

Reconstructing Biological and Digital Phylogenetic Trees in Parallel

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Abstract

In this paper, we study the parallel query complexity of reconstructing biological and digital phylogenetic trees from simple queries involving their nodes. This is motivated from computational biology, data protection, and computer security settings, which can be abstracted in terms of two parties, a *responder*, Alice, who must correctly answer queries of a given type regarding a degree- d tree, T , and a *querier*, Bob, who issues batches of queries, with each query in a batch being independent of the others, so as to eventually infer the structure of T . We show that a querier can efficiently reconstruct an n -node degree- d tree, T , with a logarithmic number of rounds and quasilinear number of queries, with high probability, for various types of queries, including *relative-distance queries* and *path queries*. Our results are all asymptotically optimal and improve the asymptotic (sequential) query complexity for one of the problems we study. Moreover, through an experimental analysis using both real-world and synthetic data, we provide empirical evidence that our algorithms provide significant parallel speedups while also improving the total query complexities for the problems we study.

2012 ACM Subject Classification Theory of computation → Parallel computing models

Keywords and phrases Tree Reconstruction, Parallel Algorithms, Privacy, Phylogenetic Trees, Data Structures, Hierarchical Clustering

Digital Object Identifier 10.4230/LIPIcs.ESA.2020.3

Related Version The full version of the paper is available at arXiv [2], <https://arxiv.org/abs/2006.15259>.

Supplementary Material The complete source code for our experiments, including the implementation of our algorithms and the algorithms we compared against, is available at <https://github.com/UC-Irvine-Theory/ParallelTreeReconstruction>.

Funding This article reports on work supported by NSF grant 1815073.

1 Introduction

Phylogenetic trees represent evolutionary relationships among a group of objects. For instance, each node in a biological phylogenetic tree represents a biological entity, such as a species, bacteria, or virus, and the branching represents how the entities are believed to have evolved from common ancestors [29, 8, 34]. (See Figure 1a.) In a digital phylogenetic tree,

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28th Annual European Symposium on Algorithms (ESA 2020).

Editors: Fabrizio Grandoni, Grzegorz Herman, and Peter Sanders; Article No. 3; pp. 3:1–3:24

 Leibniz International Proceedings in Informatics
Schloss Dagstuhl – Leibniz-Zentrum für Informatik, Dagstuhl Publishing, Germany

3:2 Reconstructing Phylogenetic Trees in Parallel

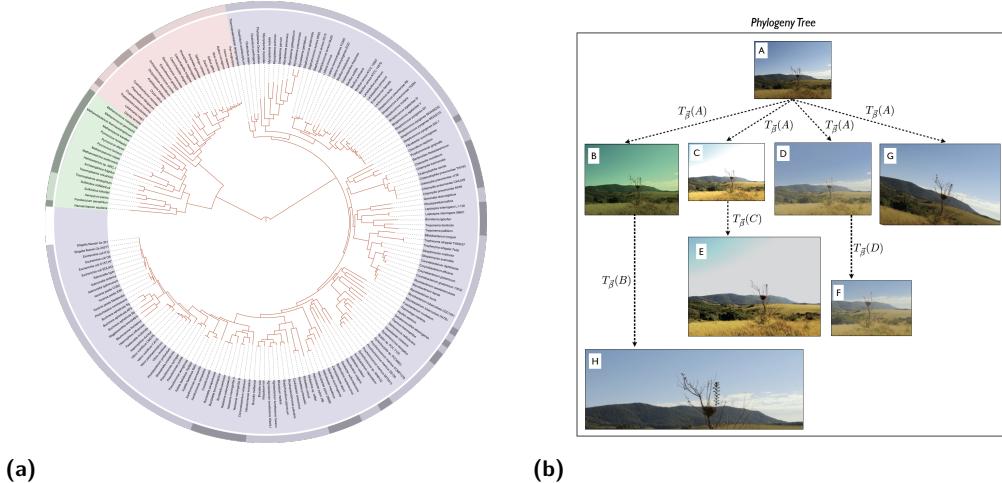


Figure 1 Two phylogenetic trees. (a) A biological phylogenetic tree of life, showing relationships between species whose genomes had been sequenced as of 2006; public domain image by Ivica Letunic, retrace by Mariana Ruiz Villarreal. (b) A digital phylogenetic tree of images, from Dias et al. [14].

on the other hand, each node represents a data object, such as a computer virus [22, 35], a source-code file [27], a text file or document [32, 40], or a multimedia object (such as an image or video) [6, 16, 15, 14] and the branching represents how these objects are believed to have evolved through edits or data compression/corruption. (See Figure 1b.)

In this paper, we are interested in studying efficient methods for reconstructing phylogenetic trees from queries regarding their structure, noting that there are differences in the types of queries one may perform on the two types of phylogenetic trees. In particular, with some exceptions,¹ in a biological phylogenetic tree we can only perform queries involving the leaves of the tree, since these typically represent living biological entities and internal nodes represent ancestors that are likely to be extinct. In digital phylogenetic trees, on the other hand, we can perform queries involving any of the nodes in the tree, including internal nodes, since these represent digital artifacts, which are often archived. The former type of phylogenetic tree has also received attention in the context of *hierarchical clustering*, where the goal is to provide a hierarchical grouping structure of items according to their similarity [18]. To support reconstruction of both biological and digital phylogenetic trees, therefore, we study both types of querying regimes in this paper.

More specifically, with respect to biological phylogenetic trees, we focus on *relative-distance* queries, where one is given three leaf nodes (corresponding to species), x , y , and z , and the response is a determination of which pair, (x, y) , (x, z) , or (y, z) , is a closest pair, hence, has the most-recent common ancestor [29]. With respect to digital phylogenetic trees, we instead focus on *path queries*, where one is given two nodes, v and w , in the tree and the response is “true” if and only if v is an ancestor of w .

The motivation for reconstructing phylogenetic trees comes from a desire to better understand the evolution of the objects represented in a given phylogenetic tree. For example, understanding how biological species evolved is useful for understanding and

¹ One notable exception to this restriction of only being able to ask queries involving leaves in a biological phylogenetic tree is for phylogenetic trees of biological viruses, for which genetic sequencing may be known for all instances; hence, ancestor-descendant path queries might also be appropriate for reconstructing some biological phylogenetic trees.

categorizing the fossil record and understanding when species are close relatives [29, 18]. Similarly, understanding how digital objects have been edited and transformed can be useful for data protection, computer security, privacy, copyright disputes, and plagiarism detection [22, 35, 27, 32, 40, 6, 16, 15, 14]. For instance, understanding the evolutionary process of a computer virus can provide insights into its ancestry, characteristics of the attacker, and where future attacks might come from and what they might look like [35].

The efficiency of a tree reconstruction algorithm can be characterized in terms of its **query-complexity** measure, $Q(n)$, which is the total number of queries of a certain type needed to reconstruct a given tree. This parameter comes from machine-learning and complexity theory, e.g., see [1, 9, 17, 42], where it is also known as “decision-tree complexity,” e.g., see [48, 5]. Previous work on tree reconstruction has focused on sequential methods, where queries are issued and answered one at a time. For example, in pioneering work for this research area, Kannan et al. [29] show that an n -node biological phylogenetic tree can be reconstructed sequentially from $O(n \log n)$ three-node relative-distance queries.

Indeed, their reconstruction algorithms are inherently sequential and involve incrementally inserting leaf nodes into the phylogenetic tree reconstructed for the previously-inserted nodes.

In many tree reconstruction applications, queries are expensive [29, 18, 22, 35, 27, 32, 40, 6, 16, 15, 14], but can be issued in batches. For example, there is nothing preventing the biological experiments [29] that are represented in three-node relative-distance queries from being issued in parallel. Thus, in order to speed up tree reconstruction, in this paper we are interested in parallel tree reconstruction. To this end, we also use a **round-complexity** parameter, $R(n)$, which measures the number of rounds of queries needed to reconstruct a tree such that the queries issued in any round comprise a batch of independent queries. That is, no query issued in a given round can depend on the outcome of another query issued in that round, although both can depend on answers to queries issued in previous rounds. Roughly speaking, $R(n)$ corresponds to the span of a parallel reconstruction algorithm and $Q(n)$ corresponds to its work. In this paper, we are interested in studying complexities for $R(n)$ and $Q(n)$ with respect to biological and digital phylogenetic trees with fixed maximum degree, d .

1.1 Related Work

The general problem of reconstructing graphs from distance queries was studied by Kannan et al. [30], who provide a randomized algorithm for reconstructing a graph of n vertices using $\tilde{O}(n^{3/2})$ distance queries.²

Previous parallel work has focused on inferring phylogenetic trees through Bayesian estimation [4]. However, we are not aware of previous parallel work using a similar query models to ours. With respect to previous work on sequential tree reconstruction, Culberson and Rudnicki [13] provide the first sub-quadratic algorithms for reconstructing a weighted undirected tree with n vertices and bounded degree d from additive queries, where each query returns the sum of the weights of the edges of the path between a given pair of vertices. Reyzin and Srivastava [38] show that the Culberson-Rudnicki algorithm uses $O(n^{3/2} \cdot \sqrt{d})$ queries.

Waterman et al. [47] introduce the problem of reconstructing biological phylogenetic trees, using additive queries, which are more powerful than relative-distance queries. Hein [24] shows that this problem has a solution that uses $O(dn \log_d n)$ additive queries, when the

² The $\tilde{O}(\cdot)$ notation hides poly-logarithmic factors.

tree has maximum degree d , which is asymptotically optimal [31]. Kannan et al. [29] show that an n -node binary phylogenetic tree can be reconstructed from $O(n \log n)$ three-node relative-distance queries. Their method appears inherently sequential, however, as it is based on an incremental approach that mimics insertion-sort. Similarly, Emamjomeh-Zadeh and Kempe [18] also give a sequential method using relative-distance queries that has a query complexity of $O(n \log n)$. Their algorithm, however, was designed for a different context, namely, hierarchical clustering.

Additionally, there exists some work (e.g. [28, 7, 25]) in an alternative perspective of the problem reconstructing phylogenetic trees, in which the goal is to find the best tree explaining the similarity and the relationship between a given fixed (or dynamic) set of data sequences (e.g. of species), using Maximum Parsimony [19, 21, 39] or Maximum Likelihood [20, 10]. This contrasts with our approach of recovering the “ground truth” tree known only to an oracle, which is consistent with its answers about the tree.

With respect to digital phylogenetic tree reconstruction, there are a number of sequential algorithms with $O(n^2)$ query complexities, including the use of what we are calling path queries, where the queries are also individually expensive, e.g., see [22, 35, 27, 32, 40, 6, 16, 15, 14]. Jagadish and Sen [26] consider reconstructing undirected unweighted degree- d trees, giving a deterministic algorithm that requires $O(dn^{1.5} \log n)$ separator queries, which answer if a vertex lies on the path between two vertices. They also give a randomized algorithm using an expected $O(d^2 n \log^2 n)$ number of separator queries, and they give an $\Omega(dn)$ lower bound for any deterministic algorithm. Wang and Honorio [46] consider the problem of reconstructing bounded-degree rooted trees, giving a randomized algorithm that uses expected $O(dn \log^2 n)$ path queries. They also prove that any randomized algorithm requires $\Omega(n \log n)$ path queries.

Our Contributions. In this paper, we study the parallel phylogenetic tree reconstruction problem with respect to the two different types of queries mentioned above:

- We show that an n -node rooted biological (binary) phylogenetic tree can be reconstructed from three-node **relative-distance queries** with $R(n)$ that is $O(\log n)$ and $Q(n)$ that is $O(n \log n)$, with high probability (w.h.p.)³. Both bounds are asymptotically optimal.
- We show that an n -node fixed-degree digital phylogenetic tree can be reconstructed from **path queries**, which ask whether a given node, u , is an ancestor of a given node, w , with $R(n)$ that is $O(\log n)$ and $Q(n)$ that is $O(n \log n)$, w.h.p. We also provide an $\Omega(dn + n \log n)$ lower bound for any randomized or deterministic algorithm suggesting that our algorithm is optimal in terms of query complexity and round complexity. Further, this asymptotically-optimal $Q(n)$ bound actually improves the sequential complexity for this problem, as the previous best bound for $Q(n)$, due to Wang and Honorio [46], had a $Q(n)$ bound of $O(n \log^2 n)$ for reconstructing fixed-degree rooted trees using path queries. Of course, our method also applies to biological phylogenetic trees that support path queries.

A preliminary announcement of some of this paper’s results, restricted to binary trees, was presented in [3]. Most of our algorithms are quite simple, although their analyses are at times nontrivial. Moreover, given the many applications of biological and digital phylogenetic tree reconstruction, we feel that our algorithms have real-world applications. Thus, we

³ We say that an event occurs with high probability if it occurs with probability at least $1 - 1/n^c$, for some constant $c \geq 1$.

have done an extensive experimental analysis of our algorithms, using both real-world and synthetic data for biological and digital phylogenetic trees. Our experimental results provide empirical evidence that our methods achieve significant parallel speedups while also providing improved query complexities in practice.

2 Preliminaries

In graph theory, an *arborescence* is a directed graph, T , with a distinguished vertex, r , called the *root*, such that, for any vertex v in T that is not the root, there is exactly one path from r to v , e.g., see Tutte [43]. That is, an arborescence is a graph-theoretic way of describing a rooted tree, so that all the edges are going away from the root. In this paper, when we refer to a “rooted tree” it should be understood formally to be an arborescence.

We represent a rooted tree as $T = (V, E, r)$, with a vertex set V , edge set E , and root $r \in V$. The *degree* of a vertex in such a tree is the sum of its in-degree and out-degree, and the degree of a tree, T , is the maximum degree of all vertices in T . So, an arborescence representing a binary tree would have degree 3. Because of the motivating applications, e.g., from computational biology, we assume in this paper that the trees we want to reconstruct have maximum degree that is bounded by a fixed constant, d .

Let us review a few terms regarding rooted trees.

► **Definition 1** (ancestry). *Given a rooted tree, $T = (V, E, r)$, we say u is **parent** of v (and v is a **child** of u) if there exists a directed edge (u, v) in E . The **ancestor** relation is the transitive closure of the parent relation, and the **descendant** relation is the transitive closure of the child relation. We denote the number of descendants of vertex s by $D(s)$. A node without any children is called a **leaf**. Given two leaf nodes, u and v in T , their **lowest common ancestor**, $\text{lca}(u, v)$, is the node, w in T , that is an ancestor of both u and v and has no child that is also an ancestor of u and v .*

We next define the types of queries we consider in this paper for reconstructing a rooted tree, $T = (V, E, r)$.

► **Definition 2.** *A **relative-distance query** for T is a function, closer , which takes three leaf nodes, u , v , and w in T , as input and returns the pair of nodes from the set, $\{u, v, w\}$, that has the lower lowest common ancestor. That is, $\text{closer}(u, v, w) = (u, v)$ if $\text{lca}(u, v)$ is a descendant of $\text{lca}(u, w) = \text{lca}(v, w)$. Likewise, we also have that $\text{closer}(u, v, w) = (u, w)$ if $\text{lca}(u, w)$ is a descendant of $\text{lca}(u, v) = \text{lca}(v, w)$, and $\text{closer}(u, v, w) = (v, w)$ if $\text{lca}(v, w)$ is a descendant of $\text{lca}(u, v) = \text{lca}(u, w)$.*

Definition 2 assumes T is a binary tree (of degree 3). Note that in this paper we restrict relative-distance queries to leaves, since these represent, e.g., current species in the application of reconstructing biological phylogenetic trees.

► **Definition 3.** *A **path query** for T is a function, path , that takes two nodes, u and v in T , as input and returns 1 if there is a (directed) path from vertex u to v , and otherwise returns 0. Also, for $u \in V$ and $W \subseteq V$, we define $\text{count}(u, W) = \sum_{v \in W} \text{path}(u, v)$, which is the number of descendants of u in W .*

We next study some preliminaries involving the structure of degree- d rooted trees that will prove useful for our parallel algorithms.

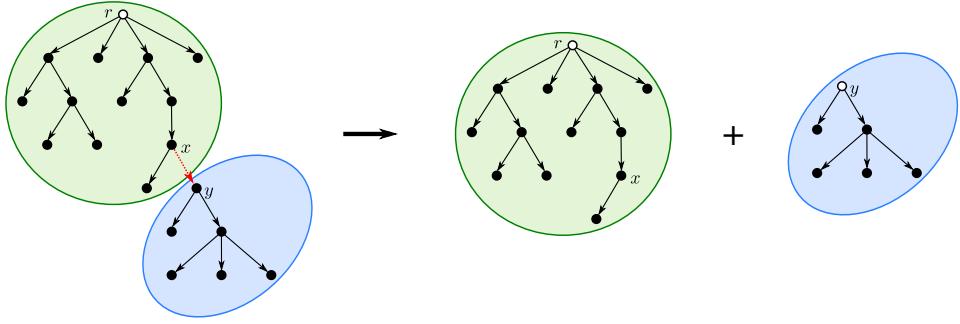


Figure 2 Illustration of a divide-conquer approach for trees. The edge (x, y) is an even-edge-separator. Note that the root of T'' is r , while y becomes root of T' .

► **Definition 4.** Let $T = (V, E, r)$ be a degree- d rooted tree. We say that an edge $e = (x, y) \in E$ is an **even-edge-separator** if removing e from T partitions it into two rooted trees, $T' = (V', E', y)$ and $T'' = (V'', E'', r)$, such that $\frac{|V|}{d} \leq |V'| \leq \frac{|V|(d-1)}{d}$ and $\frac{|V|}{d} \leq |V''| \leq \frac{|V|(d-1)}{d}$. (See Figure 2.)

► **Lemma 5.** Every rooted tree of degree- d has an even-edge-separator.

Proof. This follows from a result by Valiant [45, Lemma 2]. ◀

As we will see, this fact is useful for designing simple parallel divide-and-conquer algorithms. Namely, if we can find an even-edge-separator, then we can cut the tree in two by removing that edge and recurse on the two remaining subtrees in parallel (see Figure 2).

3 Reconstructing Biological Phylogenetic Trees in Parallel

Relative-distance queries model an experimental approach to constructing a biological phylogenetic tree, e.g., where DNA sequences are compared to determine which samples are the most similar [29]. In simple terms, pairs of DNA sequences that are closer to one another than to a third sequence are assumed to be from two species with a common ancestor that is more recent than the common ancestor of all three. In this section, for the sake of tree reconstruction, we assume the **responder** has knowledge of the absolute structure of a rooted binary phylogenetic tree; hence, each response to a *closer*(u, v, w) query is assumed accurate with respect to an unknown rooted binary tree, T . As in the pioneering work of Kannan et al. [29], we assume the distance comparisons are accurate and consistent. The novel dimension here is that we consider parallel algorithms for phylogenetic tree reconstruction.

As mentioned above, we consider relative-distance queries to occur between leaves of a rooted binary tree, T . That is, in our query model, the **querier** has no knowledge of the internal nodes of T and can only perform queries using leaves. Because T is a binary phylogenetic tree, we may assume it is a **proper** binary tree, where each internal node in T has exactly two children.

3.1 Algorithm

At a high level, our parallel reconstruction algorithm (detailed in Algorithm 1) uses a randomized divide-and-conquer approach, similar to Figure 2. In our case, however, the division process is random three-way split through a vertex separator, rather than an edge-separator-based binary split. Initially, all leaves belong to a single partition, L . Then two

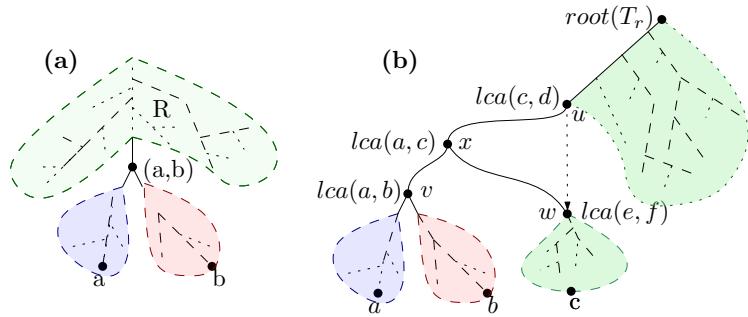


Figure 3 (a) The subgroups leaves are split into. (b) The linking step attaching T_a , T_b and T_r .

Algorithm 1 Reconstruct a binary tree of a set of leaves, L .

```

1 Function reconstruct-phylogenetic( $L$ ):
2   if  $|L| \leq 3$  then return the tree formed by querying  $L$ 
3   Pick two leaves,  $a, b \in L$ , uniformly at random
4   for each  $c \in L$  s.t.  $c \neq a, b$  do in parallel
5     Perform query  $\text{closer}(a, b, c)$ 
6     Split the leaves in  $L$  into  $R$ ,  $A$ , and  $B$  based on results
7     parallel do
8        $T_a \leftarrow \text{reconstruct-phylogenetic}(A \cup \{a\})$ 
9        $T_b \leftarrow \text{reconstruct-phylogenetic}(B \cup \{b\})$ 
10       $T_r \leftarrow \text{reconstruct-phylogenetic}(R)$ 
11      Let  $v$  be a new node, labeled “ $\text{lca}(a, b)$ ”
12      Set  $v$ ’s left child to  $\text{root}(T_a)$  and the right to  $\text{root}(T_b)$ 
13      if  $R = \emptyset$  then return tree,  $T_v$ , rooted at  $v$ 
14      else return  $\text{link}(v, T_r)$ 

```

leaves, a and b , are chosen uniformly at random from L and each remaining leaf, c , is queried in parallel against them using relative-distance queries. Notice that the lowest common ancestor of a and b splits the tree into three parts. Given a and b , the other leaves are split into three subsets (R , A , and B) according to their query result (as shown in Figure 3(a)):

- A : leaves close to a , i.e., for which $\text{closer}(a, b, c) = (a, c)$
- B : leaves close to b , i.e., for which $\text{closer}(a, b, c) = (b, c)$
- R : remaining leaves, i.e., for which $\text{closer}(a, b, c) = (a, b)$

We then recursively construct the trees in parallel: T_a , for $A \cup \{a\}$; T_b , for $B \cup \{b\}$; and T_r , for R . The remaining challenge, of course, is to merge these trees to reconstruct the complete tree, T . The subtree of T formed by subset $A \cup B$ is rooted at an internal node, $v = \text{lca}(a, b)$; hence, we can create a new node, v , label it “ $\text{lca}(a, b)$ ” and let T_a and T_b be v ’s children. If $R = \emptyset$, then we are done. Otherwise, we need to determine the parent of v in T ; that is, we need to link v into T_r using function $\text{link}(v, T_r)$.

To identify the parent of v , in T , let us assume inductively that each internal node $u \in T_r$ has a label “ $\text{lca}(c, d)$ ”, since we have already recursively labeled each internal node in T . Recall that v is labeled with “ $\text{lca}(a, b)$ ”. The crucial observation is to note if there exists an edge $(u \rightarrow w)$ in T_r , such that u is labeled “ $\text{lca}(c, d)$ ” and $\text{closer}(a, c, d) = (a, z)$ for $z \in \{c, d\}$, and w is either leaf z or an ancestor of z labeled “ $\text{lca}(e, f)$ ” with $\text{closer}(a, e, f) = (e, f)$, (See Figure 3(b)), then edge $(u \rightarrow w)$ must be where the parent of v belongs in T , and if

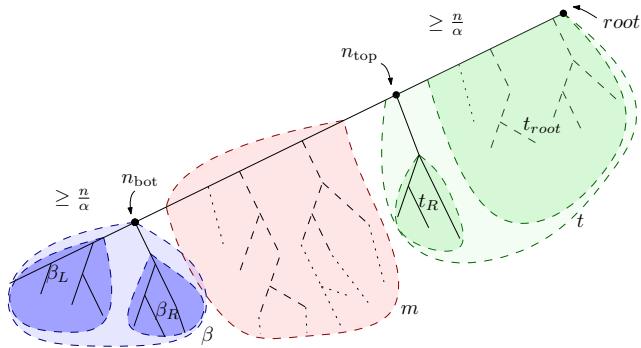


Figure 4 A left-heavy tree drawing displaying node n_{top} , node n_{bot} and the relevant partitions.

there is no such edge, the parent of v is the root of T and the sibling of v is the root of T_r . We can determine the edge $(u \rightarrow w)$ in a single parallel round by performing the query, $\text{closer}(a, c, d)$, for each each internal node $u \in T$ (where the label of u is “ $\text{lca}(c, d)$ ”). The full pseudo-code of function $\text{link}(v, T_r)$ is provided in the full version of the paper [2]. It is also worth noting that if the oracle can identify cases where all three leaves share a single lca, simple modifications to Algorithm 1 would enable it to handle trees of higher degree.

3.2 Analysis

The correctness of our algorithm follows from the way relative-distance queries always return a label for the lowest common ancestor for the two closest leaves among the three input nodes. Furthermore, executing the three recursive calls can be done in parallel, because $A \cup \{a\}$, $B \cup \{b\}$, and R form a partition of the set of leaves, L , and at every stage we only perform relative-distance queries relevant to the respective partition.

► **Theorem 6.** Given a set, L , of n leaves in a proper binary tree, T , such as a biological phylogenetic tree, we can reconstruct T using relative-distance queries with a round complexity, $R(n)$, that is $O(\log n)$ and a query complexity, $Q(n)$, that is $O(n \log n)$, with high probability.

Proof. Because the recursive calls we perform in each call to the reconstruct algorithm are done in parallel on a partition of the leaf nodes in L , we perform $\Theta(n)$ work per round. Thus, showing that the number of rounds, $R(n)$, is $O(\log n)$ w.h.p. also implies that $Q(n)$ is $O(n \log n)$ w.h.p. To prove this, we show that each round in Algorithm 1 has a constant probability of decreasing the problem size by at least a constant factor for each of its recursive calls. For analysis purposes, we consider the left-heavy representation of each tree, in which the tree rooted at the left child of any node is always at least as big as the tree rooted at its right child. (See Figure 4.) Using this view, we can characterize when a partition determines a “good split” and provide bounds on the sizes of the partitions, as follows.

► **Lemma 7.** *With probability of at least $\frac{\alpha-5}{2\alpha^2}$, a round of Algorithm 1 decreases the problem size of any recursive call by at least a factor of $\frac{\alpha-1}{\alpha}$, for a constant $\alpha > 5$, thus experiencing a good split.*

Proof. Define the *spine* to be all nodes on the path from the root to its left-most leaf in a left-heavy drawing. Let n_{bot} be the bottom-most node on the spine that has at least n/α of the nodes in its sub-tree. Conversely, let n_{top} be the parent of the top-most spine node that has at most $(1 - 1/\alpha) \cdot n$ descendants. (See Figure 4.) Consider the three resulting trees obtained from separating at the incoming edge to n_{bot} and the outgoing edge from n_{top} to

its left child. As shown in Figure 4, let t be the resulting tree retaining the root, β the tree rooted at n_{bot} and m the tree between n_{top} and n_{bot} . Within β let β_L and β_R be the trees rooted at the left and right child of n_{bot} . Similarly, for t , let t_R be the tree rooted at the right child of n_{top} . Finally, let t_{root} be the remaining tree when cut at n_{top} .

Consider the size of tree β , $|\beta|$, since this is the first tree rooted in the spine with over n/α nodes, then β_L must have had strictly under n/α nodes. Since the trees are in left-heavy order, β_R can have at most as many nodes as β_L so $\frac{n}{\alpha} \leq |\beta| < \frac{2n}{\alpha}$. Furthermore, we know that $|\beta| + |m| + |t_R| + |t_{\text{root}}| + 1 = n$. Due to the left-heavy order, $|t_R| \leq |\beta| + |m|$. By definition of n_{top} , it's necessary that $|t_{\text{root}}| < \frac{n}{\alpha}$, thus $2(|\beta| + |m|) + 1 > n - \frac{n}{\alpha}$ and $|\beta| + |m| > \left(\frac{\alpha-1}{2\alpha}\right)n - \frac{1}{2}$. Using the previous inequality and $|t| = n - |\beta| - |m|$, we find $|t| < \left(\frac{\alpha+1}{2\alpha}\right)n + \frac{1}{2}$. Also, $|m| = n - |t| - |\beta|$, so $|m| > n - \frac{5n+\alpha n}{2\alpha}$.

$$\frac{n}{\alpha} \leq |\beta| < \frac{2n}{\alpha}, \quad \frac{n}{\alpha} \leq |t| < \left(\frac{\alpha+1}{2\alpha}\right)n + \frac{1}{2}, \quad \left(\frac{\alpha-5}{2\alpha}\right)n < |m| \leq \left(\frac{\alpha-2}{\alpha}\right)n \quad (1)$$

Picking a leaf from β and another from m guarantees that $\beta \subseteq (A \cup \{a\})$ and $t \subseteq R$. Thus, using Equation (1), each of the three sub-problem sizes, $|A \cup \{a\}|$, $|B \cup \{b\}|$, and $|R|$, will be at most $\left(\frac{\alpha-1}{\alpha}\right)n$, when $\alpha > 5$. $Pr[\text{good split}] \geq Pr[\text{leaf in } \beta] \cdot Pr[\text{leaf in } m]$. Asymptotically, $Pr[\text{leaf in } \beta] \approx Pr[\text{node in } \beta]$, thus $Pr[\text{good split}] > \frac{\alpha-5}{2\alpha^2}$, which established the lemma. \blacktriangleleft

Returning to the proof of Theorem 6, let $p = \frac{\alpha-5}{2\alpha^2}$. From Lemma 7, we expect it will take $1/p$ rounds to obtain a good split. Every good split will reduce the problem-size by at least a constant factor, $\frac{\alpha-1}{\alpha}$. Thus, we are guaranteed to have just a single node left after we get $N_{\text{SPLITS}} = \log_{\frac{\alpha}{\alpha-1}}(n)$ good splits. Consider the geometric random variable, X_i , describing the number of rounds required to obtain the i -th good split, then $X = X_1 + \dots + X_{N_{\text{SPLITS}}}$ describes the total number of rounds required by the algorithm. By linearity of expectation, $E[X] = \frac{2\alpha^2}{(\alpha-5)} \cdot N_{\text{SPLITS}} = \frac{2\alpha^2}{(\alpha-5)} \cdot \log_{\frac{\alpha}{\alpha-1}}(n)$. Therefore, since $\alpha > 5$ is a constant, this already implies an expected $O(\log n)$ rounds for Algorithm 1. Moreover, by a Chernoff bound for the sum of independent geometric random variables (see [23, 33]), $Pr[X > C \cdot E[X]] \leq e^{-\frac{(C-1) \cdot p \cdot N_{\text{SPLITS}}}{5}}$ for any constant $C \geq 3$ and constant $\alpha > 5$. Thus, the probability that we take over $C \cdot E[X]$ rounds is $O(1/n^{C-1})$. Therefore, by a union bound across the n leaves, our algorithm completes in $O(\log n)$ rounds w.h.p. \blacktriangleleft

► **Corollary 8.** *Algorithm 1 is optimal when asking $\theta(n)$ queries per round.*

The query complexity of Algorithm 1 matches an $\Omega(n \log n)$ lower bound for $Q(n)$, due to Kannan et al. [29]. Besides, we need $\Omega(\log n)$ rounds if we have $\theta(n)$ processors; hence, the round complexity of Algorithm 1 is also optimal.

4 Reconstructing Phylogenetic Trees from Path Queries

Let $T = (V, E, r)$ be a rooted (biological or digital) phylogenetic tree with fixed degree, d . In this section, we show how a querier can reconstruct T by issuing $Q(n) \in O(n \log n)$ path queries in $R(n) \in O(\log n)$ rounds, w.h.p., where $n = |V|$. We provide a lower bound to prove that our algorithm is optimal in terms of query complexity and round complexity. At the outset, the only thing we assume the querier knows is n and V , that is, the vertex set for T , and that the names of the nodes in V are unique, i.e., we may assume, w.l.o.g., that $V = \{1, 2, \dots, n\}$. The querier doesn't know E or r – learning these is his goal.

4.1 Algorithms

We start by learning r , which we show can be done via any maximum-finding algorithm in Valiant's parallel model [44], which only counts parallel steps involving comparisons. The challenge, of course, is that the ancestor relationship in T is, in general, not a total order, as required by a maximum-finding algorithm. This does not actually pose a problem, however.

► **Lemma 9.** *Let A be a parallel maximum-finding algorithm in Valiant's model, with $O(f(n))$ span and $O(g(n))$ work. We can use A to find the root, r in a rooted tree $T = (V, E, r)$, using $R(n) \in O(f(n))$ rounds and $Q(n) \in O(g(n) + n)$ total queries.*

Proof. We pick an arbitrary vertex $v \in T$. In the first round, we perform queries $path(u, v)$ in parallel for every other vertex $u \in V$ to find S , the ancestor set for v . If $S = \emptyset$, then v is the root. Otherwise, we know all the vertices in a path from root to the parent of v , albeit unsorted. Still, note that for S the ancestor relation is a total order; hence, we can simulate A with path queries to resolve the comparisons made by A . We have just a single round and $O(n)$ queries more than what it takes for A to find the maximum. Thus, we can find the root in $O(f(n))$ rounds and $O(g(n) + n)$ queries. ◀

Thus, by well-known maximum-finding algorithms, e.g., see [11, 41, 44]:

► **Corollary 10.** *We can find r of a rooted tree $T = (V, E, r)$ deterministically in $O(\log \log n)$ rounds and $O(n)$ queries.*

Determining the rest of the structure of T is more challenging, however. At a high level, our approach to solving this challenge is to use a separator-based divide-and-conquer strategy, that is, find a “near” edge-separator in T , divide T using this edge, and recurse on the two remaining subtrees in parallel. The difficulty, of course, is that the querier has no knowledge of the edges of T ; hence, the very first step, finding a “near” edge-separator, is a bottleneck computation. Fortunately, as we show in Lemma 11, if v is a randomly-chosen vertex, then, with probability depending on d , the path from root r to v includes an edge-separator.

► **Lemma 11.** *Let $T = (V, E, r)$ be a rooted tree of degree d and let v be a vertex chosen uniformly at random from V . Then, with probability at least $\frac{1}{d}$, an even-edge-separator is one of the edges on the path from r to v .*

Proof. By Lemma 5, T has an even-edge-separator. Let $e = (x, y)$ be an even-edge-separator for $T = (V, E, r)$ and let $T' = (V', E', y)$ be the subtree rooted at y when we remove e . Then, every path from r to each $v \in V'$ must contain e . By Definition 4, T' has at least $|V|/d$ vertices. Therefore, if we choose v uniformly at random from V , then with probability $\frac{|V'|}{|V|} \geq \frac{1}{d}$, the path from r to v contains e . ◀

► **Definition 12 (splitting-edge).** *In a degree- d rooted tree, an edge $(parent(s), s)$ is a splitting-edge if $\frac{|V|}{d+2} \leq D(s) \leq \frac{|V|(d+1)}{d+2}$, where $D(s)$ is the number of descendants of s .*

Note that a degree- d rooted tree T always has a splitting-edge, as every even-edge-separator is also a splitting-edge and by Lemma 5, it always has an even-edge-separator – a fact we use in our tree-reconstruction algorithm, which we describe next. This recursive algorithm (given in pseudo-code in Algorithm 2), assumes the existence of a randomized method, `find-splitting-edge`, which returns a splitting-edge in T , with probability $\Omega(1/d)$, and otherwise returns `Null`. Our reconstruction algorithm is therefore a randomized recursive algorithm that takes as input a set of vertices, V , with a (known) root vertex $r \in V$, and

returns the edge set, E , for V . At a high level, our algorithm is to repeatedly call the method, `find-splitting-edge`, until it returns a splitting-edge, at which point we divide the set of vertices using this edge and recurse on the two resulting subtrees.

■ **Algorithm 2** Reconstruct a rooted tree with path queries.

```

1 Function reconstruct-rooted-tree( $V, r$ ):
2    $E \leftarrow \emptyset$ 
3   if  $|V| \leq g$  then //  $g$  is a chosen constant
4     return edges found by a quadratic brute-force algorithm
5   while true do
6     Pick a vertex  $v \in V$  uniformly at random
7     for  $z \in V$  do in parallel
8       Perform query  $path(z, v)$ 
9     Let  $Y$  be the vertex set of the path from  $r$  to  $v$ 
10    splitting-edge  $\leftarrow$  find-splitting-edge( $v, Y, V$ )
11    if splitting-edge  $\neq Null$  then
12       $(u, w) \leftarrow$  splitting-edge
13       $E \leftarrow E \cup \{(u, w)\}$ 
14      for  $z \in V$  do in parallel
15        Perform query  $path(w, z)$ 
16        split  $V$  into  $V_1, V_2$  at  $(u, w)$  using query results
17        parallel do
18           $E \leftarrow E \cup$  reconstruct-rooted-tree( $V_1, w$ )
19           $E \leftarrow E \cup$  reconstruct-rooted-tree( $V_2, r$ )
20    return  $E$ 

```

In more detail, during each iteration of a repeating **while** loop, we choose a vertex $v \in V$ uniformly at random. Then, we find the vertices on the path from r to v and store them in a set, Y , using the fact that a vertex, z , is on the path from r to v if and only if $path(z, v) = 1$. Then, we attempt to find a splitting-edge using the function `find-splitting-edge` (shown in pseudo-code in Algorithm 3). If `find-splitting-edge` is unsuccessful, we give up on vertex v , and restart the **while** loop with a new choice for v . Otherwise, `find-splitting-edge` succeeded and we cut the tree at the returned splitting-edge, (u, w) . All vertices, $z \in V$, where $path(w, z) = 1$ belong to the subtree rooted at w , thus belonging to V_1 , whereas the remaining vertices belong to V_2 and the partition containing both u and rooted at r . Thus, after cutting the tree we recursively `reconstruct-rooted-tree` on V_1 and V_2 .

The main idea for our efficient tree reconstruction algorithm lies in our `find-splitting-edge` method (see Algorithm 3), which we describe next. This method takes as input the vertex v , the vertex set Y , (comprising the vertices on the path from r to v), and the vertex set V . As we show, with probability depending on d , the output of this method is a splitting-edge; otherwise, the output is *Null*. Our algorithm performs a type of “noisy” search in Y to either locate a likely splitting-edge or return *Null* as an indication of failure.

Our `find-splitting-edge` algorithm consists of two phases. We enter **Phase 1** if the size of path Y is too big, i.e., $|Y| > |V|/K = \frac{|Y|}{C_2 \log |V|}$, where C_2 is a predetermined constant and $K = C_2 \log |V|$. The purpose of this phase is either to pass a shorter path including an even-edge-separator to the second phase or to find a splitting-edge in this iteration. The search on the set Y is noisy, because it involves random sampling. In particular, we take a random sample S of size $m = C_1 \sqrt{|V|}$ from path Y (where C_1 is a predetermined

■ **Algorithm 3** Finding a splitting-edge from vertex set, Y , on the path from vertex v to the root r .

```

1 Function find-splitting-edge( $v, Y, V$ ):
2   splitting-edge  $\leftarrow$  Null
3    $m = C_1 \sqrt{|V|}$ ,  $K = C_2 \log |V|$ 
4   Phase 1:
5     if  $|Y| > |V|/K$  then
6        $S \leftarrow$  subset of  $m$  random elements from  $Y$ 
7        $S \leftarrow S \cup \{v, r\}$ 
8       for each  $s \in S$  do in parallel
9          $X_s \leftarrow$  subset of  $K$  random elements from  $V$ 
10        Perform queries to find  $count(s, X_s)$ 
11        if  $\forall s \in S : count(s, X_s) < \frac{K}{d+1}$  then return Null
12        if  $\forall s \in S : count(s, X_s) > \frac{Kd}{d+1}$  then return Null
13        if  $\exists s \in S : \frac{K}{d+1} \leq count(s, X_s) \leq \frac{Kd}{d+1}$  then
14          return verify-splitting-edge( $s, V$ )
15        for each  $\{a, b\} \in S$  do in parallel
16          perform query  $path(a, b)$ 
17        Find  $w, z$  such that they are two consecutive nodes in the sorted order of
18         $S$  such that  $count(w, X_w) > \frac{Kd}{d+1}$  and  $count(z, X_z) < \frac{K}{d+1}$ 
19         $Y \leftarrow$  nodes from  $Y$  in the path from  $w$  to  $z$ 
20   Phase 2:
21     if  $|Y| > |V|/K$  then return Null
22     for each  $s \in Y$  do in parallel
23        $X_s \leftarrow$  subset of  $K$  random elements from  $V$ 
24       Perform queries to find  $count(s, X_s)$ 
25       if  $\exists s \in Y$  s.t.  $\frac{K}{d+1} \leq count(s, X_s) \leq \frac{Kd}{d+1}$  then
26         return verify-splitting-edge( $s, V$ )
27   return Null

```

constant). We include r and v , the two endpoints of the path Y , to S . Then, we estimate the number of descendants of s , $D(s)$, for each $s \in S$. To estimate this number for each $s \in S$, we take a random sample X_s of K elements from V and we perform queries to find $count(s, X_s)$. Here, we use $m \cdot K \in O(\sqrt{|V|} \log |V|)$ queries in a single round. Then, if all the estimates were less than $K/(d+1)$, we return *Null* as an indication of failure (we guess that all the nodes on the path Y have too few descendants to be a separator). Similarly, if all the estimates were greater than $\frac{Kd}{d+1}$, we return *Null* (we guess that all the nodes on the path Y have too many descendants to be a separator). If there exists a node s such that $\frac{K}{d+1} \leq count(s, X_s) \leq \frac{Kd}{d+1}$, we check if s is a splitting-edge by counting its descendants using a function, *verify-splitting-edge*. This function takes vertex s and the full vertex set V to return edge (*find-parent*(s, V), s) if $\frac{|V|}{d+2} \leq count(s, V) \leq |V| \cdot \frac{d+1}{d+2}$ and return *Null* otherwise.

If neither of these three cases happens, we perform queries to sort elements of S using a trivial quadratic work parallel sort which takes $O(m^2) \in O(|V|)$ queries in a single round. We know that two consecutive nodes w and z exist on the sorted order of S , where $count(w, X_w) > \frac{Kd}{d+1}$ and $count(z, X_z) < \frac{K}{d+1}$. We find all the nodes on Y starting at w and ending at z , and use this as our new path Y .

Function $\text{find-parent}(s, V)$.

```

1 find  $Y$ , ancestor set of  $s$  from  $V$  using  $|V|$  queries in parallel
2  $m = C_1 \sqrt{|V|}$ 
3 for  $i \leftarrow 1$  to  $2$  &  $|Y| > m$  do
4    $S \leftarrow$  random subset of  $Y$  with  $m$  elements
5   sort  $S$  as  $x_1 < \dots < x_m$  using  $O(m^2)$  queries in parallel
6   find  $Y' = \{u \in Y \mid u \leq x_1\}$  using  $O(|Y|)$  queries in parallel, replace  $Y$  with  $Y'$ 
7 if  $|Y| \leq m$  then
8   sort  $Y$  using  $O(m^2)$  queries in parallel
9   return (minimum of this path)
10 return Null

```

In **Phase 2**, we expect a path of size under $|Y|/K$, we will later prove this is true with high probability. Otherwise, we just return *Null*. In this phase, we estimate the number of descendants much like we did in the previous phase, except the only difference is that we estimate the number of descendants for all the nodes on our new path Y . If there exists a node $s \in Y$ such that $\frac{K}{d+1} \leq \text{count}(s, X_s) \leq \frac{Kd}{d+1}$, we verify if it is a splitting-edge, as described earlier.

Finally, let us describe how we find the parent of a node s in V . We first find, Y , the set of ancestors of v in V in parallel using $|V|$ queries. Let $x \succ y$ describe the total order of nodes in path Y , where for any $x, y \in Y$: $x \succ y$ if and only if $\text{path}(x, y) = 1$. The parent of s is the lowest vertex on the path. Then, the key idea is that if $|Y| \in O(\sqrt{|V|})$, we can sort them using $O(|V|)$ queries. If the path is greater than this amount, we instead use S , a sample of size $O(\sqrt{|V|})$ from the path. Next, we sort the sample to obtain $x_1 < \dots < x_m$ for S and then find all of the nodes in Y which are less than the smallest sample x_1 . Finally, we replace Y with these descendants of x_1 and repeat the whole procedure again. We later prove that with high probability after two iterations of this sampling, the size of the path is $O(\sqrt{|V|})$, allowing us to sort all nodes in Y to return the minimum (see Function find-parent).

4.2 Analysis

The correctness of the algorithm follows from the fact that our method first finds the root, r , of T and then finds the parent of each other node, v in T .

► **Theorem 13.** *Given a set, V , of nodes of a rooted tree, T , such as a biological or digital phylogenetic tree, with degree bounded by a fixed constant, d , we can construct T using path queries with round complexity, $R(n)$, that is $O(\log n)$ and query complexity, $Q(n)$, that is $O(n \log n)$, with high probability.*

Our proof of Theorem 13 begins with Lemma 14.

► **Lemma 14.** *In a rooted tree, $T = (V, E, r)$, let Y be a (directed) path, where $|Y| > m = C_1 \sqrt{|V|}$. If we take a sample, S , of m elements from Y , then with probability $1 - \frac{1}{|V|}$, every two consecutive nodes of S in the sorted order of S are within distance $O\left(\frac{|Y| \log |V|}{\sqrt{|V|}}\right)$ from each other in Y .*

Proof. Note that some nodes of Y may be picked more than once as we pick S in parallel. Divide the path Y into $\frac{\sqrt{|V|}}{\log |V|}$ equal size sections (the difference between the size of any two sections is at most 1). For each $1 \leq i \leq \frac{\sqrt{|V|}}{\log |V|}$, let A_i be the subset of S lying in the i^{th}

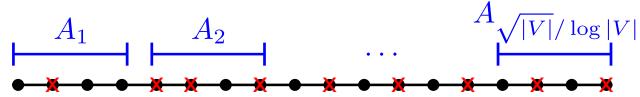


Figure 5 Illustration of how scattered sample S is on path Y . The i^{th} blue interval represents the i^{th} section of Y , the black dots correspond to the nodes on the path Y , and red crossed marks represent elements of S .

section of Y . (See Figure 5.) It is clear that each node $s \in S$ ends up in section i with probability $\frac{\log|V|}{\sqrt{|V|}}$, and therefore, for each $1 \leq i \leq \frac{\sqrt{|V|}}{\log|V|}$, $E[|A_i|] = C_1 \log|V|$. Thus, using standard a Chernoff bound, $\Pr[|A_i| = 0] < \frac{1}{|V|^2}$ for any constant $C_1 > 6 \ln 10$. Using a union bound, all the sections are non-empty with probability at least $1 - \frac{1}{|V|}$. Hence, the distance between any two consecutive nodes of S from each other in Y is at most $\frac{2|Y|\log|V|}{\sqrt{|V|}}$. \blacktriangleleft

Lemma 14 allows us to analyze the find-parent method, as follows.

► **Lemma 15.** *The `find-parent`(s, V) method outputs the parent of s with probability at least $1 - 2/|V|$, with $Q(n) \in O(n)$ and $R(n) \in O(1)$.*

Proof. The find-parent method succeeds if, after the `for` loop, the size of the set of remaining ancestors of s , Y , is $|Y| \leq m$, so it is enough to show that this occurs with probability at least $1 - 2/|V|$. By Lemma 14, the size of Y at the end of the first iteration is $|Y| \in O(m \log|V|)$, with probability at least $1 - 1/|V|$. Similarly, a second iteration, if required, further reduces the size of Y into $|Y| \in o(m)$, with probability at least $1 - 1/|V|$. Thus, by a union bound, the probability of success is at least $1 - 2/|V|$.

The query complexity can be broken down as follows, where $m \in O(\sqrt{|V|})$:

1. $O(|V|)$ queries in 1 round to determine the ancestor set, Y , of s .
2. $O(m^2) + O(|Y|) \in O(|V|)$ queries in 2 rounds for each of the (at most) 2 iterations performed in `find-parent`, whose purpose is to discard non-parent ancestors of s in Y .
3. $O(m^2) \in O(|V|)$ to find, in 1 round, the minimum among the remaining ancestors of Y (at most m w.h.p.). If $|Y| > m$, then no further queries are issued.

In total, the above amounts to $Q(n) \in O(n)$ and $R(n) \in O(1)$. \blacktriangleleft

We next analyze the `find-splitting-edge` method.

► **Lemma 16.** *Any call to `find-splitting-edge` returns true with probability $\frac{1}{2d}$; hence Algorithm 2 calls `find-splitting-edge` $O(d)$ times in expectation.*

Proof. By Lemma 11, we know that if we pick a vertex v , uniformly at random, then with probability $\frac{1}{d}$, an even-edge-separator lies on the path from r to v . We show that if there is such an even-edge-separator (Definition 4) on that path, `find-splitting-edge`(v, Y, V) returns a splitting-edge (Definition 12) with probability at least $\frac{1}{2}$, and otherwise returns *Null*. Using an intricate Chernoff-bound analysis (see full version for details [2]), we can prove that there exists a constant $C_2 > 0$, as used in line 3 of Algorithm 3 such that the following probability bounds always hold:

$$\begin{cases} \Pr\left(\text{count}(s, X_s) \geq \frac{K}{d+1}\right) \geq 1 - \frac{1}{|V|^2} & \text{if } \text{count}(s, V) \geq \frac{|V|}{d}, \\ \Pr\left(\text{count}(s, X_s) \leq K \frac{d}{d+1}\right) \geq 1 - \frac{1}{|V|^2} & \text{if } \text{count}(s, V) \leq |V| \frac{d-1}{d}, \end{cases} \quad (2)$$

$$\begin{cases} \Pr \left(\text{count}(s, X_s) < \frac{K}{d+1} \right) \geq 1 - \frac{1}{|V|^2} & \text{if } \text{count}(s, V) < \frac{|V|}{d+2}, \\ \Pr \left(\text{count}(s, X_s) > K \frac{d}{d+1} \right) \geq 1 - \frac{1}{|V|^2} & \text{if } \text{count}(s, V) > |V| \frac{d+1}{d+2} \end{cases} \quad (3)$$

It is clear that we either return a splitting-edge or *Null* when passing through verify-splitting-edge. We break the probability of returning *Null* according to the phases. We call a vertex v **ineligible** if $\text{count}(v, V) < \frac{|V|}{d+2}$ or $\text{count}(v, V) > \frac{|V|(d+1)}{d+2}$ ($(\text{parent}(v), v)$ is not a splitting-edge). On the other hand, we call vertex v **candidate** if after estimating the number of its descendants: $\frac{K}{d+1} \leq \text{count}(v, X) \leq \frac{Kd}{d+1}$. Let (a, b) be an even-edge-separator on path Y .

Phase 1:

- lines 10,11: By Definition 4, $\frac{|V|}{d} \leq \text{count}(b, V) \leq \frac{|V|(d-1)}{d}$. We add $\{r, v\}$ to S in line 6 of the algorithm (the two endpoints of path Y). Notice that $\frac{|V|}{d} \leq \text{count}(b, V) \leq \text{count}(r, V)$ and that $\text{count}(v, V) \leq \text{count}(b, V) \leq \frac{|V|(d-1)}{d}$. So, by Equation (2), with probability at least $1 - \frac{2}{|V|^2}$, $\text{count}(r, X_r) \geq \frac{K}{d+1}$ and $\text{count}(v, X_v) \leq \frac{Kd}{d+1}$, and consequently, we don't return *Null* in lines 10,11 of the algorithm.
- line 12: Equation (3) shows that an ineligible node is not a candidate with probability $1 - \frac{1}{|V|^2}$. Thus, by a union bound, none of our candidates is ineligible in line 12 with probability at least $1 - \frac{|S|}{|V|^2}$. Moreover, if there exists a candidate s in S , the algorithm outputs a splitting-edge $(\text{parent}(s), s)$ with probability at least $1 - \frac{2}{|V|}$, by Lemma 15.
- lines 15,16: Let us partition S into S_l and S_r (see Figure 6), as follows:

$$S_l = \{s \in S \mid \text{count}(s, V) > \text{count}(b, V)\}, \quad S_r = \{s \in S \mid \text{count}(s, V) < \text{count}(b, V)\}$$

Then, by definition of b :

$$\forall s \in S_l : \text{count}(s, V) > |V|/d, \quad \forall s \in S_r : \text{count}(s, V) < |V|(d-1)/d.$$

and thus, by Equation (2) and a union bound, we have with probability at least $1 - \frac{|S|}{|V|^2}$:

$$\forall s \in S_l : \text{count}(s, X_s) \geq K/(d+1), \quad \forall s \in S_r : \text{count}(s, X_s) \leq Kd/(d+1).$$

Finally, since S does not contain any candidate nodes (otherwise we would have picked them in line 12), the above inequalities imply that:

$$\forall s \in S_l : \text{count}(s, X_s) > Kd/(d+1), \quad \forall s \in S_r : \text{count}(s, X_s) < K/(d+1).$$

Therefore, $w \in S_l$ and $z \in S_r$, which implies that the subpath from w to z in Y must include vertex b . This means that with probability $1 - O(\frac{1}{|V|})$, we either find a splitting-edge in this phase or pass b to the next phase.

Now, consider Phase 2:

- line 17: Here, if $|Y| > |V|/K$, then we have passed through Phase 1. Using Lemma 14, we know that since S was a sample of size $C_1 \sqrt{|V|}$ from Y , with probability $1 - \frac{1}{|V|}$ the distance between any two consecutive nodes of S in Y was $O(|Y| \frac{\log |V|}{\sqrt{|V|}}) \in O(\sqrt{|V|} \log |V|)$. Thus, the size of path Y after passing through line 15 is at most $O(\sqrt{|V|} \log |V|)$. Thus, the probability of returning *Null* in line 17 is at most $\frac{2}{|V|}$.

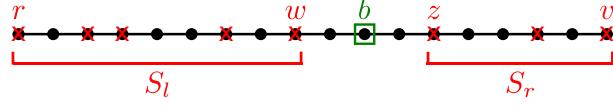


Figure 6 Illustration of the path reduction in Phase 1 of `find-splitting-edge`. At the end of this phase, the path Y is trimmed down into the subpath consisting of the nodes between w and z , which contains b w.h.p.

- line 21: By Equation (3), with probability at least $1 - \frac{|Y|}{|V|^2}$, no ineligible node is between candidate set. Besides, for a candidate node s , the algorithm outputs a splitting-edge $(parent(s), s)$ with probability at least $1 - \frac{2}{|V|}$, by Lemma 15.
- line 22: The probability that we return `Null` here is equal to the probability that our candidate set in line 21 is empty. By Equation (2), with probability at least $1 - \frac{2}{|V|^2}$, b is between candidates at line 21 and candidate set is non-empty. Thus, the total probability of failing to return a splitting-edge in this phase is at most $O(\frac{1}{|V|})$.

Therefore, for $|V|$ greater than the chosen constant g , the probability of returning `Null` in the existence of an even-edge-separator is at most $O(\frac{1}{|V|}) \leq 1/2$. Thus, the probability of returning a splitting-edge in any call to `find-splitting-edge` is at least $\frac{1}{2d}$. \blacktriangleleft

► **Lemma 17.** *The subroutine `find-splitting-edge`(v, Y, V) has query complexity, $Q(n)$, that is $O(|V|)$, and round complexity, $R(n)$, that is $O(1)$.*

Proof. The queries done by `find-splitting-edge`(v, Y, V), in the worst case, can be broken down as follows, where $m = O(\sqrt{|V|})$:

Phase 1: A total of $O(|V|)$ queries in $O(1)$ rounds, consisting of:

- $O(mK) \in O(\sqrt{|V|} \log |V|)$ queries in one round for estimating the number of descendants for the m samples.
- $O(m^2) \in O(|V|)$ queries in one round for sorting the m samples.
- $O(|Y|) \in O(|V|)$ queries in a round to find the subpath of Y that is the input for Phase 2.
- $O(|V|)$ queries in $O(1)$ rounds for determining the parent of s (see Lemma 15).

Phase 2: If we enter this phase, it spends $O(|V|)$ queries in $O(1)$ rounds:

- $|Y| \cdot K \in O(|V|)$ queries in one round to evaluate `count`(s, X_s) for each $s \in Y$.
- $O(|V|)$ queries in one round to find the number of descendants of node s .
- $O(|V|)$ queries in $O(1)$ rounds to determine the parent of s (see Lemma 15).

Overall, the above break down amounts to $Q(n) \in O(n)$ and $R(n) \in O(1)$. \blacktriangleleft

Now, recall Theorem 13: *Given a set, V , of nodes of a rooted tree, T , such as a biological or digital phylogenetic tree, with degree bounded by a fixed constant, d , we can construct T using path queries with round complexity, $R(n)$, that is $O(\log n)$ and query complexity, $Q(n)$, that is $O(n \log n)$, with high probability.*

Proof. The expected query complexity $Q(n)$ of Algorithm 2 is dominated by the two recursive calls $\left(Q\left(\frac{n}{d+2}\right)$ and $Q\left(\frac{n(d+1)}{d+2}\right)\right)$ and the calls to `find-splitting-edge`. By Lemma 16, we call `find-splitting-edge` an expected $O(d)$ times, incurring a cost of $O(dn) \in O(n)$ path queries in $O(d) \in O(1)$ rounds (see Lemma 17). Thus, $Q(n)$ and $R(n)$ are:

$$Q(n) = Q\left(\frac{n}{d+2}\right) + Q\left(\frac{n(d+1)}{d+2}\right) + O(n),$$

$$R(n) = \max \left(R \left(\frac{n}{d+2} \right), R \left(\frac{n(d+1)}{d+2} \right) \right) + O(1)$$

which shows it needs $Q(n) \in O(n \log n)$ and $R(n) \in O(\log n)$ in expectation. To prove the high probability results, note that the main algorithm is a divide-and-conquer algorithm with two recursive calls per call; hence, it can be modeled with a recursion tree that is a binary tree, B , with height $h = O(\log \frac{d+2}{d+1} n) = O(\log n)$. For any root-to-leaf path in B , the time taken can be modeled as a sum of independent random variables, $X = X_1 + X_2 + \dots + X_h$, where each X_i is the number of calls to `find-splitting-edge` (each of which uses $O(|V|)$ queries in $O(1)$ rounds) required before it returns true, which is a geometric random variable with parameter $p = \frac{1}{2d}$. Thus, by a Chernoff bound for sums of independent geometric random variables (e.g., see [23, 33]), the probability that X is more than $O(d \log \frac{d+2}{d+1} n)$ is at most $1/n^{c+1}$, for any given constant $c \geq 1$. The theorem follows, then, by a union bound for the n root-to-leaf paths in B . \blacktriangleleft

4.3 Lower Bound

We establish the following simple lower bound, which extends and corrects lower-bound proofs of Wang and Honorio [46].

► **Theorem 18.** *Reconstructing an n -node, degree- d tree requires $\Omega(dn + n \log n)$ path queries. This lower bound holds for the worst case of a deterministic algorithm and for the expected value of a randomized algorithm.*

Proof. Consider an n -node, degree- d tree, T , as shown in Figure 7, which consists of a root, r , with d children, each of which is the root of a chain, T_i , of at least one node rooted at a child of r . Since a querier, Bob, can determine the root, r , in $O(n)$ queries anyway, let us assume for the sake of a lower bound that r is known; hence, no additional information is gained by path queries involving the root. Let us denote the vertices in chain T_i as V_i . In order to reconstruct T , Bob must determine the nodes in each V_i and must also determine their order in T_i . For a given path query, $\text{path}(u, v)$, say this query is **internal** if $u, v \in V_i$, for some $i \in [1, d]$, and this query is **external** otherwise. Note that even if Bob knows the full structure of T except for a given node, v , he must perform at least $d - 1$ external queries in the worst case, for a deterministic algorithm, or $\Omega(d)$ external queries in expectation, for a randomized algorithm, in order to determine the chain, T_i , to which v belongs. Furthermore, the result of an (internal or external) query, $\text{path}(u, v)$, provides no additional information for a vertex w distinct from u and v regarding the set, V_i , to which w belongs. Thus, Bob must perform $\Omega(d)$ external queries for each vertex $v \neq r$, i.e., he must perform $\Omega(dn)$ external queries in total. Moreover, note that the results of external queries involving a vertex, v ,

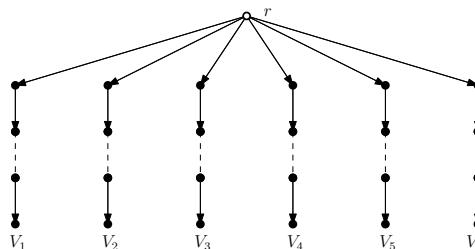


Figure 7 Illustration of the $\Omega(dn + n \log n)$ lower bound for path queries in directed rooted trees (shown for $d = 6$).

provide no information regarding the location of v in its chain, T_i . Even if Bob knows all the vertices that comprise each V_i , he must determine the ordering of these vertices in the chain, T_i , in order to reconstruct T . That is, Bob must *sort* the vertices in V_i using a comparison-based algorithm, where each comparison is an internal query involving two vertices, $u, v \in V_i$. By well-known sorting lower bounds (which also hold in expectation for randomized algorithms), e.g., see [23, 12], determining the order of the vertices in each T_i requires $\Omega(|V_i| \log |V_i|)$, as one of the chain can be as great as $n - d$ vertices, then he needs $\Omega(n \log n)$ internal queries. \blacktriangleleft

► **Corollary 19.** *Algorithm 2 is optimal for bounded-degree trees when asking $\theta(n)$ queries per round.*

The query complexity of Algorithm 2 matches the lower bound provided by Theorem 18 when d is constant. Besides, we need $\Omega(d + \log n)$ rounds if we have $\theta(n)$ processors; hence, the round complexity of Algorithm 2 is also optimal.

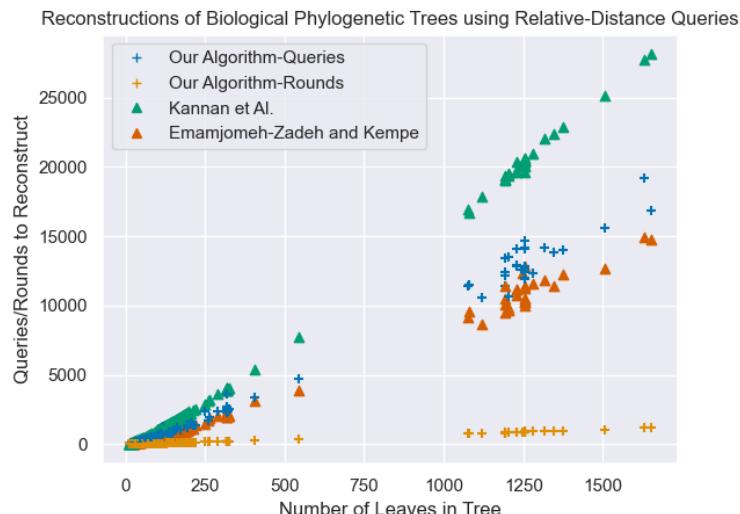
5 Experiments

Given that both of our algorithms are randomized and perform optimally with high probability, we carried out experiments to analyze the practicality of our algorithms and compare their performance with the best known algorithms for reconstructing rooted trees.⁴

5.1 Reconstructing Biological Phylogenetic Trees

In order to assess the practical performance of Algorithm 1, we performed experiments using synthetic phylogenetic trees and real-world biological phylogenetic trees from the phylogenetic library TreeBase [36], which is a database of biological phylogenetic trees, comprising over 100,000 distinct taxa in total.

⁴ The complete source code for our experiments, including the implementation of our algorithms and the algorithms we compared against, is available at github.com/UC-Irvine-Theory/ParallelTreeReconstruction.



■ **Figure 8** A scatter plot showing the number of queries and rounds for each of the three tree reconstruction algorithms for real trees from TreeBase. Since our algorithm is parallel, we include round complexity to serve as a comparison for the sequential complexity.

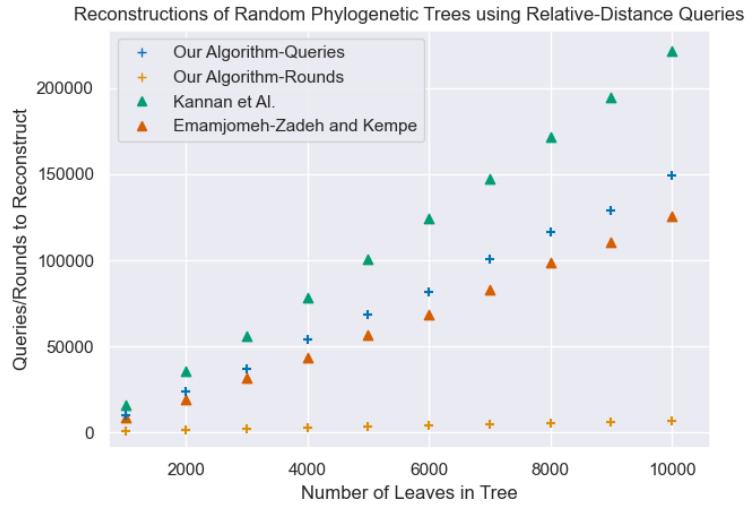


Figure 9 A plot showing the average number of queries and rounds for each of the three tree reconstruction algorithms. Each data point represents the average for 10 randomly generated trees.

We implemented an oracle interface, instantiated it with the relevant trees, and implemented our algorithm along with two other phylogenetic tree reconstruction algorithms that use relative-distance queries. The first is by Emamjomeh-Zadeh and Kempe [18], which is a randomized sequential divide-and-conquer algorithm. The second is by Kannan et al. [29], where they use a sequential deterministic procedure reminiscent of insertion-sort. All three algorithms achieve the optimal asymptotic query complexity of $\Theta(n \log n)$ in expectation.

Real Data. We instantiated our oracles with 1,220 biological phylogenetic trees from the TreeBase collection and used them to run all three algorithms. The results, shown in Figure 8, suggest that our algorithm outperforms the algorithm by Kannan et al., both in terms of its round complexity and query complexity. However our algorithm almost matches Emamjomeh-Zadeh and Kempe's in terms of total queries and we believe the small difference is a direct result of the cost incurred while parallelizing the link step of Algorithm 1. It remains clear that Algorithm 1 outperforms the two other algorithms when considering the parallel speed-up.

Synthetic Data. We also tested this algorithm using synthetic data and found similar results, detailed in Figure 9. We detail the method used to generate these random tree instances in Section 5.2, however, given our algorithm's strict focus on biological phylogenetic trees, we use only full binary trees, where each internal node has exactly two children.

5.2 Reconstructing Phylogenetic Trees from Path Queries

To assess the practical performance of our method for reconstructing (biological and digital) phylogenetic trees from path queries, we performed experiments using both synthetic and real data to compare our algorithm with the algorithm by Wang and Honorio [46], which is the best known reconstruction algorithm for phylogenetic trees from path queries. Our experimental results provide evidence that Algorithm 2 provides significant parallel speedup, while simultaneously improving the total number of queries.

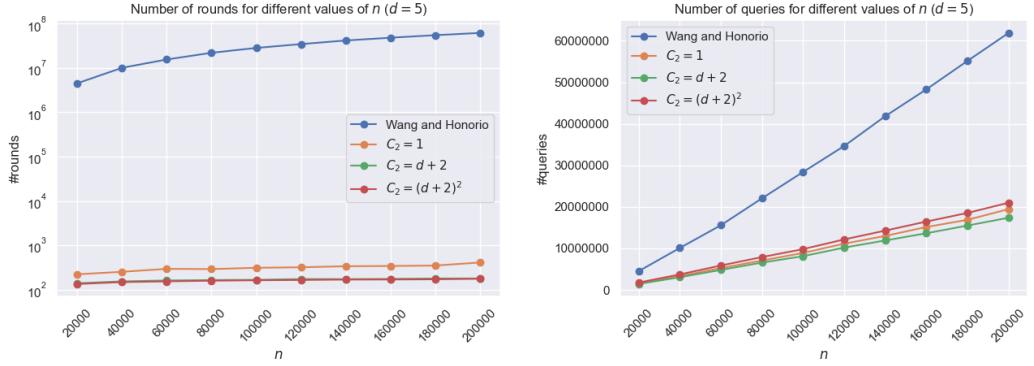


Figure 10 Comparing Our Algorithm’s number of rounds (left) and total queries (right) with Wang and Honorio’s [46], for fixed $d = 5$ and varying n .

Synthetic Data. In order to generate random instances of trees with maximum degree, d , we synthesized a data set of random degree- d trees of n nodes for different values of n and d . To generate a random tree, T , for a given n and d , we first generated a random Prüfer sequence [37] of a labeled tree, which defines a unique sequence associated with that tree, and converted it to its associated tree. In particular, each n -node tree $T = (V, E)$ has a unique code sequence s_1, s_2, \dots, s_{n-2} , where $s_i \in V$ for all $1 \leq i \leq n-2$ and every node $v_i \in V$ of degree d_i appears exactly $d_i - 1$ times in this sequence. Therefore, in order to generate random degree- d rooted trees we generate a random Prüfer sequence while imposing conditions that: (i) all vertices appear at most $d - 1$ times in the code and (ii) there is at least one node such that it appears exactly $d - 1$ times. Converting each such sequence to its associated tree gave us a random degree- d tree instance that we used in our experiments.

Since our parallel reconstruction algorithm using path queries is parameterized by a constant, C_2 , we ran our algorithm using different values for C_2 . The constant C_2 controls sample size from V used to estimate the number of descendants of a node. Furthermore, to reduce noise from randomization, each data-point will be averaged for 3 runs on 10 randomly generated trees. In Figure 10, we compare our algorithm’s rounds and total number of queries with the one by Wang and Honorio [46], for fixed degree trees $d = 5$ and varying tree-sizes. These results provide empirical evidence that our algorithm provides a noticeable speedup in parallel round complexity while also outperforming the algorithm by Wang and Honorio [46] in total number of queries.

In Figure 11, we compare Algorithm 2 with the one by Wang and Honorio [46] for fixed size and varying values of d . Again, this supports our theoretical findings that our algorithm achieves both a significant parallel speedup and a simultaneous improvement in the number of total queries.

In Figure 12, we study the behavior of Algorithm 2 under different values of C_2 , so as to experimentally find the best value for C_2 . While our high probability analysis requires $C_2 \approx (d + 2)^4$, Figure 12 suggests that we do not need that high probability reassurance in practice, and we can use smaller sample to reduce the total number of queries.

Real Data. Our experiments on real-world biological phylogenetic trees also confirm the superiority of our algorithm in terms of performance as compared to the one by Wang and Honorio [46]. Similar to our experiments using relative-distance queries, we used a dataset comprised of trees from the phylogenetic library TreeBase [36]. Figure 13 summarizes our experimental results, where each data point corresponds to an average performance of 3 runs

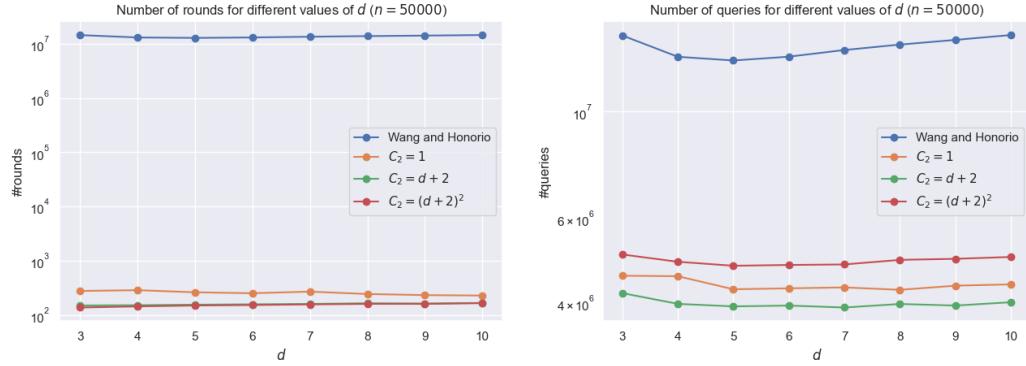


Figure 11 Comparing our algorithm's number of rounds (left) and total queries (right) with Wang and Honorio's [46], for $n = 50000$ and varying values for d .

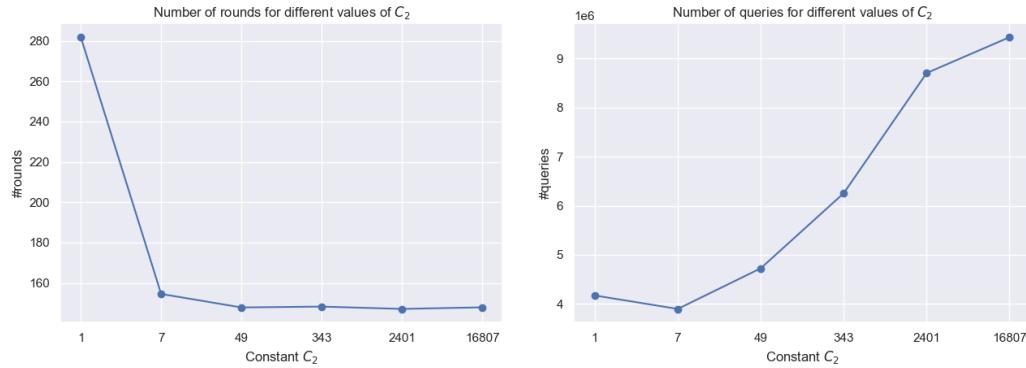


Figure 12 Change in the total number of rounds (left) and total number of queries (right) when running our algorithm for varying values of C_2 ($n = 50000$, $d = 5$).

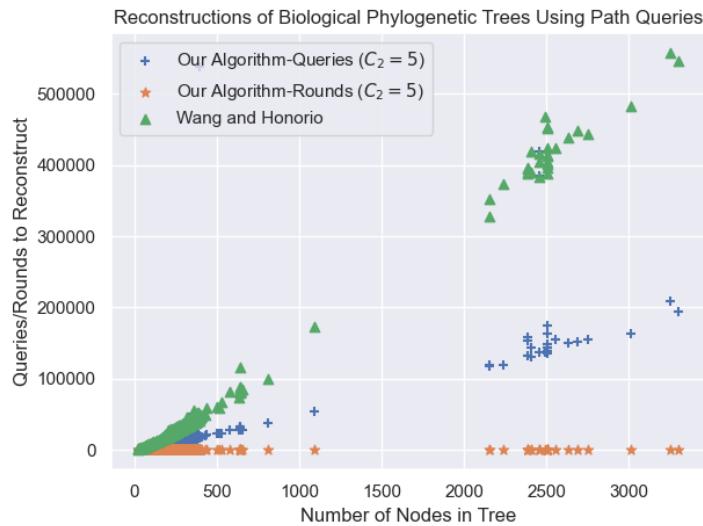


Figure 13 A scatter plot comparing the number of queries and rounds of our algorithm and with the one by Wang and Honorio [46] for real-world trees from TreeBase [36]. Since our algorithm is parallel, we include round complexity to serve as a comparison for the sequential complexity.

on the same tree. Our algorithm is superior in both queries and rounds for all the values of C_2 we tried: $C_2 \in \{1, d + 2, (d + 2)^2\}$. The best performance corresponds to $C_2 = d + 2 = 5$, which is the one illustrated in Figure 13.

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