represents a quartet of T_1 of the form $[x_1 x_2 | x_3 x_4]$ where $x_i \in W_i$. So, for example, $SBCB$ represents quartets $[x_1 x_2 | x_3 x_4]$ where $x_1 \in S$, $x_2 \in B$, $x_3 \in C$, $x_4 \in B$ (notice that this is a quartet of type-1). Recall that we can view $qd(T_1, T_2)$ as the sum of indicator random variables, each representing a quartet of type 0 or 1 in T_1 and the probability it is not compatible with T_2 . In Table 3 we list each possible quartet subtype, the number of indicator random variables (i.e. quartets) of this subtype normalized by dividing with $(1 + o(1)) \binom{n}{4}$, and the probability it is not compatible with T_2 . Using Table 3 we immediately obtain

subtype	normalized quantity	probability
$CCCC$	$(1 - \alpha - \beta)^4$	$\frac{2}{3}$
$BCCC \cup CCCB$	$4\beta(1 - \alpha - \beta)^3$	$\frac{2}{3}$
$BBCC \cup CCBB$	$3\beta^2(1 - \alpha - \beta)^2$	0
$BCCB$	$3\beta^2(1 - \alpha - \beta)^2$	$\frac{1}{2}$
$BBCB \cup BCBB \cup BBBC \cup CBBB$	$4\beta^3(1 - \alpha - \beta)$	0
$BBBB$	β^4	0
$SCCC$	$4\alpha(1 - \alpha - \beta)^3$	$\frac{2}{3}$
$SBCC \cup SCCB$	$12\alpha\beta(1 - \alpha - \beta)^2$	1
$SBBC \cup SBCB \cup SCBB$	$12\alpha\beta^2(1 - \alpha - \beta)$	1
$SBBB$	$4\alpha\beta^3$	1

Table 3: The various subtypes of quartets of type 0 or 1, the normalized quantity of quartets of each subtype or union of subtypes, and the probability it is not compatible with T_2 .

$$\begin{aligned}
\frac{1}{\binom{n}{4}(1+o(1))} \mathbb{E}[qd(T_1, T_2)] &= \frac{2}{3}(1 - \alpha - \beta)^4 \\
&+ \frac{8}{3}\beta(1 - \alpha - \beta)^3 \\
&+ \frac{3}{2}\beta^2(1 - \alpha - \beta)^2 \\
&+ \frac{8}{3}\alpha(1 - \alpha - \beta)^3 \\
&+ 12\alpha\beta(1 - \alpha - \beta)^2 \\
&+ 12\alpha\beta^2(1 - \alpha - \beta) \\
&+ 4\alpha\beta^3 .
\end{aligned}$$

Simplifying, the right hand side of the last equality is

$$g(\beta) = \alpha\beta^2 - \alpha\beta^3 - \frac{5}{2}\beta^2 + \frac{7}{3}\beta^3 + 4\alpha\beta + \frac{2}{3} - 4\alpha^2 - 8\alpha^2\beta + 4\alpha^3\beta + \frac{3}{2}\alpha^2\beta^2 + \frac{16}{3}\alpha^3 - 2\alpha^4 - \frac{1}{2}\beta^4$$

where we have named the expression $g(\beta)$ to emphasize that α is fixed. Hence using (3) our hope is to show that there exists $0 \leq \beta \leq 1 - \alpha$ such that $g(\beta) > \frac{2}{3}(1 - \alpha)^4 + \frac{8}{3}\alpha(1 - \alpha)^3$ as this will prove that

$$M_{T(S)} - \mathbb{E}[X_{T(S)}] \geq \mathbb{E}[qd(T_1, T_2)] - \mathbb{E}[X_{T(S)}] = \Theta(n^4)$$

as required. To see that the claim on $g(\beta)$ holds, first observe that $g(0) = \frac{2}{3}(1 - \alpha)^4 + \frac{8}{3}\alpha(1 - \alpha)^3$.

As g is differentiable, it suffices to prove that $g'(0) > 0$. Indeed

$$g'(\beta) = 2\alpha\beta - 3\alpha\beta^2 - 5\beta + 7\beta^2 + 4\alpha - 8\alpha^2 + 4\alpha^3 + 3\alpha^2\beta - 2\beta^3$$

so

$$g'(0) = 4\alpha - 8\alpha^2 + 4\alpha^3 = 4\alpha(1 - \alpha)^2 > 0 .$$

□

References

- [1] N. Alon, H. Naves, and B. Sudakov. On the maximum quartet distance between phylogenetic trees. *SIAM Journal on Discrete Mathematics*, 30(2):718–735, 2016.
- [2] N. Alon, S. Snir, and R. Yuster. On the compatibility of quartet trees. *SIAM Journal on Discrete Mathematics*, 28(3):1493–1507, 2014.
- [3] H. J. Bandelt and A. Dress. Reconstructing the shape of a tree from observed dissimilarity data. *Advances in Applied Mathematics*, 7:309–343, 1986.
- [4] D. Bryant and J. Lagergren. Compatibility of unrooted phylogenetic trees is FPT. *Theoretical Computer Science*, 351(3):296–302, 2006.
- [5] D. Bryant and M. Steel. Constructing optimal trees from quartets. *Journal of Algorithms*, 38(1):237–259, 2001.
- [6] B. Chor, P. L. Erdős, and Y. Komornik. A high quartet distance construction. *Annals of Combinatorics*, 23(1):51–65, 2019.
- [7] M. Csűrös. Fast recovery of evolutionary trees with thousands of nodes. *Journal of Computational Biology*, 9(2):277–297, 2002.
- [8] C. Daskalakis, E. Mossel, and S. Roch. Phylogenies without branch bounds: contracting the short, pruning the deep. *SIAM Journal on Discrete Mathematics*, 25(2):872–893, 2011.
- [9] G. F. Estabrook, F. R. McMorris, and C. A. Meacham. Comparison of undirected phylogenetic trees based on subtrees of four evolutionary units. *Systematic Zoology*, 34(2):193–200, 1985.
- [10] I. Gronau, S. Moran, and S. Snir. Fast and reliable reconstruction of phylogenetic trees with indistinguishable edges. *Random Structures & Algorithms*, 40(3):350–384, 2012. Preliminary version appeared in ACM-SIAM Symposium on Discrete Algorithms (SODA) 2008.
- [11] S. Grünewald. Slim sets of binary trees. *Journal of Combinatorial Theory, Series A*, 119(2):323–330, 2012.

- [12] S. Grünewald, P. J. Humphries, and C. Semple. Quartet compatibility and the quartet graph. *The electronic journal of combinatorics*, 15(1):103, 2008.
- [13] T. Jiang, P. Kearney, and M. Li. Orchestrating quartets: approximation and data correction. In *IEEE Symposium on Foundation of Computer Science (FOCS)*, pages 416–425, 1998.
- [14] T. Jiang, P. E. Kearney, and M. Li. A polynomial time approximation scheme for inferring evolutionary trees from quartet topologies and its application. *SIAM Journal on Computing*, 30(6):1942–1961, 2000.
- [15] C. Semple and M. A. Steel. *Phylogenetics*. Oxford University Press, 2003.
- [16] S. Snir and R. Yuster. A linear time approximation scheme for maximum quartet consistency on sparse sampled inputs. *SIAM Journal on Discrete Mathematics*, 25(4):1722–1736, 2011. Preliminary version appeared in APPROX 2011.
- [17] S. Snir and R. Yuster. Reconstructing approximate phylogenetic trees from quartet samples. *SIAM Journal on Computing*, 41(6):1466–1480, 2012. Preliminary version appeared in SODA 2010.
- [18] M. Steel. The complexity of reconstructing trees from qualitative characters and subtrees. *Journal of Classification*, 9(1):91–116, 1992.
- [19] M. Steel and D. Penny. Distributions of tree comparison metrics—some new results. *Systematic biology*, 42(2):126–141, 1993.
- [20] K. Strimmer and A. von Haeseler. Quartet Puzzling: a quartet maximum-likelihood method for reconstructing tree topologies. *Molecular Biology and Evolution*, 13(7):964–969, 1996. Software available at <ftp://ftp.ebi.ac.uk/pub/software/unix/puzzle/>.