On the compatibility of quartet trees

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Abstract

Phylogenetic tree reconstruction is a fundamental biological problem. Quartet trees, trees over four species, are the minimal informational unit for phylogenetic classification. While every phylogenetic tree over $n$ species defines $\binom{n}{4}$ quartets, not every set of quartets is compatible with some phylogenetic tree.

Here we focus on the compatibility of quartet sets. We provide several results addressing the question of what can be inferred about the compatibility of a set from its subsets. Most of our results use probabilistic arguments to prove the sought characteristics. In particular we show that there are quartet sets $Q$ of size $m = cn \log n$ in which every subset of cardinality $\epsilon n / \log n$ is compatible, and yet no fraction of more than $1/3 + \epsilon$ of $Q$ is compatible. On the other hand, in contrast to the classical result stating when $Q$ is the densest, i.e. $m = \binom{n}{4}$ the consistency of any set of 3 quartets implies full consistency, we show that even for $m = \Theta\left(\binom{n}{4}\right)$ there are (very) inconsistent sets for which every subset of large constant cardinality is consistent.

Our final result, relates to the conjecture of Bandelt and Dress regarding the maximum quartet distance between trees. We provide asymptotic upper and lower bounds for this value.

1 Introduction

The study of evolution and the construction of phylogenetic (evolutionary) trees are classical subjects in biology. A phylogeny, the evolutionary history of a set of species, is normally represented by a tree where the species under study are mapped to the leaves of the tree and the tree structure represents evolutionary relationships. Frequently, it is desirable to combine several trees over overlapping sets of species. This task is called the supertree task [6, 5] where the goal is to find a tree over the full set of species that satisfies most of the partial input trees. We distinguish between rooted and unrooted settings. In the rooted setting a rooted triplet tree (Figure 1:a) is the basic unit of information. We denote the triplet over leaves $\{a, b, c\}$ as $[a|bc]$ if the lowest common ancestor (LCA) for $a, b$ is a (proper) descendant of the LCA for all $\{a, b, c\}$. However, the more prevailing setting is the unrooted setting. In the unrooted setting, the notion of LCA is meaningless and therefore the basic unit of information is a quartet tree (Figure 1:b).

We denote a quartet over leaves $\{a, b, c, d\}$ as $[ab|cd]$ - meaning that there is an edge in the underlying tree separating $a$ and $b$ from $c$ and $d$.

![Figure 1](image_url)

Figure 1: In a rooted setting, a rooted triplet is the smallest informative tree versus an unrooted quartet in the unrooted setting. (a) - a rooted triplet tree [12;3]. (b) - an unrooted quartet tree [12;34].

For its fundamental role in phylogenetics, a vast research effort has been devoted to phylogenetic tree reconstruction from quartets, a field denoted as quartet-based reconstruction (see e.g. [3, 4, 25, 31, 28, 33] among many). Here, accurate trees over four species are constructed, normally using some quartet oracle [12, 13, 17, 21], from a (possibly partial) set of 4-sets. These trees are subsequently combined together into the big tree on the full species set. The latter problem, however, deciding whether there exists a tree satisfying all the quartets in an arbitrary given set, is NP-complete [32]. Moreover, the ideal case in which all quartets agree on a single tree, is very rare. This raises the problem of finding a tree maximizing the number of compatible quartets - maximum quartet compatibility (MQC) [27]. MQC is obviously NP-hard and therefore several approximation algorithms have been suggested [4, 8, 24, 29, 30], but the best
approximation to the general problem is still obtained by a naive “random tree” with expected approximation ratio of $1/3$.

A possible direction to follow in this respect, is to check compatibility of relatively small subsets of the ground set as “witnesses” for compatibility, under the trivial observation that if the ground set is compatible (agreeing on some tree), then necessarily every subset of it is compatible. Of course the number of such subsets is exponentially large, but one might suspect that a sampling approach can lead to a randomized algorithm for set compatibility. In this work we address the question of how much can we infer about a quartet set just by examining its constituting subsets. We examine this question in several settings, all of which are abstract and asymptotically large. We use probabilistic arguments to base our claims, allowing us to show large incompatibility in (relatively sparse) sets of quartets, despite the compatibility of all their (rather large) subsets. One consequence of the results here is that no sampling algorithm, even one based on $m/polylog(m)$ subsets, cannot guarantee even relative compatibility (compatibility of a large fraction) of the ground set. This result extends a result of [23] showing an example of a constant size incompatible quartet set all of whose subsets are compatible. We can use the same blowup technique we use here on that example, to get a big incompatible set (of magnitude a constant fraction of $\binom{n}{4}$), but the size of the compatible subsets this way will only be limited to 5.

Compatibility is inherently linked to the subject of closure operations on a quartet set [7, 10, 15, 16, 23]. These operations rely on inference rules allowing a recursive augmentation of a set of quartets with quartets that are implied by the existing set. A quartet set $Q$ is closed when it contains all the quartets induced by all the trees satisfying $Q$. Part of our work is also related and relies on these inference rules, used here in Section 4.

Our last result touches compatibility from a different angle. We tackle the question of how much can a compatible set be violated. In particular we are interested in answering what fraction of the largest, unambiguous, compatible, set - the full set of $\binom{n}{4}$ compatible quartets - can be violated. This question has significance when measuring similarity between trees based on quartet similarity [20]. It was presented by Bandelt and Dress [2] where they conjectured that this value tends to $2/3$. We give upper and lower bounds on this fraction.

We end the paper with open problems and further research questions arising as a result of this work.

2 Preliminaries
A binary rooted tree is a tree whose edges are directed, every internal vertex has two children and every vertex but one distinguished vertex, the root, has a single ancestor. In a binary undirected (also called unrooted) tree, edges are undirected (and hence parenthood does not exist), and all internal vertices have three neighbors each. Such a tree is also called a trivalent tree. Throughout this paper, unless stated otherwise, all trees are assumed to be unrooted binary trees, with leaves labeled bijectively by a taxa (species) set $X$ of size $n$. Such trees are called phylogenetic trees. For a tree $T = (V, E)$, the set of leaves of $T$ is denoted by $\mathcal{L}(T)$.

The removal of an edge $e$ in a tree splits the tree into two subtrees and therefore induces a split among the leaves of the tree. We identify an edge $e$ by the
split \((U, \mathcal{L}(T) \setminus U)\) it generates on the set of leaves, and denote the split by \(U_e\). As external edges (edges adjacent to leaves) induce trivial splits, we refer only to internal edges.

Let \(T\) be a tree and \(A \subset \mathcal{L}(T)\) a subset of the leaves of \(T\). We denote by \(T|_A\), the topological subtree of \(T\) induced by \(A\) where all leaves in \(\mathcal{L}(T) \setminus A\) and paths leading exclusively to them are removed, and subsequently internal vertices with degree two are contracted.

For two trees \(T\) and \(T'\), we say that \(T\) satisfies \(T'\) (or, equivalently, that \(T'\) is satisfied by \(T\)), if \(\mathcal{L}(T') \subset \mathcal{L}(T)\) and \(T|_{\mathcal{L}(T')} = T'\). Otherwise, \(T'\) is violated by \(T\). Let \(T = \{T_1, \ldots, T_k\}\) be a set of trees with possibly overlapping leaves, and denote by \(\mathcal{L}(T) = \bigcup_i \mathcal{L}(T_i)\), the union of the set of leaves of all trees \(T_i \in T\). Then for a tree \(T\) with \(\mathcal{L}(T) = \mathcal{L}(T_1)\), we denote by \(T_s(T)\) the set of trees in \(T\) that satisfy \(T\). We say that \(T\) is compatible if there exists a tree \(T^*\) over the set of leaves \(\mathcal{L}(T)\) that satisfies every tree \(T_i \in T\), i.e. \(T_s(T^*) = T\) (see Figure 2). We denote by \(co(T)\) the set of trees that satisfy \(T\), \(co(T) = \{T : T_s(T) = T\}\).

Further, we say that \(T^*\) is defined by \(T\) if \(co(T)\) is the singleton \(\{T^*\}\). If there is no such compatible tree \(T^*\), (i.e. \(co(T) = \emptyset\)), we say that \(T\) is incompatible.

Figure 2: (a) A phylogenetic tree over five leaves. (b) Two quartets compatible with the tree on the left.

A quartet tree (or just a quartet for short), is a phylogenetic tree over four leaves \(\{a, b, c, d\}\). We denote a quartet over \(\{a, b, c, d\}\) as \([ab|cd]\) if there exists an edge \(e\) whose corresponding split \(U_e\) satisfies \(a, b \in U\) and \(c, d \notin U\). Quartets are the most elementary informational unit in an unrooted tree, as a pair corresponds to a path in a tree and a triplet to a vertex. Every phylogenetic tree \(T\) with \(n\) leaves uniquely defines \(\binom{n}{4}\) quartets, one for each set of four leaves. Let \(Q(T)\) denote this full quartet set of \(T\). Obviously, \(Q(T)\) uniquely defines \(T\).

We mention two basic problems and results regarding quartet based reconstruction. When a set of trees \(T\) is incompatible, it is desirable to find a tree \(T^*\) over \(\bigcup_i \mathcal{L}(T_i)\) that maximizes some objective function. This meta-problem is commonly known as the supertree problem and a corresponding solution \(T^*\) is a supertree. An important case of the supertree problem is when the set of input trees is a set of quartet trees \(Q\) and the task is to find a tree \(T\) such that \(|Q_s(T)|\) (the subset of \(Q\) maximized by \(T\)) is maximized. This problem is called maximum quartet compatibility (MQC).

**Problem 2.1. (MQC)** Given a set of quartets \(Q\) with leaves labeled by a taxa set \(X\), find a tree \(T\) with leaves labeled bijectively by \(X\) that satisfies the maximum number of elements of \(Q\).

We note that MQC is NP-hard. In fact, the decision problem of whether \(Q\) is compatible is NP-Complete [32].

Let \(T\) be any tree with \(n\) leaves labeled by a taxa set \(X\). Consider a random bijection \(\pi\) between a taxa set \(X\) of size \(n\) and the leaves of \(T\). The corresponding labeled tree is denoted by \(T^\pi\). As each of the \(n!\) possible bijections is equally likely, we notice that a quartet \([ab|cd]\) with labels from \(X\) is satisfied by \(T^\pi\) with probability \(1/3\). We therefore have, by linearity of expectation:

**Lemma 2.1.** Let \(Q\) be an arbitrary set of quartets over a taxa set \(X\) of size \(n\), and let \(T^n\) be a random bijection between the leaves of a tree \(T\) and \(X\). Then the expected number of elements in \(Q\) satisfied by \(T\) is \(|Q|/3\).

Lemma 2.1 immediately yields an efficient (randomized) \(1/3\) approximation algorithm for MQC. This naive solution is presently the best known approximation ratio for general instances of MQC that can be achieved by a polynomial time algorithm.

3 Subset compatibility does not imply set compatibility

Our first result shows that even when all relatively large subsets of a given set are compatible, the whole set can still be very far from compatible.

**Theorem 3.1.** There exists a set \(Q\) of \(\Theta(n \log n)\) quartets such that every subset \(Q' \subset Q\) of size \(\Theta\left(\frac{n}{\log n}\right)\) is compatible, yet \(Q\) is (very) incompatible, that is, no subset consisting of more than a \(1/3 + \epsilon\) fraction of its quartets is compatible.

In the following we prove the existence of \(Q\) in Theorem 3.1 via probabilistic arguments.
DEFINITION 3.1. (RANDOM QUARTET SET) A set of $m$ quartets $Q$ is a random quartet set if it is constructed by the following process. A quartet $q$ is composed by first sampling four distinct taxa $a,b,c,d \in \{1,\ldots,n\}$ uniformly at random. Then, $q$ is set to be one out of the three possible quartets over $\{a,b,c,d\}$ (namely, one of $[ab][cd],[ac][bd],[ad][bc]$) with equal probability. Finally, $q$ is added to $Q$. The process repeats $m$ times (observe that $Q$ is constructed with replacement, so it may be a multiset; however, the probability of having a repeated element in $Q$ tends to zero as $n$ grows, assuming $m = o(n^2)$).

LEMMA 3.1. Fix $\epsilon > 0$. Let $Q$ be a random quartet set of size $|Q| = m \geq \frac{1}{3}n \log n$. Then, with probability at least $2/3$, there is no phylogenetic tree satisfying more than a fraction of $1/3 + \epsilon$ quartets of $Q$.

Proof. Let $T$ be any phylogenetic tree over the taxa set $X = \{1,\ldots,n\}$ and let $Q_s(T)$ be the quartets of $Q$ satisfied by $T$. Clearly, by the construction of $Q$, a quartet $q$ is satisfied with probability $1/3$ and by linearity of expectation, $E[m - |Q_s(T)|] = 2m/3$. By a Chernoff bound (cf. [1], Theorem A.1.13)

$$Pr[|Q_s(T)| - \frac{m}{3} > \epsilon m] = Pr[(m - |Q_s(T)|) - \frac{2m}{3} < -\epsilon m] < e^{-\frac{\epsilon^2m^2}{4m}} \leq \frac{1}{n^{3m}}.$$

Now, a phylogenetic tree with $n$ leaves has $2n - 2$ vertices and it is well known that there are exactly $(2n - 2)^{2n-4}$ (not necessarily phylogenetic) labeled trees with $2n - 2$ vertices. Hence, using the union bound, we obtain that the probability that any phylogenetic tree satisfies more than $m/3 + \epsilon m$ quartets is less than

$$(2n - 2)^{2n-4} \cdot \frac{1}{n^{3m}} \ll \frac{1}{3}. $$

We next prove the existence of a set $Q$ all of whose subsets of size $O(n/\log n)$ are compatible. Again, we use probabilistic arguments to establish the desired properties.

DEFINITION 3.2. (QUARTET COVER) Let $Q'$ be a set of quartets. Let $\text{cover}(Q')$ denote the set of taxa contained in some quartet of $Q'$. If $X' \subseteq \text{cover}(Q')$, then we say that $Q'$ covers $X'$.

LEMMA 3.2. Let $Q'$ be a random quartet set of size $m'$. For $k \leq n$,

$$Pr[|\text{cover}(Q')| \leq k] \leq \left( \frac{k}{n} \right)^{4m'-k} e^k. \tag{3.1}$$

Proof. For a given subset $X'$ of $k$ taxa, we consider the event that $\text{cover}(Q') \subseteq X'$. The probability that a random quartet has all its taxa in $X'$ is

$$\frac{k(k-1)(k-2)(k-3)}{n(n-1)(n-2)(n-3)} \leq \left( \frac{k}{n} \right)^4. \tag{3.2}$$

Hence, $Pr[|\text{cover}(Q')| \subseteq X'] \leq \left( \frac{k}{n} \right)^{4m'}$. As there are $\binom{n}{k}$ possible choices for $X'$, we have

$$Pr[|\text{cover}(Q')| \leq k] \leq \binom{n}{k} \left( \frac{k}{n} \right)^{4m'} \leq \binom{m}{k} \left( \frac{k}{n} \right)^{4m'} \leq \left( \frac{me}{k} \right)^k \left( \frac{k}{n} \right)^{4m'} \leq \left( \frac{k}{n} \right)^{4m' - k} e^k. \tag{3.3}$$

Notice that the proof works seamlessly when $Q'$ is a multiset.

Equation (3.1) bounds the probability that a given random quartet set $Q'$ satisfies $|\text{cover}(Q')| \leq k$. As our ground set of $m$ quartets $Q$ is also random, so is every subset of $Q$. We want to bound the probability of having a small value of $|\text{cover}(Q')|$ for any subset $Q'$ of $Q$ of size $m'$. As there are $\binom{m}{m'}$ subsets to consider, we immediately obtain the following corollary from Lemma 3.2.

COROLLARY 3.1. Let $Q$ be a random quartet set of size $m$. For $m' \leq m$, the probability that there exists some subset $Q'$ of $Q$ of size $m'$ with $|\text{cover}(Q')| \leq k$ is at most

$$\binom{m}{m'} \left( \frac{k}{n} \right)^{4m'^{-k}} e^k \leq \left( \frac{me}{m'} \right)^{m'} \left( \frac{k}{n} \right)^{4m'^{-k}} e^k = \left( \frac{m}{m'} \right)^{m'} \left( \frac{k}{n} \right)^{4m'^{-k}} e^{k+m'}. \tag{3.4}$$

On the one hand, the larger $k$ is, the stronger the result in Theorem 3.1 is. On the other hand, making $k$ too large makes it more difficult to maintain compatibility. The next few claims establish a value of $k$ which is relatively large, while guaranteeing compatibility.
**Definition 3.3.** A quartet set $Q$ satisfies twofold coverage (TFC) if $|\text{cover}(Q)| > 2|Q|$. 

The following lemma can also be deduced from a result of Grünewald [22] but the proof presented here is simpler.

**Lemma 3.3.** Let $Q'$ be a set of quartets with the property that every nonempty subset $Q \subset Q'$ satisfies TFC, then $Q'$ is compatible.

**Proof.** Suppose that every nonempty subset $Q' \subset Q'$ satisfies TFC. We first note that any such $Q$ has at least one taxon covered by a single quartet of $Q$. Indeed, the average number of quartets containing a specific taxon is precisely

\[
\frac{4|Q|}{|\text{cover}(Q)|} \leq \frac{4|Q|}{2|Q|} = 2
\]

and so at least one taxon is contained in less than two quartets of $Q$, namely in one.

**Observation 3.1.** Let $T$ be a tree over a set $\mathcal{X}$ and let $q$ be a quartet over $\{a,b,c,d\}$ s.t. $|\{a,b,c,d\} \setminus \mathcal{X}| \geq 1$. Then it is possible to construct a tree (over $\{a,b,c,d\} \cup \mathcal{X}$) satisfying both $q$ and $T$.

**Proof.** We consider the case $|\{a,b,c,d\} \setminus \mathcal{X}| = 1$, if this cardinality is bigger the argument is simpler. WLOG let $q = [ab|cd]$ and assume $d \notin \mathcal{X}$. Let $T'$ be constructed from $T$ as follows. Split the edge incident with $c$ in $T$ by adding a new internal vertex $v$, and attach a new edge connecting $v$ and $d$. Hence, $T'$ satisfies both $T$ and $q$.

As any nonempty $Q \subset Q'$ satisfies TFC and thus has a taxon $x$ covered by a single quartet of $Q$, the last observation shows that if we already have a tree over the rest of the taxa $\mathcal{X} \setminus x$ that satisfies all $Q' \setminus q$, we can construct a tree over the whole set $\mathcal{X}$ by adding $x$ such that $q$ is satisfied and hence all $Q'$ is satisfied.

We now construct a tree satisfying $Q'$. The proof follows by induction on the size of $Q'$. The basis of the induction is trivial, $Q'$ is a single quartet and such is the tree. In order to prove the induction step, we need some auxiliary observation.

**Observation 3.2.** For a quartet set $Q'$ such that every nonempty subset $Q \subset Q'$ satisfies TFC, it is possible to order $Q'$ as $(q_i)$ such that every $q_i$ contains a new taxon, i.e. a taxon not contained in any quartet $q_j$ for $j < i$.

**Proof.** We build the ordering backward, starting from the complete set $Q'$. Since, $Q'$ satisfies TFC, there must be a quartet $q'$ with a taxon covered only by $q'$. Then we take out $q'$ to be the last in the ordering. Since $Q' \setminus \{q'\}$ also satisfies the TFC, we can repeat this process all the way until $Q'$ is depleted.

We can now prove the induction step. Since every $q_i$ in the ordering $(q_i)$ contains a taxon not covered by any $q_j$, for $j < i$, by Observation 3.1 it can be added to the existing tree. 

It now remains to establish the probability of the event described by the conditions of Lemma 3.3 for the values of interest.

**Lemma 3.4.** Let $C \geq 1$ be a constant and let $n$ be sufficiently large as a function of $C$. Let $Q$ be a random quartet set of size $m \leq Cn \log n$. Then the probability that every subset $Q' \subset Q$ of size at most $n^2/(4e^4m)$ is compatible is at least $2/3$.

**Proof.** By Corollary 3.1 the probability that there exists a quartet subset of size $m'$ (of a set of $m$ quartets) that covers at most $k$ taxa is at most

\[
\left(\frac{m}{m'}\right)^{m'} \left(\frac{k}{n}\right)^{4m' - k} e^{k + m'}.
\]

As we wish to use the properties of TFC, we set $k = 2m'$. The probability in the last equation becomes

\[
(3.2) \left(\frac{m}{m'}\right)^{m'} \left(\frac{2m'}{n}\right)^{4m' - 2m'} e^{3m'} = \left(\frac{4e^3 mm'}{n^2}\right)^{m'}.
\]

However, we need to bound the above probability not for a single value of $m'$, but for all values $m' = 1, \ldots, m^*$ where $m^* = n^2/(4e^4m)$. Thus, by (3.2) and the union bound, we must prove:

\[
\sum_{m' = 1}^{m^*} \left(\frac{4e^3 mm'}{n^2}\right)^{m'} \leq \frac{1}{3}.
\]

Indeed, such a bound implies that with probability at least $2/3$, every subset of quartets of size $m' \leq m^*$ covers more than $k = 2m'$ quartets, and hence satisfies TFC. Consequently, by Lemma 3.3, every such subset is compatible.

To bound the left hand side of the last inequality note that for $m' = 1$ we have $4e^3 mm'/n^2 = O(\log n/n)$ and for each $2 \leq m' \leq \log n$ we have $(4e^3 mm'/n^2)^{m'} = O((\log^2 n)/n^2)$. For bigger values of $m'$ the assumption that
m' \leq n^2/(4e^4m) \text{ implies } (4e^3mm'/n^2)^{m'} \leq (1/e)^{m'} \leq \frac{1}{n}. \text{ Therefore the sum is at most}
\[ O\left(\frac{\log n}{n}\right) + \sum_{2\leq i\leq \log n} O\left(\frac{\log^2 n}{n}\right) + \sum_{i>\log n} \left(\frac{1}{e}\right)^i \]
\[ = O\left(\frac{\log n}{n}\right), \]

which is smaller than 1/3 provided n is sufficiently large. \[ \blacksquare \]

**Proof (Theorem 3.1):** Let \( \epsilon > 0 \) and let \( C = 4/\epsilon^2 \). Let n be sufficiently large as a function of \( \epsilon \) (and hence C). Let \( Q \) be a random quartet set of size \(|Q| = m = 2^n n \log n\). Then, by Lemma 3.1, with probability at least \( 2/3 \) there is no phylogenetic tree satisfying more than a fraction of \( 1/3 + \epsilon \) quartets of \( Q \). By Lemma 3.4, with probability at least \( 2/3 \), every subset of \( Q \) of size at most \( \frac{1}{16\epsilon^2 \log n} \) is compatible. Since with probability at least \( 1/3 \) (namely, positive probability) both lemmata hold for a randomly chosen \( Q \), the theorem follows. \[ \blacksquare \]

4 Tri-compatibility implies compatibility

In Section 3 we have shown that even when all quartet subsets of a fairly large magnitude are compatible, the whole quartet set \( Q \) may still be very far from compatible. In this section we observe that when \( Q \) is very dense, this cannot happen. As before, our taxa set is of size \( n \). Recall that a full quartet set has size \( \binom{n}{4} \) where every four taxa induce a single quartet. The following proposition is a direct consequence of a result of Colonius and Schulze [11].

**Proposition 4.1.** Let \( Q \) be a full quartet set. If every subset of three quartets (a quartet triplet) is compatible, then \( Q \) is compatible.

The motivation to study quartet triplets stems from the following reason. Trivially, a single quartet is compatible, and by our assumption (that every four taxa induce a single quartet) and Observation 3.1, also a pair of quartets is compatible. This, however, changes when considering three or more quartets. For example, the set \([ab|cd],[ac|ed],[ae|cd]\) is easily seen to be incompatible. Figure 3:a shows two compatible quartets inducing a tree over five taxa whereas Figure 3:b shows a quartet triplet that is incompatible - every pair of quartets induces a different tree. We denote trees over five taxa as quintets and usually mark quintets by \( r \) (as \( q \) is reserved for quartets). Observe that all unlabeled phylogenetic trees on five leaves are isomorphic. Precisely two pairs of leaves have a common neighbor (such a pair is called a cherry). We therefore have the following definition.

**Definition 4.1.** A quintet is an unrooted phylogenetic tree over five taxa. We mark a quintet \( r = [12\{34,5\}] \) denoting that \{1,2\} and \{4,5\} are the two cherries and 3 is the remaining leaf.

**Proof (Proposition 4.1):** For a quartet set \( Q \), let \([ab*cd]\) denote that \([ac|bd] \notin Q \) and \([ad|bc] \notin Q \). The following result has been proved in [11]

Let \( Q \) be a quartet set. If for every five taxa \( \{a,b,c,d,e\} \) the following holds:

\[ [ae|bc] \lor [ae*cd] \Rightarrow ([ab*cd] \Rightarrow [be|cd]) \]

then \( Q \) is consistent.

Since in Proposition 4.1 we assume that \( Q \) is a full quartet set, we can rephrase this condition as

\[ [ae|bc] \lor [ae|cd] \Rightarrow ([ab|cd] \Rightarrow [be|cd]). \]

It is easy to verify that indeed each five taxa \( \{a,b,c,d,e\} \) obey this rule (see also [27], Ch. 6, Ex. 19). Indeed, if \([ae|bc]\) and also \([ab|cd]\) then the quintet must \([ae|bc|cd] \Rightarrow [be|cd]\) holds. Similarly, if \([ae|cd]\) and \([ab|cd]\) then the quintet is either \([qb|e|cd]\) or \([ae|bc|cd] \Rightarrow [be|cd]\) holds in any case. \[ \blacksquare \]

5 Extension to dense inputs

In the previous sections we have shown that when the quartet set is rather sparse, specifically \( O(n \log n) \)
quartets, it is possible that even if every relatively large subset of it is compatible, the entire set may still be very far from compatible. On the other hand, if the set is the full \( \binom{n}{4} \) quartet set, then it is enough that every quartet triplet is compatible, to force compatibility of the entire set. A natural question to ask is how far can we push up the size of the ground set, that is, increasing the number of quartets towards \( \binom{n}{4} \), and still obtain a negative result while requiring that all non-negligible size subsets are compatible. In this section we show that even for size \( \Theta\left(\binom{n}{4}\right) \) there are (very) incompatible sets of this size in which every subset of large constant cardinality is compatible.

**Theorem 5.1.** For any \( \gamma > 0 \) there exists \( \delta \leq \gamma \) and there exists quartet sets of size \( \delta n^4 \) that are incompatible, and yet have the property that every subset of size \( \Theta\left((1/\delta)^{1/3}\right) \) is compatible. \(^1\)

We give a short overview of the proof. We start with a small constant size basic set \( \mathcal{X}^* \) of \( N \) taxa that is big enough for Theorem 3.1 to hold. We therefore have a quartet set of size \( \Theta(N \log N) \) for which we know that it is not compatible and yet every subset of size \( \Theta(N/\log N) \) is compatible. Next, we use a blowup argument to expand the basic set to a set of taxa \( \mathcal{X} \) of size \( n \) and \( \Theta\left(\binom{n}{4}\right) \) quartets. We prove that the expanded quartet set is still very far from being compatible yet any appropriate large constant size subset of it is compatible. Adjusting the parameter \( \gamma \) and hence \( \delta \) controls the size of \( N \) and the blowup scale, and the theorem folloew. We proceed with the details.

**Proof.** By the proof of Theorem 3.1 we know that for any \( \epsilon > 0 \) there exists \( N_0 = N_0(\epsilon) \) such that for all \( N > N_0 \) there exists a quartet set \( Q \) over a taxa set of size \( N \) with \( |Q| = \frac{1}{4} N \log N \) with the following properties: No tree satisfies more than a fraction of \( 1/3 + \epsilon \) elements of \( Q \) and yet every subset of \( Q \) with at most \( \epsilon^2 N/(16e^4 \log N) \) elements is compatible. For \( \gamma > 0 \), let \( \epsilon > 0 \) be the largest constant for which \( N_0 = N_0(\epsilon) \) satisfies

\[
\gamma \geq \frac{4 \log N_0}{\epsilon^2 N_0^3} .
\]

Let \( N \geq N_0 \) be the smallest constant which satisfies

\[
\left(\frac{1}{\delta(\log \frac{1}{\delta})^4}\right)^{1/3} \leq \frac{\epsilon^2 N}{16e^4 \log N}
\]

where

\[
\delta = \frac{4 \log N}{\epsilon^2 N^3} .
\]

Observe that indeed \( \delta \leq \gamma \).

Let \( \mathcal{X}^* \) be a ground set of \( N \) taxa and let \( Q^* \) be a set of \( |Q^*| = \frac{1}{4} N \log N \) quartets over \( \mathcal{X}^* \) with the following properties: No tree satisfies more than a fraction of \( 1/3 + \epsilon \) elements of \( Q^* \) and yet every subset of \( Q^* \) with at most \( \epsilon^2 N/(16e^4 \log N) \) elements is compatible.

Let \( \mathcal{X} \) be obtained from \( \mathcal{X}^* \) by replacing each taxon \( x \in \mathcal{X}^* \) with \( k \) copies denoted \( x_1, \ldots, x_k \) where \( k = n/N \). Observe that \( |\mathcal{X}| = n \). Correspondingly, construct a quartet set \( Q = \{Q^*\}_k \) by constructing, for each \( q = [ab|cd] \in Q^* \) a set of \( k^4 \) copies of the form \( q_{i,j,\ell,p} = [a_i b_j | c_\ell d_p] \) for \( i, j, \ell, p = 1, \ldots, k \). Notice that

\[
|Q| = k^4 |Q^*| = \left(\frac{n}{N}\right)^4 \frac{4}{\epsilon^2} N \log N = \delta n^4 .
\]

We next show that \( Q \) is (very) incompatible. Let \( Q' \subset Q \) be any set of size least \( (1/3 + \epsilon)|Q| \). We show that \( Q' \) is incompatible. We can partition \( Q' \) into \( k^4 \) equivalence classes \( Q'(i,j,\ell,p) \) according to the indices of the quartets in it. A quartet \([a_i b_j | c_\ell d_p]\) belongs to the class \( Q'(i,j,\ell,p) \). By averaging, there is some equivalence class, say \( WLOG Q'(1,1,1,1) \), of size at least

\[
\frac{|Q'|}{k^4} \geq \frac{(1/3 + \epsilon)|Q|}{k^4} = \frac{(1/3 + \epsilon)|Q^*|}{(n/N)^4} = (1/3 + \epsilon)|Q^*| .
\]

But \( Q'(1,1,1,1) \) is isomorphic to a subset of quartets of \( Q^* \) (simply ignore the indices), and by the properties of \( Q^* \) we have that no subset of more than a fraction of \( 1/3 + \epsilon \) elements of it is satisfied, and hence \( Q'(1,1,1,1) \) is incompatible. Thus, \( Q' \) is incompatible.

It remains to prove that every subset of \( Q \) of size \( \left(\frac{1}{\delta(\log \frac{1}{\delta})^4}\right)^{1/3} \) is compatible. Indeed, let \( Q' \) be such a subset. If we ignore the indices of the taxa we get that the index-free \( Q' \) is a (multi) set of \( Q^* \) of size at most \( \left(\frac{1}{\delta(\log \frac{1}{\delta})^4}\right)^{1/3} \), and hence, by (5.3) and by the property of \( Q^* \), it is compatible. Let \( T' \) be a tree satisfying the index-free \( Q' \) over \( \mathcal{X}^* \). Replace every leaf (taxa) in \( T' \) with a tree on its \( k \) copies, as shown in Figure 4, to obtain a tree over \( \mathcal{X} \) satisfying \( Q' \). \( \blacksquare \)

## 6 Maximum violation of compatible quartets

The issue of tree similarity is central in phylogenetics. The most common tree distance measure between two trees is the Robinson-Foulds metric that counts how many distinct bipartitions (a bipartition is the taxa partition of a tree resulting from the removal of an edge) are induced by exactly one of the two trees [20].

Another common measure that involves quartet compatibility is quartet distance [19]. Let \( T \) be a tree over \( n \) leaves and let \( Q(T) \) be its full quartet set of \( \binom{n}{4} \).
quartets. For another tree $T'$ with $n$ leaves, let $qd_T(T')$ denote the number of quartets out of $Q(T)$ satisfied by $T'$. Clearly, $qd_T(T) = \binom{n}{4}$ and $qd_T(T') = qd_T(T)$. A natural question to ask is how small can $qd_T(T')$ be. It is clear that a tree over four taxa, i.e. a quartet $q$, can easily be violated by another quartet $q'$, simply by rewiring (permuting) the taxa of $q$, yielding $qd_q(q') = 0$. However, as we show next, for larger trees, the problem gets significantly more involved.

We now define the problem rigorously using, for convenience, the following notation. Let $f(n)$ denote the maximum cardinality of a set of compatible quartets $Q$ over $n$ taxa such that there is some tree which violates all of $Q$. Trivially, $f(n) \leq \binom{n}{4}$ and $f(4) = 1$. A classical conjecture of Bandelt and Dress [2] states that $f(n)/\binom{n}{4}$ converges to $2/3$.

The simplest non trivial tree is a quintet. As we have seen in Section 4, there is a single unlabeled structure for a quintet so for $n = 5$, we can only rewrite the labels on the leaves. Observe that the quintet $r' = [15|3|24]$ violates all the quartets defined by the quintet $r = [12|3|45]$ thereby showing that $f(5) = 5$ (or, equivalently, that $qd_r(r') = 0$). However, as we shall see in Lemma 6.1, already for $n = 6$ we no longer have total violation, as $f(6) = 14 < \binom{6}{4}$. This was also proved in [2] but the proof here is a bit simpler. The main result of this section provides upper and lower bounds for $f(n)$.

**Theorem 6.1.** $\frac{a}{10}^{\binom{n}{4}}(1 + o(1)) \geq f(n) > \frac{2}{3}^{\binom{n}{4}}$.

We first establish the following lemma (see also [2]).

**Lemma 6.1.** $f(6) = 14$.

**Proof.** There are two non-isomorphic unlabeled phylogenetic trees on 6 leaves. One with three cherries and another with two cherries, which we denote as the flower and the caterpillar respectively (see Figure 5). Let $T$ and $T'$ be two labeled trees on the 6 taxa $\{1, 2, 3, 4, 5, 6\}$. We need to show that at least one quartet is satisfied by both of them.

Figure 4: (a) A tree $T'$ on taxa set $X' = \{a, b, c, d, e\}$. (b) The tree $T'$ on taxa set $X$ after replacing each leaf with its $k$ copies ($k = 3$ in this example).

Figure 5: (a) The 6-flower tree. (b) The 6-caterpillar tree [12|3|4|56].

Assume first that at least one of $T$ or $T'$ is a flower. WLOG $T$ is a flower. Observe that the flower has the property that for any two of its taxa $x, y$, there is at least one quartet of the form $[xy|ab]$. Indeed, if $\{a, b\}$ is a cherry not involving $x$ or $y$, then the quartet on $\{x, y, a, b\}$ has this form. Now, for any cherry $\{x, y\}$ of $T'$, and for any cherry $\{a, b\}$ of $T$ which does not involve $x, y$, the quartet $[xy|ab]$ is satisfied by both $T$ and $T'$.

We may now assume that both $T$ and $T'$ are caterpillars. Assume WLOG that $\{1, 2\}, \{5, 6\}$ are the cherries of $T$ and that 3 is the “non-cherry” closer to $\{1, 2\}$. For convenience, we can denote $T$ by [12|3|4|56].

Now, if 1 and 2 are not in opposite cherries in $T'$ (namely $T'$ is not of the form $[x|y|a|b|c|2d]$), then there is at least one quartet in $T'$ of the form $[12|ab]$, as we can take $a, b$ to be a cherry of $T'$ not involving 1, 2.

So, we may now assume that 1 and 2 are in opposite cherries in $T'$, and, symmetrically, we can assume that 5 and 6 are in opposite cherries in $T'$. So, either $T'$
is equivalent to one of $[15|3|4|26]$ or $[15|4|3|26]$. In the first case, $[13|46]$ is the only quartet satisfied by both trees and in the second case, $[23|45]$ is the only quartet satisfied by both trees, proving that, in fact $f(6) = 14$.

Proof (Theorem 6.1): We first prove that $f(n) > \frac{4}{3} \binom{n}{4}$.

Let $T$ be any tree on the $n$-taxa set $X$. Let $Q = Q(T)$ be the full quartet set of $T$. In particular, any subset of $Q$ is a compatible set. Let $T^\pi$ be obtained from $T$ by randomly permuting the labels on the leaves. Then, for any quartet $Q'$ in $Q$, the probability that it is satisfied by $T^\pi$ is $1/3$. By linearity of expectation, the expected number of quartets of $Q$ satisfied by $T^\pi$ is $\binom{n}{4}/3$. As the random variable (that counts the number of quartets of $Q$ satisfied by $T^\pi$) is non-constant, we get that there is a permutation on the leaves such that the resulting $T^\pi$ does not satisfy more than $\frac{4}{3} \binom{n}{4}$ quartets of $Q$.

We next prove that $f(n) \leq \frac{9}{10} \binom{n}{4}(1 + o(1))$. Recall that an $r$-uniform hypergraph on $n$ vertices is a subset of $r$-sets of $\{1, \ldots, n\}$ (the $r$-sets are the edges of the hypergraph). An $r$-uniform hypergraph is complete if it contains all $\binom{r}{4}$ possible edges. Denote by $K^r_k$ the complete $r$-uniform hypergraph on $k$ vertices. For positive integers $r < k < n$, let $T(n, k, r)$ denote the maximum possible number of edges in an $r$-uniform hypergraph that does not contain $K^r_k$ as a subgraph. A result of de Caen [14] asserts that $T(n, 6, 4) \leq \frac{9}{10} \binom{n}{4}(1 + o(1))$.

Given two trees $T$ and $T^*$ on the $n$ taxa set $\{1, \ldots, n\}$, construct the following 4-uniform hypergraph $H$ whose vertices are the taxa. For any 4-set $\{a, b, c, d\}$, we make $\{a, b, c, d\}$ an edge of $H$ if and only if the quartet on $\{a, b, c, d\}$ in $T^*$ is different from the quartet on $\{a, b, c, d\}$ in $T$. By Lemma 6.1, we have that $H$ does not contain $K^4_6$ as a subgraph. Hence, the number of edges of $H$ is at most $T(n, 6, 4) \leq \frac{9}{10} \binom{n}{4}(1 + o(1))$.

7 Further research and open problems

In this work we presented several results regarding quartet subset compatibility. We drew a direct linkage between the density of the incompatible ground quartet set and the gap to its compatible constituting subsets. Our results rely on probabilistic arguments and hence do not necessarily provide explicit examples for the given proofs of existence.

As mentioned in the introduction, one consequence of the results here is that no sampling algorithm can effectively be used to determine the compatibility of the given quartet set, or estimate the maximum cardinality of a compatible subset of it.

The results presented here have tight link to quartet set closure as studied extensively in [9, 16, 23]. Recall that $co(Q)$ is the set of trees that satisfy $Q$. Then the closure of $Q$, $cl(Q)$ is defined as,

$$cl(Q) = \bigcap_{T \in co(Q)} Q(T).$$

That is, $cl(Q)$ is the quartet set that exists in every tree compatible with $Q$. There is no polynomial time algorithm known to compute $cl(Q)$. An implied property of $cl(Q)$ is that it cannot be extended by any quartet inference rule such as the dyadic closure rules presented below. In [23] an explicit set of six quartets over $n = 8$ taxa is given. This set has the property that it is incompatible yet every subset of it is compatible and closed. The example demonstrates that there are cases in which no quartet rule can be applied on any compatible subset, in order to arrive at a conflict at the ground set. However, it is not shown how this example can be extended to any $n$.

In this respect, it is interesting to find whether we can extend our compatible subsets by applying some quartet rules. We give here a partial answer to this question that extends our result from Theorem 3.1. We say that a set $Q$ is 2-closed if it cannot be extended by any of the two following two obvious rules (denoted as the dyadic closure, introduced first by [15] and used further in [17, 18]).

Definition 7.1. The dyadic closure of a quartet set $Q$, denoted as $cl_2(Q)$, is a minimal set of quartets that contains $Q$ and satisfies the following two rules:

1. dc1: $[ab|cd], [ab|ce] \in cl_2(Q) \Rightarrow [ab|de] \in cl_2(Q)$.
2. dc2: $[ab|cd], [bc|de] \in cl_2(Q) \Rightarrow [ab|ce], [ab|de], [ac|de] \in cl_2(Q)$.

Observe that, indeed, any tree which satisfies the quartets on the l.h.s. of a dyadic rule, must also satisfy the r.h.s. of the rule. Hence, $Q$ is 2-closed if $Q = cl_2(Q)$. Below is a restatement of Theorem 3.1 with the restriction to 2-closed sets.

Theorem 7.1. There exists a set $Q$ of $m$ quartets, such that $m = \Theta(n \log n)$ and every subset $Q' \subset Q$ of size $m' = O\left(\frac{n}{\log n}\right)$ is compatible and 2-closed, yet $Q$ is incompatible.

Proof. We need to show that in no subset of $Q$ we can apply one of the dyadic rules. Note that to apply each
of these rules we need to have jointly three taxa in both quartets. We need to show that there exists such a set, satisfying the conditions of Theorem 3.1 and also no two quartets share the same three taxa.

Observation 7.1. If $Q$ is a set of $\Theta(n \log n)$ random quartets, the probability of two quartets sharing the same three taxa, is $o(1)$.

Proof. For three taxa $a, b, c$, the probability of being selected in a quartet is $\frac{1}{n(n-1)(n-2)} \binom{3}{1} 3! = \Theta\left(\frac{1}{n^3}\right)$, and for being selected in two quartets $q_1$ and $q_2$, $\Theta\left(\frac{1}{n^7}\right)$. Since we have $\binom{n}{3}$ triplets of taxa, the probability of any three taxa appearing in two quartets is $\Theta\left(\frac{n^2}{n^7}\right)$. Finally, since the size of $Q$ is $\Theta(n \log n)$, there are $\Theta(n^2 \log^2 n)$ pairs of quartets, so the total probability is at most $O\left(\frac{\log^2 n}{n}\right) = o(1)$.

Since the probability to find such a pair of quartets is so low, it is clear that this constraint does not affect the existence of such a set $Q$ as we showed in Theorem 3.1.

The order of a closure inference rule is the minimal number of quartets necessary to derive the inference (i.e., number of quartets on the left side of the rule). Theorem 7.1 answers only partially the question of under what order our subsets are closed, that is, what are the closure inference rules that cannot be applied to them. In particular, if no inference rule can be applied to these subsets, they are fully closed. While using similar arguments to those used here can push the limit a bit upward, it seems that a different approach is necessary to prove/disprove full closeness.

As the majority of this work provides negative results regarding the inability to infer set compatibility based on subset compatibility, it would be beneficial to expand the positive result of Section 4 to other cases. It is noteworthy that compatibility of the full quartet set can be checked in polynomial time [2], and therefore the result of Section 4 is not of direct practical algorithmic use, and is mostly a structural result.

On the realm of quartet fit measure studied in Section 6, the task of closing the gap between the two bounds remains open. This is essential for providing a normalization means for this measure, representing the relative (as opposed to the absolute) quartet violation between trees.

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