Species Trees are Recoverable from Unrooted Gene Tree Topologies Under a Constant Rate of Horizontal Gene Transfer∗

Constantinos Daskalakis† Sebastien Roch‡

March 3, 2022

Abstract

Reconstructing the tree of life from molecular sequences is a fundamental problem in computational biology. Modern data sets often contain a large number of genes, which can complicate the reconstruction problem due to the fact that different genes may undergo different evolutionary histories. This is the case in particular in the presence of horizontal genetic transfer (HGT), where a gene is inherited from a distant species rather than an immediate ancestor. Such an event produces a gene tree which is distinct from, but related to, the species phylogeny.

In previous work, a natural stochastic models of HGT was introduced and studied. It was shown, both in simulation and theoretical studies, that a species phylogeny can be reconstructed from gene trees despite surprisingly high rates of HGT under this model. Rigorous lower and upper bounds on this achievable rate were also obtained, but a large gap remained. Here we close this gap, up to a constant. Specifically we show that a species phylogeny can be reconstructed correctly from gene trees even when, on each gene, each edge of the species tree has a constant probability of being the location of an HGT event. Our new reconstruction algorithm, which relies only on unrooted gene tree topologies, builds the tree recursively from the leaves and runs in polynomial time.

We also provide a matching bound in the negative direction (up to a constant) and extend our results to some cases where gene trees are not perfectly known.

∗Keywords: Phylogenetic Reconstruction, Horizontal Gene Transfer, Gene Tree/Species Tree, Distance Methods.
†Department of Electrical Engineering and Computer Science at MIT. Supported by a Microsoft Research faculty fellowship and NSF Award CCF-0953960 (CAREER) and CCF-110149. This work was done while CD was visiting the Simons Institute for Theoretical Computer Science.
‡Department of Mathematics at the University of Wisconsin–Madison. Supported by NSF grant DMS-1149312 (CAREER) and DMS-1614242. This work was done while SR was visiting the Simons Institute for Theoretical Computer Science.
1 Introduction

A major challenge in the reconstruction of the tree of life from modern molecular datasets is that different genes often tell conflicting stories about the evolutionary history of a group of organisms [Mad97, DBP05, Nak13]. Consider the example in Figure 1. On the left-hand side is depicted a species phylogeny, where branchings (i.e., internal nodes) represent past speciation events and leaves correspond to contemporary species [SS03]. Imagine that, at some point in the past history of these species, a gene was transferred by a virus from a donor species (the gray node labeled $D$) to a recipient species (the gray node labeled $R$), a biological process known as transduction [HJ98], and eventually replaced that gene in the recipient species. This event is referred to as a horizontal gene transfer (HGT). From a phylogenetic point of view, the result of this transfer is that, in the tree representing the history of this transferred gene, the middle branch is now more closely related to the right subtree of the root (where the donor species lies) than to the left subtree of the root—in direct conflict with the species history. This new tree, depicted on the right-hand side of Figure 1, is called a gene tree.

In datasets comprising multiple genes, each gene has its own history—embodied by its own gene tree. An abundance of reconstruction algorithms have been developed to infer such gene trees using DNA sequences extracted from a reference individual of each leaf species [Fel04]. In particular much is known about the rigorous, theoretical properties of these single-gene inference methods. See e.g., [SS02, Mos03, Mos04, MRS11, ESSW99a, DMR11a, DMR11b, Roc10, ESSW99b, CGG02, MR05, DR10, DR13, ADHR10, ADHR12] for a sample of results. In some parts of the tree of life, e.g., in bacteria, it is common for a significant fraction of gene trees to be in conflict with the species phylogeny. See [ZGC+06] for an example. Although individual gene histories are interesting in their own right, a fundamental goal is to reconstruct the species history (which is not directly measurable), i.e., the sequence of speciation events that have produced the current diversity of species. (We ignore past extinctions, which cannot be inferred purely from contemporary data.) Therefore, a key problem in modern phylogenetics is: how to infer a species phylogeny from a collection of (possibly discordant) gene trees?

The answer to this question depends on the mechanism(s) responsible for the discordances, which include HGT as well as gene tree estimation errors, incomplete lineage sorting, gene duplications and losses, etc. [Mad97]. In the current work, we focus solely on HGT. One possible reconstruction approach is to identify genes or loci which are believed to have undergone little or no HGT, such as 16S ribosomal RNA sequences [FSH80]. However such sequences are typically short, leading to unreliable tree estimates [SS02, Mos03]. Moreover a single-gene approach ignores much of the available data. Here we con-

Figure 1: An HGT event. On the left, the species phylogeny is shown with the donor ($D$) and recipient ($R$) locations. On the right, the resulting (unweighted) gene tree is shown after the HGT event.
sider inference methods based on multiple genes that explicitly model the discordances produced by HGT. A stochastic model of HGT was introduced by Roch and Snir [RS12], inspired by work of Kim and Salisbury [KS01] and Galtier [Gal07]. In this model, for each gene independently, HGT events occur at random along the phylogeny according to a Poisson point process (see Section 2 for details). The goal is then to recover the species phylogeny from a collection of gene trees, each of which can be thought of as a “randomly scrambled” instance of the species phylogeny. A related model was studied in [LRvH07, SLHS13, SS13]. In particular, Steel et al. [SLHS13] shed light on some of the challenges arising in this context by showing that applying a majority rule to all triples of species may fail to recover the correct topology.

A natural question is: when is there too much HGT to recover the species phylogeny? It was proved in [RS12] that surprisingly high rates of HGT can in fact be tolerated, in agreement with simulation results of Galtier [Gal07]. Roughly, under assumptions that will be detailed in Section 2, a species phylogeny with $n$ leaves can be recovered from a logarithmic number of genes when the HGT rate is at most $O(1/\log n)$ per unit time. On the other hand, it was also shown in [RS12] that there are species phylogenies that cannot be distinguished with constant probability from the same number of genes when the HGT rate is of the order of $\Omega(\log \log n)$ per unit time.

Here we close the gap. That is, under the same assumptions, we show that in fact a constant rate of HGT can be tolerated, with a matching bound (up to constants) in the negative direction. The algorithmic result in [RS12] is based on the observation that, under the assumptions made there, for any gene the subtree spanned by any four leaves is unlikely to be the location of an HGT event when the rate is $O(1/\log n)$. By taking a majority vote across genes, the corresponding subtree of the species phylogeny can be obtained with high probability. Then, using standard techniques [SS03], the full species phylogeny can be derived from all four-leaf subtrees, also called quartet topologies or simply quartets. This argument fails when the rate of HGT is constant. Instead, we use a recursive approach which progressively builds the species phylogeny from the leaves up, using the information obtained from partially reconstructed subtrees to reach further into the past. This recursive approach is reminiscent of recent work in the single-gene context where tight results were obtained using this type of approach [Mos04, DMR06, Roc10]. The negative result, on the other hand, follows from a coupling argument.

The rest of the paper is organized as follows. The stochastic model of gene trees under HGT is described in Section 2, alongside a statement of the main results. The proof of the algorithmic result is first presented in a special case in Section 3. The full proof is then derived in Section 4. The impossibility result is detailed in Section 5.

## 2 Definitions and Results

In this section we introduce the stochastic model of horizontal gene transfer (HGT), which is based on models of Kim and Salisbury [KS01, GWK05] and of Galtier [Gal07, GD08]. In essence, we assume that HGT events occur at random along the species phylogeny. We follow roughly the presentation in [RS13]. See also [Suc05, JNST06, LRvH07] for related models. After introducing the model in Section 2.1, we proceed with the formal statement of our main results.

**Notation**  Recall that, for functions $f(n), g(n)$, $f = O(g)$ means that there is constant $C > 0$ such that $f(n) \leq Cg(n)$ for all $n$ large enough. Similarly, $f = \Omega(g)$ indicates $f(n) \geq C'g(n)$ for $C' > 0$. In addition $f = \Theta(g)$ is equivalent to $f = O(g)$ and $f = \Omega(g)$. By polynomial in $n$, we mean $O(n^{C''})$ for some constant $C'' > 0$. We use the notation $\mathbb{P}[E_0 | E_1]$ for the conditional probability of $E_0$ given $E_1$. 

2.1 Stochastic Model of HGT

A species phylogeny is a graphical representation of the speciation history of a collection of organisms. The leaves correspond to extant species. Each branching indicates a speciation event. To each edge is associated a positive value corresponding to the time elapsed along that edge.

**Definition 1 (Species phylogeny)** A species phylogeny $T_s = (V_s, E_s; r, \tau)$ is a directed tree rooted at $r$ with vertex set $V_s$, edge set $E_s$ and $n$ labelled leaves $L = [n] = \{1, \ldots, n\}$ such that 1) the degree of all internal vertices $V_s - L$ is exactly 3 except the root $r$ which has degree 2, and 2) the edges are assigned inter-speciation times $\tau : E_s \to (0, +\infty)$. We assume that $T_s$ is ultrametric, that is, from every node, the path lengths with respect to $\tau$ from that node to all its descendant leaves are equal. (This is equivalent to assuming that all leaves are contemporaneous.)

Phylogenies are naturally equipped with a notion of distance between leaves (or more generally vertices). Such metrics are useful in reconstructing phylogenies.

**Definition 2 (Species metric)** A species phylogeny $T_s = (V_s, E_s; r, \tau)$ induces a metric $\tau$ on the leaves defined as follows, for all $u, v \in L$:

$$\tau(u, v) = \sum_{e \in p(u, v)} \tau(e),$$

where $p(u, v)$ is the unique path between leaves $u, v$ in the phylogeny, viewed as a set of edges. We call $\tau$ the species metric.

To infer a species phylogeny, we first reconstruct gene trees, that is, trees of ancestor-descendant relationships for orthologous genes (or, more generally, loci). Phylogenomic studies have revealed extensive discordance between gene trees, in particular, as a result of HGT as we describe below (e.g., [BSL+05, DB07]).

**Definition 3 (Gene tree)** A gene tree $T_g = (V_g, E_g; \rho, \omega_g)$ for gene $g$ is a directed tree rooted at $\rho$ with vertex set $V_g$, edge set $E_g$ and the same leaf-set $L = \{1, \ldots, n\}$ as the species phylogeny such that 1) the degree of every internal vertex is either 2 or 3, and 2) the edges are assigned branch lengths $\omega_g : E_g \to (0, +\infty)$. Similarly to Definition 2, we let $\omega_g(u, v)$ be the sum of the branch lengths on the path between $u$ and $v$.

As we will discuss below, gene trees are derived from—or “evolve” on—the species phylogeny. In our model, their branch lengths represent expected numbers of substitutions. Their topology and branch lengths may differ from those of the species phylogeny as a result of HGT events. Our stochastic model of HGT requires a rooted species phylogeny as time plays a key role in constraining valid HGT events. Indeed such events necessarily involve contemporaneous locations in the species phylogeny. See, e.g., [JNST09]. In particular our results rely on the ultrametricity property of the species phylogeny.

We now formalize a stochastic model of HGT. First some notation. Let $T_s = (V_s, E_s; r, \tau)$ be a fixed species phylogeny. By a location in $T_s$, we mean any position along $T_s$ seen as a continuous object, that is, a point $x$ along an edge $e \in E_s$. We write $x \in e$ in that case. We denote the set of locations in $T_s$ by $\mathcal{X}_s$. We say that $x \in \mathcal{X}_s$ is an ancestor of $y \in \mathcal{X}_s$ if $x$ is on the path between $y$ and $r$ in $T_s$ (in which case $y$ is also a descendant of $x$). For any two locations $x, y$ in $\mathcal{X}_s$, we let $\text{MRCA}(x, y)$ be their most recent common ancestor (MRCA) in $T_s$ and we let $\tau(x, y)$ be the length of the path connecting $x$ and $y$ in $T_s$ under the metric naturally defined by the weights $\{\tau(e), e \in E_s\}$, interpolated linearly to locations along an edge. In words $\tau(x, y)$, which we refer to as the $\tau$-distance between $x$ and $y$, is the sum of times to $x$ and $y$ from $\text{MRCA}(x, y)$. We say that two locations $x, y$ are contemporaneous if their respective $\tau$-distance to the root $r$ is identical, that is,

$$\tau(x, r) = \tau(y, r).$$
We let
\[ C_x = \{ y \in X_s : \tau(r, x) = \tau(r, y) \} \]
be the set of locations contemporaneous to \( x \).

We associate to each edge \( e \in E_s \) in \( T_s \) a rate of horizontal gene transfer \( 0 < \lambda(e) < +\infty \). We let \( \Lambda(e) = \lambda(e) \tau(e), e \in E_s \). We note that, since \( \lambda(e) \) is the HGT rate on \( e \), \( \Lambda(e) \) gives the expected number of HGT events along \( e \). Further, we let
\[ \Lambda_{\text{tot}} = \sum_{e \in E_s} \Lambda(e), \]
be the total HGT weight of the phylogeny.

Our model of HGT is as follows. From a topological point of view, an HGT event is equivalent to a subtree-prune-and-regraft (SPR) operation [SS03]. The recipient location, that is, the location receiving the gene transfer, is the point of pruning. The donor location is the point of regrafting. In other words, on the gene tree, a new internal node is created at the donor location with two children nodes, one being the original endpoint of the corresponding edge and the other being the node immediately under the recipient location in the species phylogeny. The original edge going to the latter node is removed. Refer to Figure 1 for an illustration.

Before describing the model formally, we need some further notation. As will become clear from the description of the HGT process below (see the example in Figure 1), each edge \( e \) of the gene tree \( T_g \) corresponds to a full or a partial edge of the species phylogeny \( T_s \). In particular, there exists a mapping (\( \eta, \zeta_b, \zeta_f : E_g \rightarrow E_s \times \mathbb{R}_+ \times \mathbb{R}_+ \)), mapping an edge \( e \in E_g \) to an edge \( \eta(e) \in E_s \) and a pair of times \( 0 \leq \zeta_b(e) \leq \zeta_f(e) \leq \tau(\eta(e)) \). The quantities \( \zeta_b(e) \) and \( \zeta_f(e) \) represent times of HGT events on edge \( \eta(e) \), as we will define below. Finally, for each gene \( g \) and each edge \( e \in E_s \) in the species tree, we associate a rate of substitution \( 0 < \mu_g(e) < +\infty \).

**Definition 4 (Stochastic model of HGT)** Let \( T_s = (V_s, E_s; r, \tau) \) be a fixed species phylogeny. A gene tree \( T_g \) is generated according to the following continuous-time stochastic process, which gradually modifies the species phylogeny starting at the root. There are two components to the process:

1. **HGT locations.** The recipient and donor locations of HGT events are selected as follows:
   - **Recipient locations.** Starting from the root, along each branch \( e \) of \( T_s \), locations are selected as recipient of a gene transfer according to a continuous-time Poisson process with rate \( \lambda(e) \). Equivalently, the total number of HGT events is Poisson with mean \( \Lambda_{\text{tot}} \) and each such event is located independently according to the following density. For a location \( x \) on branch \( e \), the density at \( x \) is \( \Lambda(e) / \Lambda_{\text{tot}} \).
   - **Donor locations.** If \( x \) is selected as a recipient location, the corresponding donor location \( y \) is chosen uniformly at random in \( C_x \). The HGT transfer is then obtained by performing an SPR move from \( x \) to \( y \), that is, the subtree below \( x \) in \( T_s \) is moved to \( y \) in \( T_g \).

   The probability that a recipient or donor location coincides with a node of \( T_s \) is 0.

2. **Executing the HGT Process:** We perform gene transfers chronologically from the root:
   - We initialize the gene tree as follows: \( V_g = V_s, E_g = E_s \).
   - We also initialize the mappings (\( \eta, \zeta_b, \zeta_f \)) as follows, for all \( e \in E_g \): \( \eta(e) = e \); \( \zeta_b(e) = 0 \); \( \zeta_f(e) = \tau(e) \).
   - We process the HGT events chronologically as follows:
Suppose the next event to process has \( x \in e \in E_s \) as recipient location and \( y \in e' \in E_s \) as donor location.

(b) We find the unique edges \( e_x, e_y \in E_g \) such that:
- \( \eta(e_x) = e \) and \( \eta(e_y) = e' \); and
- \( \zeta_b(e_x) \leq \tau_x \leq \zeta_f(e_x) \) and \( \zeta_b(e_y) \leq \tau_y \leq \zeta_f(e_y) \);

where \( \tau_x \) is the time between \( x \) and its most recent ancestor in \( T_s \), and similarly for \( \tau_y \).

(c) We introduce a new node \( v \), splitting \( e_y \) into two consecutive edges, \( e_{y_1} \) and \( e_{y_2} \), with the following features:
- \( \eta(e_{y_1}) = \eta(e_{y_2}) = e' \);
- \( \zeta_b(e_{y_1}) = \zeta_b(e_y) ; \zeta_f(e_{y_1}) = \tau_y \);
- \( \zeta_b(e_{y_2}) = \tau_y ; \zeta_f(e_{y_2}) = \zeta_f(e_y) \).

(d) If \( e_x = (u, w) \), we update it to \( e_x = (v, w) \), and change \( \zeta_b(e_x) = \tau_x \).

After all HGT events have been processed, the weights on the resulting gene tree \( T_g \) are defined as follows. For all \( e \in E_g \), \( \omega_g(e) = (\zeta_f(e) - \zeta_b(e)) \cdot \mu_g(\eta(e)) \).

Observe that HGT events may disconnect subtrees of the species phylogeny from their original roots, connecting them to other branches of the gene tree, thereby creating nodes of degree 2 in the gene tree. We allow internal vertices of degree 2 in a gene tree to potentially delineate between two consecutive species phylogeny edges. Each gene tree branch length \( \omega_g(e) \) represents the expected number of substitutions on the (possibly partial) edge of the species phylogeny corresponding to edge \( e \) of the gene tree, which is determined by the substitution rate \( \mu_g(\eta(e)) \), as well as the times \( \zeta_b(e) \) and \( \zeta_f(e) \).

2.2 Species phylogeny reconstruction under constant HGT rate

Let \( T_s = (V_s, E_s; r, \tau) \) be an unknown species phylogeny. We assume that \( N \) independent gene trees \( T_{g1}, \ldots, T_{gN} \), corresponding to homologous genes \( g_1, \ldots, g_N \), were generated according to the process of Definition 4. Our overall goal is to reconstruct the species phylogeny, given the gene trees.

Problem statement However, given that the gene trees are ultimately reconstructed from genetic sequences, we assume that we have imperfect knowledge of these trees. To formalize this further, we make the following definitions.

Definition 5 (Real subtree) Given a rooted tree \( T \), we call a subtree \( T' \) of \( T \) real if all leaves of \( T' \) are leaves of \( T \). Given a node \( u \) of \( T \), we denote by \( u \downarrow T \) the subtree of \( T \) rooted at \( u \).

Definition 6 (Leafomorphic trees) Given two leaf-labeled rooted, directed trees \( T = (V, E) \) and \( T' = (V', E') \) we call them leafomorphic if there exists a leaf-label respecting isomorphism between the trees \( \tilde{T} \) and \( T' \) obtained from \( T \) and \( T' \) respectively, after replacing all maximal directed paths \( \langle u, u_1, \ldots, u_k, v \rangle \) whose internal vertices have in- and out-degree 1 by a single directed edge \( \langle u, v \rangle \).

With the above definitions we can formalize the information that our algorithm is given.

- Contracted unrooted gene tree topologies. We assume that we are given unrooted gene tree topologies where only those edges on a path between two leaves are kept and degree 2 vertices are suppressed. In addition, we note that the HGT process can produce gene tree branch lengths that are arbitrarily short, and therefore, that may be hard to reconstruct from DNA sequences. Hence we also assume that a subset of edges (possibly all) whose length is below a threshold \( \epsilon \) are contracted. Namely, for each gene \( g \), we are given an \( \epsilon \)-contraction of its gene tree, defined as follows.
**Definition 7 (ε-Contractions)** For ε ≥ 0, an ε-contraction of a gene tree $T_g = (V_g, E_g; r, ω_g)$ is a unrooted, unweighted tree topology $T'_g = (V'_g, E'_g)$ on the same set of leaves $L$ as $T_g$ obtained from the following construction. We start by unrooting $T_g$, removing all edges of $T_g$ that are not on a path between two leaves, and replacing all maximal paths $(u, u_1, \ldots, u_k, v)$ whose internal vertices have degree 2 by a single edge $(u, v)$ whose weight is the sum of the weights of the edges on the path. We then contract a subset of edges (possibly all) whose weight is ≤ ε, i.e., for each chosen edge, we remove the edge and fuse its endpoints into a single new vertex. We then discard the weights. The result is $T'_g$.

See [DMR11b] for a reconstruction algorithm that produces such a contraction from sequences at the leaves. We use the notation $d_g(u, v)$ and $d'_g(u, v)$ for the graph distances between $u$ and $v$ on $T_g$ and $T'_g$ respectively.

The **Species Phylogeny Reconstruction Problem in the Presence of HGT** is the following:

Given ε-contractions $T'_{g_1}, \ldots, T'_{g_N}$ of $N$ independent gene trees generated under the process of Definition 4, reconstruct the topology $T_s$ of the phylogeny, namely reconstruct the rooted tree $(V_s, E_s)$ up to a leaf-label respecting isomorphism.

Our main focus in this work is on the rate of HGT that can be sustained without obscuring the phylogenetic signal.

**Main result** To derive asymptotic results, we make some assumptions on the underlying model. The following assumptions were introduced in [DR10, DR13] and are related to commonly made assumptions in the mathematical phylogenetics literature.

**Definition 8 (Bounded-rates model)** Let $0 ≤ \rho_λ ≤ 1$, $0 < \rho_τ$, $ρ_μ ≤ 1$, and $0 < \tau, \lambda, \mu < +∞$ be constants. Under the bounded-rates model, we consider the set of phylogenies $T_s = (V_s, E_s; r, \tau)$ on $n$ extant leaves with rates of transfer $λ(e)$ and rates of substitution $μ_g(e)$ such that the following conditions are satisfied: $∀ e \in E_s$ and all genes $g$, $\lambda \equiv \rho_λ \lambda ≤ \lambda(e) ≤ \lambda$, $\tau \equiv r_τ \tau ≤ \tau(e) ≤ \tau$, and $μ \equiv \rho_μ \mu ≤ μ_g(e) ≤ \mu$.

Finally, our main result is the following.

**Theorem 1 (Algorithmic result: ε-contractions)** Fix constants $0 ≤ \rho_λ ≤ 1$, $0 < \rho_τ ≤ 1$, $0 < \rho_μ ≤ 1$, $0 < \tau, \mu < +∞$ and $0 ≤ ε < τμ$. Under the bounded-rates model, it is possible to reconstruct the topology of the species phylogeny with probability at least $1 - \frac{1}{\text{poly}(n)}$ from ε-contractions of $N = \Omega(\log n)$ independent gene trees generated under the process of Definition 4, as long as $\lambda$ is a sufficiently small constant not depending on $n$.

Our reconstruction algorithm is detailed in the proof of Theorem 1. The condition on $ε$ in Theorem 1 corresponds to the requirement that branches with no transfer are present in the gene tree, that is, are not contracted.

**Proof sketch** We first prove the result in an easier case, the ultrametric case with partial branch length information.¹ That is, we assume that the rate of substitution satisfies $μ_g(e) = μ$ for all $e$ for some $μ > 0$ and that we are given an $ε$-distortion of the resulting gene tree metric.

¹Theorem 2 was announced without proof in extended abstract form in [DR16].
Definition 9 (ε-Distortion) For $\epsilon \geq 0$, an $\epsilon$-distortion of a gene tree $T_g = (V_g, E_g; r, \omega_g)$ is a rooted, directed tree $T'_g = (V'_g, E'_g; r', \omega'_g)$ on the same set of leaves $L$ whose internal vertices have out-degree 2 which is obtained as follows. We remove all edges of $T_g$ that are not on a path between two leaves and replace all maximal paths $(u, u_1, \ldots, u_k, v)$ whose internal (non-root) vertices have degree 2 by a single edge $(u, v)$ whose weight is the sum of the weights of the edges on the path. Moreover, the edge weights $\omega'_g$ of $T'_g$ define a metric on the leaves that is $\epsilon$-close to the metric defined by $\omega_g$, namely for all pairs of leaves $v, w \in L$: $|\omega_g(v, w) - \omega'_g(v, w)| \leq \epsilon$.

Theorem 2 (Algorithmic result: ultrametric $\epsilon$-distortions) Fix constants $0 \leq \rho_\lambda \leq 1$, $0 < \rho_\tau \leq 1$, $0 < \tau, \mu < +\infty$ and $0 \leq \epsilon < \frac{\mu}{2}$. Under the bounded-rates model where we further assume that $\mu_g(\epsilon) = \mu$ for all $\epsilon$, it is possible to reconstruct the topology of the species phylogeny with probability at least $1 - \frac{1}{\text{poly}(n)}$ from $\epsilon$-distortions of $N = \Omega(\log n)$ independent gene trees generated under the process of Definition 4, as long as $\overline{\lambda}$ is a sufficiently small constant not depending on $n$.

Our reconstruction algorithm, which is detailed in the proof of Theorem 2, is recursive: it reconstructs the species phylogeny a few “levels” from the leaves at a time. To give some insights into how it works, we first observe that it is infeasible to use the approach of [RS13] under the conditions of Theorem 2. Indeed, in [RS13], the induced species phylogeny topology on every subset of four leaves $\{a, b, c, d\} \subset L$, also known as a quartet, is determined directly by using the majority induced topology on these four leaves across gene trees. When HGT rates are low enough, it can be shown that most such induced gene tree topologies coincide with the species phylogeny [RS13]. The full species phylogeny can then be reconstructed from the collection of all quartets using standard techniques (see e.g. [SS03]). But Theorem 2 allows an expected $\Omega(\log n)$ HGT events on every path from the root to a leaf, making the argument in [RS13] invalid. Instead, we work our way up the tree, obtaining stronger evidence for the state of quartets as we get firmer knowledge of the lower levels of the tree. A related approach has proved very powerful in the context of phylogeny reconstruction from a single gene (see e.g. [Mos04, DMR11a]).

The proof of Theorem 2 contains several steps:

1. **Reconstructing the recent past:** We first show how to use pairwise distance information to reconstruct the species phylogeny in the “recent past.” The basic idea is to show that, for each pair of leaves at “short distance” in the species phylogeny, the median distance across all genes is a good estimate of the actual distance in the species phylogeny (Lemma 1). We then use standard distance-based techniques to reconstruct the shallow part of the species phylogeny (Lemma 2).

2. **Going deeper into the tree:** We then bootstrap the previous argument to reach deeper parts of the species phylogeny. The main problem is to identify corresponding vertices in the gene trees and in the reconstructed parts of the species phylogeny. Because of the extensive HGT, such a task is far from trivial. We show that, for each vertex at the frontier of the reconstructed phylogeny and for each gene, one can find with high probability a certain type of subtree rooted at the corresponding vertices, called a diluted subtree, which has not undergone HGT and, therefore, is shared by the gene tree and the species phylogeny (Lemma 3). We then show how to use such diluted subtrees to estimate the distance between close-by pairs of vertices deep inside the reconstructed phylogeny (Proposition 1).

3. **Computing diluted trees and recursing:** We show how to compute diluted subtrees in Proposition 2. The algorithm is based on a dynamic programming approach. The final details of the proof are described in Section 3.4 where the main induction step is implemented.

To prove Theorem 1, we make use of graph distances rather than distortions and we employ a related “unrooted” approach, cherry picking, which is detailed in Section 4.
2.3 An impossibility result

We also provide evidence that the reconstruction problem becomes significantly harder when the HGT rate is larger than a high enough constant. Specifically, we show that considerably more data is needed in that regime.

**Theorem 3 (Impossibility result)** Fix $\rho = 0$. Under the bounded-rates model, for all $\rho_\tau$, $\rho_\mu$, $\bar{\tau}$ and $\bar{\mu}$, there is a constant $\lambda$ large enough such that for any $n$ there exists two species phylogenies which produce the same $N = \Omega(n^{1/6})$ gene trees with probability at least $1/2$.

The proof uses a coupling argument which is presented in Section 5. We point out that we were unable to obtain a provably correct reconstruction algorithm in this regime, even assuming that the number of genes satisfies the conditions of Theorem 3—or, in fact, even if $N = +\infty$. In particular, the question of the identifiability of the model remains an outstanding open problem in this area.

3 Algorithmic result: $\epsilon$-distortions

In this section we provide the proof of Theorem 2. In particular, we assume that $\mu_g(e) = \mu$ for all $e$. Throughout this section, our **Operating Assumptions** are the following: We are given $\epsilon$-distortions $T_{g1}', \ldots, T_{gN}'$ of gene trees $T_{g1}, \ldots, T_{gN}$, generated independently according to the random HGT model of Definition 4 from a species phylogeny $T_s = (V_s, E_s; r, \tau)$ with rates of horizontal transfer $\lambda(e)$ and a constant rate of substitution $\mu$ satisfying the bounded rates model of Definition 8. We assume in particular that $\epsilon < \frac{\mu}{2\lambda}$. Additionally $N \geq C \log n$ for a large enough constant $C$, and $\lambda$ a small enough constant, as required by all the lemmas established in this section. In particular, we will skip stating these assumptions in the statements of all lemmas. To simplify the notation, we let

$$\omega_s(u, v) = \mu \cdot \tau(u, v).$$

The proofs of the lemmas below can be found in Section 3.5.

3.1 Reconstructing the Recent Past

In this section, we show that the signal from the distorted gene trees is strong enough to reconstruct the recent past from the leaves of the species phylogeny. We use a distance-based approach. The key observation, encapsulated in the following lemma, is that median distances provide accurate estimates of “short distances.” This intuitively follows from the fact that, at small enough rates of HGT, the path between two close-by leaves is unlikely to be the site of an HGT event. In fact, the lemma says a bit more: median distance estimates of long distances are also guaranteed to exceed a threshold.

**Lemma 1 (Median distances are accurate estimates of short distances)** For any constant $d_0 > 0$, under our operating assumptions, for all $u, v \in L$, the following are true with probability at least $1 - \frac{1}{\text{poly}(n)}$:

1. Short distances. If $\omega_s(u, v) \leq d_0$, then $\text{median}_{i=1,\ldots,N} \{\omega_{gi}'(u, v)\} = \omega_s(u, v) \pm \epsilon$;

2. Long distances. If $\omega_s(u, v) > d_0$, then $\text{median}_{i=1,\ldots,N} \{\omega_{gi}'(u, v)\} > d_0 - \epsilon$.

How do we use Lemma 1 to reconstruct the recent past? Let us first formalize what we mean by the “recent past.” In essence, we truncate the species phylogeny at a fixed time in the past—which produces a forest. However, because of the distorted nature of our input, such a truncation must be defined with care. We will need the following notation. Given a rooted tree $T$ and a subset of its leaves $L'$, we denote by $T|L'$ the restriction of $T$ to leafset $L'$, i.e., the smallest connected subgraph of $T$ that contains $L' \cup \{\text{MRCA}(L')\}$.
Definition 10 (Truncation of a phylogeny) Given a phylogeny $T_s = (V_s, E_s; r, τ)$ with leaf-set $L = [n]$ and some $D > ϵ > 0$, a $(D, ϵ)$-truncation of $T_s$ is a leaf-labeled forest $T_s^D = (V_s', E'_s)$ with leaf-set $L = [n]$, satisfying the following properties:

- Disjoint forest. For some $k ≤ n$, $T_s^D$ comprises $k$ rooted trees, with disjoint leaf-sets $L_1, \ldots, L_k$ which, further, correspond to clusters in the species phylogeny, that is, for all $1 ≤ i ≤ j ≤ k$: $\text{MRCA}_{T_s}(L_i ∪ L_j) ≠ \text{MRCA}_{T_s}(L_i), \text{MRCA}_{T_s}(L_j)$.
- Truncation. Every pair of leaves $u, v ∈ L$, such that $ω_s(u, v) ≤ D − 2ϵ$ belong to the same $L_i$, and every pair of leaves $u, v ∈ L$ such that $ω_s(u, v) > D$ belong to different $L_i$'s.
- Faithfulness. For all $i = 1, \ldots, k$, the leaf-labeled tree $T_s^D|L_i$ is isomorphic to the leaf-labeled tree $T_s|L_i$, under a leaf-label respecting isomorphism.

To reconstruct a truncation of the species phylogeny, we appeal to standard distance-based concepts. See in particular [KZZ03, Mos07]. We first recall a well-known approach for reconstructing ultrametric species phylogeny.

To reconstruct a truncation of the species phylogeny, we appeal to standard distance-based concepts. See in particular [KZZ03, Mos07]. We first recall a well-known approach for reconstructing ultrametric species trees. An ultrametric tree naturally defines a system of nested clusters, sometimes called clades (see, in particular [KZZ03, Mos07]). Indeed, for each vertex $v$ trees. An ultrametric tree naturally defines a system of nested clusters, sometimes called clades (see, in particular [KZZ03, Mos07]). We first recall a well-known approach for reconstructing ultrametric species phylogeny.

To reconstruct a truncation of the species phylogeny, we appeal to standard distance-based concepts. See in particular [KZZ03, Mos07]. We first recall a well-known approach for reconstructing ultrametric species trees. An ultrametric tree naturally defines a system of nested clusters, sometimes called clades (see, e.g., [SS03]). Indeed, for each vertex $v$ in a species phylogeny $T_s$, consider the set $A_v$ of all leaves below $v$, that is, leaves for which $v$ is an ancestor. For all pairs of vertices $u, v$ in $T_s$, we have that either $A_u ∩ A_v = ∅$ (neither $u$ nor $v$ is an ancestor of the other one), $A_u ⊆ A_v$ ($v$ is an ancestor of $u$) or $A_v ⊆ A_u$ ($u$ is an ancestor of $u$). We say that such sets are nested. Reconstructing the topology of $T_s$ is equivalent to reconstructing this system of nested clusters. If one is given a species metric $ω_s$, obtaining these clusters is straightforward using, for instance, single-linkage clustering: iteratively join the closest pair of reconstructed clusters, where the distance between two clusters is defined as the shortest distance between their respective elements.

However, we are not given $ω_s$—what we have is an estimate that is reliable only over short distances

$$∀u, v ∈ L, \quad \hat{d}(u, v) := \text{median}_{i=1,\ldots,N} \{ω'_{g_i}(u, v)\}. \quad (1)$$

Moreover, we only seek to reconstruct a truncation of the species phylogeny. We explain how to do this in the next lemma.

Lemma 2 (Building a truncation) Assume that $\hat{d}$, as defined in (1), satisfies the statement of Lemma 1 with $ε < \frac{d_0}{2}$ for some $d_0$. Then a $(d_0, ε)$-truncation of $T_s$ can be computed in polynomial-time (e.g., by single-linkage clustering).

3.2 Reaching Deeper into the Past

Our goal in this section is to reach deeper into the species phylogeny. The minimum distance scheme in Formula (4) is unfortunately not accurate beyond a large constant. Instead, our basic idea is to bootstrap the median estimator in (1). However, there is a significant hurdle. Although the leaves of a gene tree and of the species phylogeny trivially match, the same does not hold deeper into the past because of the extensive HGT observed under the rates we consider here. Rather we introduce a notion of “conserved” subtrees. For this purpose, we borrow a combinatorial concept of diluted subtrees from [Mos01]. We use diluted subtrees to show that, for any given gene and any given internal vertex of the species phylogeny, with probability close to 1 there is a “dense” subtree of the species phylogeny which has not been modified by the HGT process and, therefore, is shared between the gene tree and the species phylogeny.

Definition 11 (Diluted subtree) Let $T$ be a binary tree rooted at $r$. A subtree $T'$ of $T$ is called a diluted subtree of $T$ if $T'$ is rooted at $r$ and, for all nodes $u$ in both $T'$ and $T$, if $u$ is at (topological) depth the $ℓ$
from $r$ with $\ell \mod 3 = 0$, then the number of descendants of $u$ at depth $\ell + 1$ in $T$ and $T'$ are equal, the number of descendants of $u$ at depth $\ell + 2$ in $T$ and $T'$ are also equal, and the number of descendants of $u$ at depth $\ell + 3$ in $T$ and $T'$ are within 1.

**Definition 12 (Containing a diluted subtree)** Given a leaf-labeled tree $T$ rooted at $u$, we say that a leaf-labeled rooted tree $T'$ contains a diluted subtree of $T$ if a real subtree of $T'$ is leafsomorphic to a diluted subtree of $T$.

**Lemma 3 (Conserved subtrees)** Consider the leaf labeled tree $u \downarrow T_s$, rooted at some node $u \in V_s$ of phylogeny $T_s$, and a gene tree $T_g$ generated from $T_s$ according to the process of Definition 4. For all $\delta > 0$, under our operating assumptions, $T_g$ contains a diluted subtree of $u \downarrow T_s$, with probability at least $1 - \delta$. In particular, with probability at least $1 - \delta$ for any given gene, there exists a diluted subtree of $u \downarrow T_s$ that does not receive any recipient locations during the HGT process of Definition 4.

With the concept of a diluted subtree and Lemma 3, we can generalize Lemma 1 to the following statement. Note that this proposition is only existential. We show how to actually compute the diluted subtrees and the corresponding cluster distances in the next subsection. We extend $\omega_s$ to clusters as before. That is, letting $u$ and $v$ be vertices in $T_s$ neither of which is an ancestor of the other and letting $A_u$ and $A_v$ be the corresponding clusters (i.e., descendant leaves), we have $\omega_s(A_u, A_v) = \min_{a \in A_u, b \in A_v} \omega_s(a, b)$.

**Proposition 1 (Induction step: Diluted subtrees and distance estimates)** Consider constants $d_0, \eta > 0$ and a pair of nodes $u, v$ of the phylogeny $T_s$, neither of which is an ancestor of the other. Under our operating assumptions, a distorted gene tree $T_g'$ satisfies the following with probability at least $1 - \eta$:

- Diluted subtree at $u$. $T_g'$ contains a real subtree $T_u'$ rooted at some node $u'$ that is leafsomorphic to a diluted subtree of $u \downarrow T_s$; moreover, any such subtree $T_u'$ has the same root;
- Diluted subtree at $v$. $T_g'$ contains a real subtree $T_v'$ rooted at some node $v'$ that is leafsomorphic to a diluted subtree of $v \downarrow T_s$; moreover, any such subtree $T_v'$ has the same root.

Moreover, for any such subtrees $T_u'$ and $T_v'$:

- If $\omega_s(u, v) \leq d_0$, $\omega_g'(\ell_1, \ell_1') = \omega_s(A_u, A_v) \pm \epsilon$ for any leaves $\ell_1$ of $T_u'$ and $\ell_1'$ of $T_v'$;
- If $\omega_s(u, v) > d_0$, $\omega_g'(\ell_1, \ell_1') > \omega_s(A_u, A_v) - \omega_s(u, v) + d_0 - \epsilon$ for any leaves $\ell_1$ of $T_u'$ and $\ell_1'$ of $T_v'$.

### 3.3 Computing Diluted Subtrees

It remains to show how to compute diluted subtrees.

**Proposition 2 (Induction step: Computing diluted subtrees)** Given a leaf-labeled tree $T$ rooted at $u$ and another leaf-labeled tree $T'$ rooted at $u'$, where both $T$ and $T'$ have the same leaf-set $L$ and they both have internal nodes of outdegree 2, we can identify in polynomial-time a real subtree of $T'$ that is leafsomorphic to a diluted subtree of $T$, if such a subtree exists in $T'$.

### 3.4 Theorem 2

Using Propositions 1 and 2, we are now ready to prove Theorem 2.
Proof (Theorem 2): For every pair \( u, v \in V_s \) neither of which is an ancestor of the other, it follows from Proposition 1 and standard concentration inequalities [MR95] that, with probability at least \( 1 - \frac{1}{\text{poly}(n)} \):

\[
\omega_s(u, v) \leq d_0 \implies \text{median}_{i \in N_{u,v}} \{ \omega'_g(\ell_i, \ell'_i) \} = \omega_s(A_u, A_v) \pm \epsilon; \tag{2}
\]

\[
\omega_s(u, v) > d_0 \implies \text{median}_{i \in N_{u,v}} \{ \omega'_g(\ell_i, \ell'_i) \} > \omega_s(A_u, A_v) - \omega_s(u, v) + d_0 - \epsilon; \tag{3}
\]

where \( N_{u,v} \) is the subset of distorted gene trees that contain a diluted subtree of \( u \downarrow T_s \) and of \( v \downarrow T_s \). For every such gene tree we let \( \ell_i, \ell'_i \) be arbitrary leaves of subtrees that are leafsomorphic to a diluted subtree of \( u \downarrow T_s \) and \( v \downarrow T_s \) respectively. Since there are \( O(n^2) \) pairs of \( u, v \in V_s \), by a union bound, Equations (2) and (3) simultaneously hold for all pairs of \( u, v \in V_s \), with probability at least \( 1 - \frac{1}{\text{poly}(n)} \). We condition on this event.

We now describe our high-level reconstruction algorithm. We proceed similarly to the proof of Lemma 2, although we employ a slightly different implementation of single-linkage clustering. But, instead of the update formula (4), whenever a new cluster is formed, we compute a diluted subtree of the corresponding tree and use it to estimate inter-cluster distances using the median as above. More precisely:

1. Let \( \mathcal{F} = \{ \{u\} : u \in [n] \} \), set \( \tilde{d} \) as in (1) and, for all \( u \in [n] \), let \( T_{\{u\}} \) be the tree composed of only \( u \).
2. Until \( \mathcal{F} = \{ [n] \} \):
   (a) Let \( A, B \) be two clusters in \( \mathcal{F} \) achieving the minimum \( \tilde{d} \) distance.
   (b) Update \( \mathcal{F} \) by removing \( A, B \) and adding \( A \cup B \).
   (c) Let \( T_{A \cup B} \) be the tree corresponding to the cluster \( A \cup B \). Let \( \rho_{A \cup B} \) be the root of \( T_{A \cup B} \).
   (d) For each gene \( i \in N \), compute a real subtree \( \tilde{T}_{A \cup B}^i \) of \( T_{g_i} \) that is leafsomorphic to a diluted subtree of \( T_{A \cup B} \), if such a subtree exists, as detailed in the proof of Proposition 2. Let \( \ell'_{A \cup B} \) be an arbitrary leaf of \( \tilde{T}_{A \cup B}^i \).
   (e) Update: for each \( F \in \mathcal{F} \) with \( F \neq A \cup B \), set \( \hat{d}(F, A \cup B) := \text{median}_{i \in N_{g_F, \rho_{A \cup B}}} \{ \omega'_g(\ell_F, \ell'_{A \cup B}) \} \).

Arguing as in Lemma 2 and using (2) and (3), it follows that running the above algorithm up to any distance \( D \) produces a \((D, \epsilon)\)-truncation of \( T_s \). That concludes the proof. \[ \blacksquare \]

3.5 Proofs

Proof (Lemma 1): First, we will need the following claim. For a pair of locations \( x, y \in X_s \), we let \( p_s(x, y) \) be the path between \( x \) and \( y \).

Claim 1 For all \( \tau^* > 0 \) and \( \delta^* < 1 \), there is \( \lambda > 0 \) small enough so that the following holds. For all pairs of locations \( x, y \in X_s \) such that \( x \) is an ancestor of \( y \) and \( \tau(x, y) \leq \tau^* \): the probability that, on a gene tree, no recipient or donor location lies on \( p_s(x, y) \) is at least \( 1 - \delta^* \).

Proof: For all \( z \) on \( p_s(x, y) \), let \( N_z = |C_z| \) be the number of contemporaneous locations to \( z \). Let \( z_1, \ldots, z_k \) be the locations on \( p_s(x, y) \) where \( N_z \), as a function of \( z \), has jumps and let \( N^0, \ldots, N^k \) be the values of \( N_z \) on the segments so obtained. Let \( z_0 = x \) and \( z_{k+1} = y \). The recipient locations on \( p_s(x, y) \) form a nonhomogeneous Poisson process with rate bounded by \( \lambda \). To ther other hand, for \( i = 0, \ldots, k \), the donor locations on \( (z_i, z_{i+1}) \) also form an independent nonhomogeneous Poisson process, which can be thought of as the superposition (over the contemporaneous branches) of thinned nonhomogeneous Poisson processes (where the thinning accounts for the choice of donor branch). The total rate of that process is bounded above by

\[
(N^i - 1) \times \frac{1}{N^i} \times \lambda \leq \lambda,
\]
where the first term on the LHS counts the number of contemporaneous branches to \((z_i, z_{i+1})\) (recall that, under our model, recipient and donor locations cannot coincide), the second term is the probability of picking \((z_i, z_{i+1})\) as donor, and the last term bounds the rate of transfer. The donor processes on \((z_i, z_{i+1}), i = 0, \ldots, k\), are independent by the independent increments property of Poisson processes. Hence, overall, the transfer locations (both recipient and donor) on \(p_s(x, y)\) form a Poisson process with rate bounded above by \(2\bar{X}\). The probability of observing no transfer location on \(p_s(x, y)\) is therefore at least \(e^{-2\bar{X}\epsilon}\). Taking \(\bar{X}\) small enough gives the result. ■

Fix \(\tau_0 = \frac{d_0}{\mu}\). We proceed to show the claims of the lemma. We first show that each gene tree distance satisfies the desired bound with high enough probability.

**Short distances:** By definition, \(\omega_s(u, v) \leq d_0\) implies \(\tau(u, v) \leq \tau_0\). Hence, if \(x = \text{MRCA}(u, v)\), \(\tau(u, x) = \tau(v, x) \leq \tau_0/2\). During the generation of a gene tree \(T_g\) from \(T_s\) according to the process of Definition 4, by Claim 1 with probability at least 0.99 (given our operating assumption that \(\bar{X}\) is small enough), no recipient locations between \(x\) and \(u\) or between \(x\) and \(v\) are chosen. Then it follows from Definition 4 that the resulting gene tree \(T_g\) satisfies \(\omega_g(u, v) = \omega_s(u, v)\), hence the distorted tree satisfies \(\omega'_g(u, v) = \omega_s(u, v) \leq \epsilon\).

**Long distances:** Suppose \(\omega_s(u, v) > d_0\). Viewing \(T_s\) as a continuous object, let \(x \neq y \in T_s\) be the unique points (guaranteed to exist and be distinct) such that \(\omega_s(x, u) = \omega_s(y, v) = d_0/2\). It follows that, \(\tau(x, u), \tau(y, v) \leq \tau_0/2\). Let now \(\bar{x}\) (resp. \(\bar{y}\)) be the closest ancestor of \(x\) (resp. \(y\)) that belongs to \(V_s\). Then, \(\tau(\bar{x}, u), \tau(\bar{y}, v) \leq \tau_0/2 + \epsilon\). During the generation of a gene tree \(T_g\) from \(T_s\) according to the process of Definition 4, by Claim 1 with probability at least 0.99 (given our operating assumption that \(\bar{X}\) is small enough), no recipient locations between \(\bar{x}\) and \(u\) or between \(\bar{y}\) and \(v\) are chosen. Then, by Definition 4, the resulting gene tree \(T_g\) will contain nodes \(\bar{x}, \bar{y}\), the path between \(u, v\) in \(T_g\) will go through these nodes, and \(\omega_g(\bar{x}, u) = \omega_s(\bar{x}, u)\) and \(\omega_g(\bar{y}, v) = \omega_s(\bar{y}, v)\). Hence, \(\omega_g(u, v) \geq d_0\) and the distorted tree satisfies \(\omega'_g(u, v) \geq d_0 - \epsilon\).

Given that a gene tree generated according to the process of Definition 4 satisfies the claims of the lemma with probability at least 0.99, the lemma follows from the choice of \(N\), and standard concentration bounds [MR95]. ■

**Proof (Lemma 2):** We apply single-linkage clustering, as described above the statement of Lemma 2, up to distance \(d_0 - \epsilon\). More precisely, we start with each leaf being in a cluster of its own with the distance \(d\) as defined in (1). At each iteration, we merge the two closest clusters. When a new cluster is formed, we update \(d\) by letting the distance between the new cluster \(A\) and any other remaining cluster \(B\) be defined as

\[
\hat{d}(A, B) := \min_{a \in A, b \in B} \hat{d}(a, b).
\]  

(4)

We stop when no pair of clusters is at distance at most \(d_0 - \epsilon\).

Let \(C_s\) be the set of all clusters of \(T_s\) and let \(C_s[M]\) be those clusters in \(C_s\) whose elements are at distance at most \(M\) under \(\omega_s\). We claim that the algorithm described above reconstructs a collection of clusters \(\hat{C}\) which satisfies

\[
\hat{C} = \left\{ A \in C_s : \min_{a_1, a_2 \in A} \hat{d}(a_1, a_2) \leq d_0 - \epsilon \right\},
\]  

(5)

and, furthermore,

\[
C_s[d_0 - 2\epsilon] \subseteq \hat{C} \subseteq C_s[d_0].
\]  

(6)

Note that the sets in \(\hat{C}\) are then nested, as those in \(C_s[d_0]\) are nested. These conditions together ensure that the output is equivalent to a \((d_0, \epsilon)\)-truncation of \(T_s\) as in Definition 10. The claim follows from Lemma 1 and
an induction argument on the steps of the algorithm. See for example [Roc10, Theorem 1 (Supplementary Materials)] for such an argument. We omit the details. ■

**Proof (Lemma 3):** Recall that, under the HGT process, a subtree moves away from its location in the species phylogeny if it is the recipient location of an HGT event. By our assumptions and Claim 1, the probability that this event occurs on any given edge of the species phylogeny is bounded by a constant, which can be made arbitrarily small. Hence, we can think of the subtree of \( u \downarrow T_s \) which is conserved under the HGT process as a *percolation process*, where an edge is open (independently from the other edges) if it does not contain a recipient location of the HGT process. All other edges are said to be closed. The open subtree of \( u \downarrow T_s \) then corresponds to a subtree which is shared between the species phylogeny and the gene tree. The result then follows directly by adapting Lemmas 6–8 in [Mos01]. ■

**Proof (Proposition 1):** Consider the generation of gene tree \( T_g \) from \( T_s \). According to Lemma 3, with probability at least \( 1 - 2\delta \), for \( \delta = \eta/4 \), there exist diluted subtrees \( \tilde{T}_u \) of \( u \downarrow T_s \) and \( \tilde{T}_v \) of \( v \downarrow T_s \) that do not receive any recipient locations in the process of Definition 4. We condition on this event in the remainder. By the definition of the HGT process, this means that \( T_g \) contains trees \( T_u \) and \( T_v \) that are leafsomorphic to \( \tilde{T}_u \) and \( \tilde{T}_v \), respectively. Moreover, these trees are rooted at nodes \( u \) and \( v \) of \( T_g \) (which we identify with the corresponding nodes of \( T_s \)). In particular observe that, for any leaf \( \ell_1 \) of \( \tilde{T}_u \) (and \( T_u \), we have that

\[
\omega_s(\ell_1, u) = \omega_g(\ell_1, u),
\]

and similarly for \( \tilde{T}_v \). In addition, by an analysis analogous to the proof of Lemma 1, it follows that, with probability at least \( 1 - 2\delta \), independently w.r.t. the event considered above:

\[
\begin{align*}
\text{If } \omega_s(u,v) \leq d_0, \text{ then } \omega_g(u,v) &= \omega_s(u,v); \\
\text{If } \omega_s(u,v) > d_0, \text{ then } \omega_g(u,v) &> d_0.
\end{align*}
\]

Finally, given that \( T'_g \) is leafsomorphic to \( T_g \), it follows that \( T'_g \) will contain real subtrees \( T'_u \), \( T'_v \) that are leafsomorphic to \( \tilde{T}_u \) and \( \tilde{T}_v \), respectively.

Let \( T''_u \) and \( T''_v \) be arbitrary real subtrees of \( T'_g \) that are leafsomorphic to some diluted subtree \( \tilde{T}_u \) of \( u \downarrow T_s \) and some diluted subtree \( \tilde{T}_v \) of \( v \downarrow T_s \) respectively. We claim that \( T'_u \) and \( T''_u \) have the same root, and similarly for \( T'_v \) and \( T''_v \). To show this, we first notice the following:

**Claim 2** \( \tilde{T}_u \) and \( \tilde{T}_v \) share two disjoint paths from their common root \( u \) to a pair of shared leaves. The same is true for \( \tilde{T}_v \) and \( \tilde{T}_v \).

**Proof (Claim 2):** Follows immediately by the Pigeonhole principle and the diluted tree degree requirements. ■

Consider the pair of disjoint paths \( p_1, p_2 \) shared by \( \tilde{T}_u \) and \( \tilde{T}_u \) by Claim 2. Suppose \( p_1 \) connects the root \( u \) to some leaf \( \ell_1 \) and \( p_2 \) connects the root \( u \) to some leaf \( \ell_2 \). Since \( T'_u \) is leafsomorphic to \( \tilde{T}_u \), it must also contain disjoint paths from its root to leaves \( \ell_1 \) and \( \ell_2 \). The same is true for \( T''_u \), as it is leafsomorphic to \( \tilde{T}_u \). Since \( T'_u \) and \( T''_u \) are real subtrees of the same tree \( T'_g \) they must have the same roots. Similarly, \( T'_v \) and \( T''_v \) have the same roots. So we have established the first two claims of the proposition.

It remains to prove the distance claims. Suppose that \( \omega_s(u,v) \leq d_0 \). For any leaf \( \ell_1 \) of \( T_u \) and \( \ell'_1 \) of \( T_v \) we have by (7) and (8) that

\[
\omega_g(\ell_1, \ell'_1) = \omega_s(\ell_1, \ell'_1) = \omega_s(A_u, A_v).
\]

Suppose that \( u' \) and \( v' \) are the roots of \( T'_u \) and \( T'_v \) in \( T'_g \) as defined above. Let again \( T''_u \) and \( T''_v \) be arbitrary real subtrees of \( T'_g \) that are leafsomorphic to some diluted subtree \( \tilde{T}_u \) of \( u \downarrow T_s \) and some diluted subtree \( \tilde{T}_v \) of \( v \downarrow T_s \).
Lemma 4
Suppose \( T \) is leafsomorphic to \( T' \). Let us make an easy observation:

Proof (Lemma 4):

- diluted subtrees \( T \)
- Definition 13 (3-Ball)
- \( \omega_g(\ell_1, \ell'_1) = \omega_g(\ell_2, \ell'_2) \), \( \omega_g(x, y) = \omega_g(x, y) \pm \epsilon \).

Combining Equations (10), (11) and (12), we obtain

\[ \omega_g(\ell_1, \ell'_1) = \omega_g(\ell_2, \ell'_2) = \omega_s(A_u, A_v) \pm \epsilon, \]

as desired. A similar argument holds if \( \omega_s(u, v) > d_0 \). We leave out the details. ■

Proof (Proposition 2): The diluted subtree can be computed using dynamic programming. Our algorithm proceeds from the leaves of the tree \( T' \) towards the root \( u' \). Letting \( T = (V, E) \) and \( T' = (V', E') \), for each node \( v' \in V' \), we identify whether a real subtree of \( v' \downarrow T' \) is leafsomorphic to a diluted subtree of a tree \( v \downarrow T \) for some node \( v \) of \( T \). If this is the case, we store the identity of \( v \) in some set-valued function \( f \) that are leafsomorphic to \( T_1, T_2 \) of \( w \downarrow T \). Then \( w'_1 = w'_2 \).

Proof (Lemma 4): By the Pigeonhole principle and the degree requirements of diluted subtrees, it follows that \( T_1 \) and \( T_2 \) share two disjoint paths from their common root \( w \) to a pair of shared leaves \( \ell_1, \ell_2 \). Since \( T'_1 \) is leafsomorphic to \( T_1 \) it must also have two disjoint paths from its root \( w'_1 \) to leaves \( \ell_1, \ell_2 \). The same is true for \( T'_2 \). Hence, \( w'_1 = w'_2 \). ■

Let us also introduce a definition.

Definition 13 (3-Ball)
Given a node \( u \) of \( T \), its 3-Ball denoted \( B_T(u, 3) \) is the subgraph of \( T \) containing \( u \)'s children (if any), grandchildren (if any), and great-grandchildren (if any). A subgraph of \( B_T(u, 3) \) is called an almost 3-Ball of \( u \) if it is the same as \( B_T(u, 3) \), except that it might be missing a single node at depth 3 from the root, if any.

We are now ready to compute \( f \). Given Lemma 4, for all \( v \in V \), there is at most one node \( v' \in V' \) such that \( v \in f(v') \). The initialization of \( f \) at the leaves of \( T' \) is clear:

\[ v \in f(v') \iff \begin{cases} \text{v' is a leaf of } T', \ v \text{ is a leaf of } T, \text{ and } v, v' \text{ have the same labels} \end{cases} \]

For each non-leaf node \( v' \) of \( T' \), working our way up the tree, we initialize \( f(v') = \emptyset \). Then, for all \( v \in V \), we set \( f(v') := f(v') \cup \{v\} \) if the following computation succeeds.

1. Let \( G \) be the great-grandchildren of \( v \). We check the subtree of \( T' \) rooted at \( v' \) to identify for each great-grandchild \( w \in G \) of \( v \) its inverse \( w' = f^{-1}(w) \), if any, inside the subtree. Recall that such \( w' \) is unique, if it exists. If more than one great-grandchild of \( v \) fail to have inverses in the subtree of \( T' \) rooted at \( v' \), we output failure. Otherwise let \( I \) be the set of inverses of great-grandchildren of \( v \).
2. For all leaves \( \mathcal{L} \) in \( B_T(v, 3) \) that are also leaves in \( T \) and are at depth \( \leq 2 \) from \( v \), we check to see if they are also leaves in the subtree of \( T' \) rooted at \( v' \). If any of them fails to be a leaf in the subtree of \( T' \) rooted at \( v' \), we output failure.

3. For all subsets \( I' \subseteq I \) of size \( |I'| = |\mathcal{G}| - 1 \), we find the minimal subtree \( T'' \) of \( T' \) that includes nodes in \( I' \cup \mathcal{L} \cup \{ v' \} \). If \( T'' \) is leafsomorphic (only preserving labels in \( \mathcal{L} \)) to an almost 3-Ball of \( v \) such that, whenever a node \( w' \in I' \) is mapped to a node \( w \) of the almost 3-Ball, \( w \in f(w') \), we output success. If all tried sets \( I' \) fail (or none of the right size exists), then we output failure. If we succeed for some \( I' \), we also store the corresponding sets \( I', \mathcal{L}, \) tree \( T'' \) and leafsomorphism, indexing them by \( (v', v) \). (We only need to store these for one successful \( I' \), if any.)

It is clear from its description that \( f \) can be computed in polynomial time in the size of \( T' \) and \( T \), in a bottom-up fashion.

When the computation of \( f \) is over, we identify the node \( u' \in V' \), if any, such that \( u \in f(u') \). If no such \( u' \) is found, we output that there is no real subtree of \( T' \) that is leafsomorphic to a diluted subtree of \( T \). If such a \( u' \) is found, then we construct a real subtree of \( u' \downarrow T' \) that is leafsomorphic to a diluted subtree of \( T \), by picking nodes iteratively as follows:

- We pick \( u' \) and associate it with \( u \), if \( u \) is not a leaf.
- For each picked node \( v' \) of \( T' \), we check to see if we have associated a node \( v \) of \( T \) with \( v' \). If not, we do nothing for \( v' \). If yes and \( v \) is not a leaf, then:
  - we pick all the nodes in the stored tree \( T'' \) indexed by \( (v', v) \);
  - for all nodes in the set \( I' \) indexed by \( (v', v) \) we associate them with their corresponding nodes in \( T \) according to the leafsomorphism indexed by \( (v', v) \).

Clearly the above procedure takes time linear in all stored information.

Let us now justify the correctness of the computation of \( f \), as well as the returned subtree of \( T' \), if any. The correctness of the computation of \( f \) can be shown inductively from the leaves. Clearly, the values computed for the leaves are correct. Inductively, suppose all values at the subtree rooted at \( v' \) have been computed correctly. Let us argue that the value computed for \( v' \) also correct.

- **No false-negatives.** Suppose there exists a diluted subtree \( T_w \) of \( v \downarrow T \) that is leafsomorphic to a real subtree \( T'_{v'} \) of \( v' \downarrow T' \). We will argue that when processing nodes \( v', v \) our algorithm will add \( v \) to \( f(v') \).

  Consider the set \( \mathcal{G} \) of great-grandchildren of \( v \). The diluted tree definition implies that there exists a subset \( \mathcal{G}' \subseteq \mathcal{G} \) of great-grandchildren of \( v \) of size \( |\mathcal{G}'| \geq |\mathcal{G}| - 1 \), such that all great-grandchildren in \( \mathcal{G}' \) are included in \( T_w \). Moreover, by the definition of a diluted tree, the subtree \( T_w \) of \( T_v \) rooted at some node \( w \in \mathcal{G}' \) is a diluted subtree of \( w \downarrow T \). Restricting the leafsomorphism between \( T_v \) and \( T'_{v'} \) to the subtree \( T_w \) of \( T_v \), we obtain a subtree \( T'_{w} \) of \( T'_{v'} \) rooted at some descendant \( u' \) of \( v' \) that is leafsomorphic to \( T_w \). Hence, assuming by induction that the value of \( f \) at \( u' \) has been computed correctly, \( w \in f(u') \). So Step 1 of our algorithm will not declare failure, and correctly compute set \( I' \).

  Next, consider the set \( L_v \) of all leaves in \( T \) at (topological) distance at most 2 from \( v \). It is clear that Step 2 of our algorithm will set \( \mathcal{L} = L_v \). Moreover, since \( T'_{v'} \) is leafsomorphic to \( T_v \), it must be that all leaves in \( \mathcal{L} \) are descendants of \( v' \) in \( T' \). So Step 2 will also not declare failure.

  Finally, for each great-grandchild \( w \in \mathcal{G}' \) that is not a leaf in \( T \), let us pick two leaves \( \ell^-_1, \ell^-_2 \) in \( T_w \) such that the paths from \( \ell^-_1, \ell^-_2 \) to \( w \) are disjoint. Such pair of leaves is guaranteed to exist by
the diluted tree requirements. Since $T_w$ and $T_w'$ are leafsomorphic, $\ell_1^w, \ell_2^w$ also belong to $T_w'$, where $w' = f^{-1}(w)$, and the paths from these leaves to $w'$ are also disjoint. If $w \in \mathcal{G}'$ is a leaf in $T$, set $\ell_1^w = \ell_2^w = w$. Now consider the set of leaves $\mathcal{L}' = \mathcal{L} \cup (\cup_{w \in \mathcal{G}'} \{\ell_1^w, \ell_2^w\})$. These leaves are a subset of the leaves of $T_v$ and $T'_v$. Let $T_v\mathcal{L}'$ be the restriction of $T_v$ to leaves $\mathcal{L}'$, i.e. the minimal subtree of $T_v$ that contains the nodes in $\mathcal{L}' \cup \{v\}$. Since $T_v$ is leafsomorphic to $T'_v\mathcal{L}'$, it must be that $T_v\mathcal{L}'$ is leafsomorphic to $T'_v\mathcal{L}'$. By our choice of leaves $\ell_1^w, \ell_2^w$, this means that the tree $T''$ constructed in Step 3 will be deemed leafsomorphic to an almost 3-Ball of $v$. So our algorithm will output Success.

- **No false-positives.** Conversely, we show that, if our algorithm adds $v$ to $f(v')$, then it must be that a real subtree of $v' \downarrow T'$ is isomorphic to a diluted subtree of $v \downarrow T$. This follows almost immediately from the description of our algorithm. For $v$ to be included in $f(v')$, it must be that when our algorithm processes $v', v$, it finds out that all but at most one $w \in \mathcal{G}$ (the set of great-grandchildren of $v$) have an inverse $f^{-1}(w)$ that is a descendant of $v'$ in $T'$, and moreover, all children and grandchildren of $v$ that are leaves in $T$ are also descendants of $v'$ in $T'$. Let $\mathcal{I}$ be the set of inverses computed in Step 1, and let $\mathcal{L}$ be the set of leaves computed in Step 2. In Step 3 our algorithm finds a subset $\mathcal{I}' \subseteq \mathcal{I}$ of size $|\mathcal{G}| - 1$ such that the minimal subtree $T''$ of $T'$ that contains the nodes in $\mathcal{I}' \cup \mathcal{L}$ is leafsomorphic (only preserving labels in $\mathcal{L}$) to an almost 3-Ball $AB(v, 3)$ of $v$. Do the following operation on $T''$ and $AB(v, 3)$: For each leaf $w'$ of $T''$ that belongs to $\mathcal{I}'$, root at $w'$ a real subtree of $w' \downarrow T'$ that is leafsomorphic to a diluted subtree $T_w$ of $w \downarrow T$, where $w$ is the leaf of $AB(v, 3)$ such that $w \in f(w')$. Also, root $T_w$ at leaf $w$ of $AB(v, 3)$. Call $\text{grown}(T'')$ and $\text{grown}(AB(v, 3))$ the trees resulting from the above operations. It is clear that $\text{grown}(T'')$ and $\text{grown}(AB(v, 3))$ are leafsomorphic, $\text{grown}(AB(v, 3))$ is a diluted subtree of $v \downarrow T$, and $\text{grown}(T'')$ is a real subtree of $v' \downarrow T'$. So we did well to include $v$ to $f(v')$.

Given that the computation of $f$ is correct, it is clear from the above analysis that determining a real subtree of $T'$ that is isomorphic to a diluted subtree of $T$ is also done correctly.

## 4 Algorithmic result: $\varepsilon$-contractions

In this section we provide the proof of our main algorithmic result, Theorem 1. (In particular, unlike the previous section, we do not assume here that the substitution rate is constant.) Throughout this section, our **Operating Assumptions** are the following: We are given $\varepsilon$-contractions $T'_1, \ldots, T'_N$ of gene trees $T_{g1}, \ldots, T_{gN}$, generated independently according to the random HGT model of Definition 4 from a species phylogeny $T_s = (V_s, E_s; r, \tau)$ with rates of horizontal transfer $\lambda(e)$ and rates of substitution $\mu_g(e)$ satisfying the bounded rates model of Definition 8. We assume that $0 \leq \varepsilon < \frac{1}{\mu}$. Additionally $N \geq C \log n$ for a large enough constant $C$, and $\bar{\lambda}$ a small enough constant, as required by all the lemmas established in this section. In particular, we will skip stating these assumptions in the statements of all lemmas.

We let $d_s(u, v)$, $d_g(u, v)$ and $d'_g(u, v)$ denote the graph distances between $u$ and $v$ on $T_s$, $T_g$ and $T_g'$ respectively. (Under $d_s(u, v)$, we ignore the root of $T_s$.) Recall that a **cherry** is a pair of leaves at graph distance 2, that is, a pair of leaves that are “siblings.” Similarly to Section 3, the proof contains several steps:

1. **Reconstructing cherries:** The first key idea is to show that, for each pair of leaves at “short distance” in the species phylogeny, the median graph distance across the genes is equal to the actual graph distance in the species phylogeny with high probability (Lemma 5). We then use the median to reconstruct the cherries of the species phylogeny (Lemma 6).

2. **Going deeper into the tree:** We then bootstrap the previous argument to reach deeper into the species phylogeny. We adapt the diluted approach of Section 3 to identify corresponding vertices in the gene
trees and in the reconstructed parts of the species phylogeny. We then show how to use such diluted subtrees to estimate the graph distance between close-by pairs of vertices deep inside the reconstructed phylogeny (Proposition 3).

3. **Computing diluted trees and recursing:** Following the dynamic programming approach of Section 3 to compute diluted subtrees, the final details of the proof are described in Section 4.4 where the main induction step is implemented.

The proofs of the lemmas below can be found in Section 4.5.

### 4.1 Reconstructing cherries

We first show how to reconstruct “short distances” from the contracted gene trees. We use the fact that, at small enough rates of HGT, the path between two close-by leaves is unlikely to be the site of an HGT event. We also show that median distance estimates of “long distances” are guaranteed to exceed a threshold. Compared to Lemma 1 in the distorted case, there is a new complication. Because we work with graph distance we must ensure that, at short distances, not only is there no transfer on the path between the leaves of interest, but also that the “subtrees hanging from that path” continue to have a representative among the leaves.

**Lemma 5 (Median distances are accurate estimates of short distances)** For any constant integer $d_0 > 0$, under our operating assumptions, for all $u, v \in L$, the following are true with probability at least $1 - \frac{1}{\text{poly}(n)}$:

1. **Short distances.** If $d_s(u, v) \leq d_0$, then $\text{median}_{i=1,\ldots,N}\{d'_{g_i}(u, v)\} = d_s(u, v)$;
2. **Long distances.** If $d_s(u, v) > d_0$, then $\text{median}_{i=1,\ldots,N}\{d'_{g_i}(u, v)\} > d_0$.

Our reconstruction algorithm first reconstructs all cherries using Lemma 5. Then it proceeds by reconstructing “cherries of cherries,” and so forth. However, as the illustration of our reconstruction method in Figures 2 and 3 shows, we cannot guarantee that the reconstruction is consistent with the rooting in the species tree. Instead, we maintain what we call a **pruning**, as defined next.

**Definition 14 (Pruning of a phylogeny)** Given a phylogeny $T_s = (V_s, E_s; r, \tau)$ with leaf-set $L = \{1, \ldots, n\}$ and some integer $D > 0$, a $D$-pruning of $T_s$ is a collection $\mathcal{F}$ of rooted subtrees $T_i = (V_i, E_i; r_i), i = 1, \ldots, \ell$, of $T_s$ satisfying the following properties:

- **Disjoint forest.** The trees $T_i, i = 1, \ldots, \ell$, are disjoint, that is, do not share edges as subtrees of $T_s$.
- **Size.** The number of edges in $\mathcal{F}$, as a subforest of $T_s$, is $D$.
- **Fullness.** For all $i = 1, \ldots, \ell$, the tree $T_i$, as a subtree of $T_s$, is full. That is, there is a neighbor $r'_i$ of $r_i$ in $T_s$ such that, if $T_s$ were (re-)rooted at $r'_i$, then $T_i$ would correspond exactly to the subtree of $T_s$ rooted at $r_i$.

We reconstruct an initial pruning using the median estimator:

$$\forall u, v \in L, \quad \hat{d}(u, v) := \text{median}_{i=1,\ldots,N}\{d'_{g_i}(u, v)\}. \quad (13)$$

Formally:

**Lemma 6 (Building an initial pruning)** Let $D$ be twice the number of cherries of $T_s$. Assume that $\hat{d}$, as defined in (13), satisfies the statement of Lemma 5. Then a $D$-pruning of $T_s$ can be computed in polynomial-time.
4.2 Reaching Deeper into the Past

We now show how to bootstrap the median estimator in (13). We rely on the concepts of diluted and conserved subtrees defined in Section 3.2. As in the previous subsection, the main new hurdle is that the use of the graph distance requires controlling the HGTs in the “subtrees hanging from the path” between two internal vertices of interest. We use ideas from percolation for that purpose.

**Proposition 3 (Induction step: Diluted subtrees and distance estimates)** Let $\mathcal{F} = \{T_1, \ldots, T_\ell\}$ be a pruning of $T_s$. Consider constants $d_0, \eta > 0$ and a pair of distinct roots $r_i, r_j$ of $\mathcal{F}$ (with respective trees $T_i$ and $T_j$). Under our operating assumptions, a contracted gene tree $T'_g$ satisfies the following with probability at least $1 - \eta$:

- **Diluted subtree at $r_i$.** $T'_g$ contains a real subtree $T'_i$ rooted at some node $r'_i$ that is leafsomorphic to a diluted subtree of $T_i$; moreover, any such subtree $T''_i$ has the same root $r'_i$;

- **Diluted subtree at $r_j$.** $T'_g$ contains a real subtree $T'_j$ rooted at some node $r'_j$ that is leafsomorphic to a diluted subtree of $T_j$; moreover, any such subtree $T''_j$ has the same root $r'_j$.

Moreover, for any such subtrees $T''_i$ and $T''_j$:

- **Short distances.** If $d_s(r_i, r_j) \leq d_0$ then $d'_g(r'_i, r'_j) = d_s(r_i, r_j)$;

- **Long distances.** If $d_s(r_i, r_j) > d_0$ then $d'_g(r'_i, r'_j) > d_0$.

4.3 Computing Diluted Subtrees

It remains to show how to compute diluted subtrees.

**Proposition 4 (Induction step: Computing diluted subtrees)** Given some node $r'_i$ of $T'_g$ and a tree $T_i$ from a pruning $\mathcal{F}$ of $T_s$, we can identify in polynomial-time a real subtree of $T'_g$ rooted at $r'_i$ that is leafsomorphic to a diluted subtree of $T_i$, if such a subtree exists in $T'_g$.

---

Figure 2: A species tree.
Figure 3: Steps of the reconstruction algorithm for the species tree $T_s$ in Figure 2. Roots of the prunings are in blue. Note that in the last step, re-rooting $T_s$ at $v$ shows that the left subtree in the pruning satisfies the fullness condition.

4.4 Phylogenies from Contracted Gene Trees

Using Propositions 3 and 4, we are now ready to prove Theorem 1.

**Proof (Theorem 1):** For every pair $r_i, r_j \in V_s$ and full, disjoint subtrees $T_i, T_j$ of $T_s$ rooted respectively at $r_i$ and $r_j$, it follows from Proposition 3 and standard concentration inequalities [MR95] that, with probability at least $1 - \frac{1}{\text{poly}(n)}$:

$$d_s(r_i, r_j) \leq d_0 \implies \text{median}_{\ell \in N_{r_i, r_j}} \{d'_{q_{rl}}(r_i, r_j)\} = d_s(r_i, r_j);$$

$$d_s(r_i, r_j) > d_0 \implies \text{median}_{\ell \in N_{r_i, r_j}} \{d'_{q_{rl}}(r_i, r_j)\} > d_0;$$

where $N_{r_i, r_j}$ is the subset of contracted gene trees that contain a diluted subtree of $T_i$ and of $T_j$. Since there are $O(n^2)$ pairs of $u, v \in V_s$, by a union bound, Equations (14) and (15) simultaneously hold for all pairs of $u, v \in V_s$, with probability at least $1 - \frac{1}{\text{poly}(n)}$. We condition on this event.

We now describe our high-level reconstruction algorithm. We proceed similarly to Lemma 6. But whenever a new subtree is formed, we identify diluted subtrees of this subtree in the contracted gene trees and use these diluted subtrees to estimate inter-root distances using the median as above. More precisely:
1. For all \( u \in [n] \), let \( T_{\{u\}} \) be the tree composed of only \( u \), with root \( \rho_{\{u\}} = u \). Let \( \mathcal{F} = \{ T_{\{u\}} : u \in [n] \} \). Set \( \hat{d} \) as in (13).

2. Until the number of edges in \( \mathcal{F} \) is \( 2n - 4 \):
   
   (a) Let \( T_A, T_B \) be two subtrees in \( \mathcal{F} \) with \( \hat{d} \)-distance between their roots equal to 2.
   
   (b) Let \( T_{A \cup B} \) be the tree obtained by attaching the trees \( T_A \) and \( T_B \) at the roots by a cherry. Let \( \rho_{A \cup B} \) be the root of \( T_{A \cup B} \), that is, the middle vertex of the new cherry.
   
   (c) Update \( \mathcal{F} \) by removing \( T_A, T_B \) and adding \( T_{A \cup B} \).
   
   (d) For each gene \( i \in N \), compute a real subtree \( T_{A \cup B}^i \) of \( T_{g_i} \) that is leafsomorphic to a diluted subtree of \( T_{A \cup B} \), if such a subtree exists, as detailed in the proof of Proposition 4. Let \( \hat{\rho}_{A \cup B}^i \) be the root of \( T_{A \cup B}^i \).
   
   (e) Update: for each \( T_F \in \mathcal{F} \) with \( F \neq A \cup B \), set
   
   \[
   \hat{d}(\rho_F, \rho_{A \cup B}) := \text{median}_{i \in N_{\rho_F, \rho_{A \cup B}} \{d_{g_i}(\hat{\rho}_{F,i}, \hat{\rho}_{A \cup B,i})\}},
   \]

   where \( N_{\rho_F, \rho_{A \cup B}} \) is the subset of contracted gene trees that contain a diluted subtree of \( T_F \) and of \( T_{A \cup B} \).

3. Add an edge connecting the roots of the two trees in \( \mathcal{F} \).

At initialization, \( \mathcal{F} \) is a 0-pruning. By (14) and (15), at each step we identify a cherry of \( T_s \) where the trees in \( \mathcal{F} \) have been pruned. Such a cherry always exists because, by fullness and disjointness of the pruning, the above operation produces a binary tree. Moreover, after adding a cherry as described in the algorithm, we preserve fullness and disjointness and the number of edges in \( \mathcal{F} \) grows by 2. The process therefore terminates with the topology of \( T_s \) in a polynomial number of steps. That concludes the proof. \( \blacksquare \)

### 4.5 Proofs

**Proof (Lemma 5):** Fix \( \tau_0 = d_0 \tau \). As the proof is similar to that of Lemma 1, we only summarize the argument.

- **Short distances:** Suppose that \( d_s(u,v) \leq d_0 \). Then \( \tau(u,v) \leq d_0 \tau = \tau_0 \). Arguing as in the proof of Lemma 1, by Claim 1 for \( \bar{\lambda} \) small enough there is no transfer on \( p_s(u,v) \) with probability at least 0.99. Note, however, that this is not enough to guarantee the result. In particular, if an entire subtree hanging from the path from \( u \) and \( v \) is transferred away, then the ancestor of this subtree on \( p_s(u,v) \) is not present as a vertex in the gene tree, which decreases the graph distance between \( u \) and \( v \). We argue that such problematic transfers do not occur with high probability. Let \( x = \text{MRCA}(u,v) \), let \( w_0, w_1, \ldots, w_\ell \) be the vertices on \( p_s(u,v) \) with \( w_0 = u \) and \( w_\ell = v \), and note that \( \ell \leq d_0 \). For \( i = 1, \ldots, k - 1 \) such that \( w_i \neq x \), let also \( y_i \) be a leaf descendant of \( w_i \) such that the path \( p_s(w_i, y_i) \) does not intersect \( p_s(u,v) \). For \( i \) such that \( w_i = x \), let \( y_i \) be a leaf descendant of the parent of \( x \) such that \( p_s(y_i, w_i) \) does not intersect \( p_s(u,v) \). Then, letting \( y_0 = y_\ell = x \), we have

   \[
   \max \{ \tau(w_i, y_i) : i = 0, \ldots, \ell \} \leq \tau_0 / 2 + 2 \tau,
   \]

   where the worst case is achieved for \( w_i = x \) when all branch lengths are \( \tau \). Arguing as in the proof of Lemma 1, by Claim 1 for \( \bar{\lambda} \) small enough there is no transfer on \( p_s(w_i, y_i) \) for all \( i = 0, \ldots, \ell \) with probability at least 0.99. Then it follows that the resulting gene tree \( T_g \) satisfies \( d'_g(u,v) = d_g(u,v) = d_s(u,v) \).
• **Long distances:** The argument in the case of long distances is similar to the proof of Lemma 1, as modified in the short distances case above. The details are left out.

The lemma then follows from standard concentration bounds [MR95]. ■

**Proof (Lemma 6):** We take $d_0 = 2$. Lemma 5 immediately implies that all cherries of $T_s$ can be identified with high probability. The collection $F$ of these cherries forms a D-pruning. ■

**Proof (Proposition 3):** The first part of the claim follows from the argument in the proof of Proposition 1. The second part, we argue similarly to Lemma 5. We only detail the short distances case. The other case is similar.

Fix $\tau_0 = \tau d_0$. Suppose that $d_s(r_i, r_j) \leq d_0$. Then $\tau(r_i, r_j) \leq \tau_0$. Let $w_0, w_1, \ldots, w_\ell$ be the vertices on $p_s(r_i, r_j)$ with $w_0 = r_i$ and $w_\ell = r_j$ and note that $\ell \leq d_0$. Fix $i = 1, \ldots, k - 1$, let $Y_i$ be the subtree of $T_s$ hanging from $p_s(r_i, r_j)$ at $w_i$ (where we think of $T_s$ as being unrooted). By Claim 1, for $\lambda$ small enough, the probability of a transfer on any given edge of $Y_i$ can be made arbitrarily small. If we imagine running a percolation process on $Y_i$ where an edge is open if there is no transfer involving that edge, then with constant probability arbitrarily close to 1 (for $\lambda$ small enough) there exists an open path from $w_i$ to some leaf $y_i$ of $Y_i$. We choose $\lambda$ such that this holds with probability at least $1 - \eta/2$ for all $i = 0, \ldots, \ell$. Then it follows that the resulting gene tree $T_g$ satisfies $d_g(r_i', r_j') = d_g(r_i', r_j') = d_s(r_i, r_j)$. ■

**Proof (Proposition 4):** For each neighbor $r_i''$ of $r_i$ in $T_g'$, root $T_g'$ at $r_i''$ and apply the procedure described in Proposition 2 to $T_i$ and $r_i' \downarrow T_g'$. ■

## 5 Impossibility result

We now prove Theorem 3. Similarly to [RS12], our improved impossibility result uses a coupling argument. Specifically, we run the HGT processes jointly on two different phylogenies simultaneously and show that they output the same gene tree with high probability. See, e.g., [Lin92] for more on coupling. Our construction also uses percolation on trees techniques. See e.g. [Per99] for more on percolation.

**Proof (Theorem 3):** Fix $\rho_\lambda = 0$, $\rho_r = 1$, and $\bar{\tau} = 1$. Let $T$ be a complete binary tree with $n = 2^H$ leaves labeled $\{1, \ldots, n\}$ and with fixed edge lengths $\bar{\tau}$. Let $\overline{T}$ be the same tree as $T$ with the same leaf labels, except for the following change: in the canonical planar representation of $T$, swap the first and third subtrees, $T_1$ and $T_3$, of $T$ on level $\frac{2}{3} \log_2 n$ (which for simplicity we assume is integer-valued) from the root. Denote by $L_1$ and $L_3$ the respective leaf sets of $T_1$ and $T_3$ in $T$. Similarly, we let $\overline{T}_1$ and $\overline{T}_3$ be the first and third subtrees on level $\frac{2}{3} \log_2 n$ of $\overline{T}$ with respective leaf sets $L_3$ and $L_1$. Observe that $|L_1| = |L_3| = n^{1/3}$. Fix $\lambda(e) = 0$ for all edges not in $T_1$ and $T_3$ and let $\lambda(e) = \bar{\lambda}$ for all edges in $T_1$ and $T_3$. Do the same on $\overline{T}$.

We couple the HGT processes in $T$ and $\overline{T}$ as follows. We first run the process on $T$. The HGT events in $\overline{T}$ are picked as follows: any transfer in $T$ can be described by the leaf set $L_R$ of the recipient location, the leaf set $L_D$ of the donor location and the distance from the root; for any such transfer in $T$, we perform the exact same transfer in $\overline{T}$, i.e., using the same distance from the root and the same sets $L_R$, $L_D$. Observe that this is always possible because at any fixed time for the root, $T$ and $\overline{T}$ share the same subtrees, although some of them are arranged differently. By symmetry, this process is then a coupling of the two HGT processes. We show below that, with probability at least $1 - 1/2N$, the produced gene trees are identical. That implies the theorem.

We make a series of claims.

• **No in-moves.** Note that only the subtrees of $T_1 / T_3$ and $\overline{T}_1 / \overline{T}_3$ can be transferred, as the HGT rate is 0 everywhere else. Let $L_{\{1,3\}} = [n] - L_1 \cup L_3$. We define two types of transfer. In an out-move,
$L_D \subseteq L_{\{1,3\}}$. In an in-move, $L_D \subseteq L_1 \cup L_3$. By the definition of the process, for any given transfer, the probability that it is an in-move is $2/n^{2/3}$. For a constant $0 < \lambda < +\infty$, the total HGT weight $\Lambda_{\text{tot}}$ of $T_1$ and $T_3$ is $\Theta(n^{1/3})$. Here we used that a binary tree with $n^{1/3}$ leaves has $O(n^{1/3})$ edges. Because the number of transfers is Poisson with mean $\Lambda_{\text{tot}}$, for any given transfer, the probability that it is an in-move is $2/n^{2/3}$. For a constant $0 < \bar{\lambda} < +\infty$, the total HGT weight $\Lambda_{\text{tot}}$ of $T_1$ and $T_3$ is $\Theta(n^{1/3})$. Here we used that a binary tree with $n^{1/3}$ leaves has $O(n^{1/3})$ edges. Because the number of transfers is Poisson with mean $\Lambda_{\text{tot}}$, for any $\alpha > 0$, the probability that more than $n^{1/3} + \alpha$ transfers occur overall is at most $O(n^{-\alpha})$ by Markov’s inequality [MR95]. The probability that any transfer is an in-move is then at most $O(n^{-1/6} + n^{-1/3} + \alpha)$ = $O(n^{-1/6})$ by the law of total probability, where we chose $\alpha = 1/6$. Let $E_1$ be the event that there is no in-move.

- **Existence of a cut.** We say that there is transfer cut in $T_1$ if, for each leaf $\ell_1$ in $T_1$, there is at least one transfer on the path between $\ell_1$ and the root of $T_1$; and similarly for $T_3$. Let $p_\lambda$ be the probability that a transfer occurs on an edge of $T_1$. Note that, by choosing $\lambda$ large enough (but constant), we can make $p_\lambda$ to be a constant as close to 1 as we desire. We associate to the HGT process a percolation process to show that, for $\lambda$ large enough, a transfer cut exists in both $T_1$ and $T_3$ with high probability. Consider $T_1$. We say that an edge of $T_1$ is closed if it contains the recipient location of at least one transfer. Otherwise it is open. Let $L'_1$ be the subset of $L_1$ connected to the root of $T_1$ by an open path. Because each edge is open independently with probability $1 - p_\lambda$, the expected size of $L'_1$ is $(1 - p_\lambda)^{H' n^{1/3}}$ where $H' = \frac{1}{3} \log_2 n$. By Markov’s inequality again, the probability that $L'_1$ is non-empty, i.e., that $|L'_1| \geq 1$, is at most $(1 - p_\lambda)^{H' n^{1/3}} = O(n^{-1/6})$ by choosing $\lambda$ to be a large enough constant. The same holds for $T_3$. Let $E_2$ be the event that there is a transfer cut in both $T_1$ and $T_3$.

- **Same output.** Condition on the events $E_1$ and $E_2$, which are guaranteed to occur simultaneously with probability at least $1 - O(n^{-1/6})$. The existence of transfer cuts and the absence of in-moves imply that all leaves of $T_1$ and $T_3$ (and similarly for $\overline{T}_1$ and $\overline{T}_3$) have been transferred into the shared part of $T$ and $\overline{T}$ (and have possibly subsequently moved within the shared part). Because under our coupling the donor locations of the transfers are chosen to be the same in $T$ and $\overline{T}$, the output gene trees are then identical.

That concludes the proof. ■
References

[ADHR10] Alexandr Andoni, Constantinos Daskalakis, Avinatan Hassidim, and Sébastien Roch. Global alignment of molecular sequences via ancestral state reconstruction (extended abstract). In *ICS*, pages 358–369, 2010.

[ADHR12] Alexandr Andoni, Constantinos Daskalakis, Avinatan Hassidim, and Sebastien Roch. Global alignment of molecular sequences via ancestral state reconstruction. *Stochastic Processes and their Applications*, 122(12):3852 – 3874, 2012.

[BSL+05] E Bapteste, E Susko, J Leigh, D MacLeod, RL Charlebois, and WF Doolittle. Do orthologous gene phylogenies really support tree-thinking? *BMC Evol Biol*, 5:33, 2005.

[CGG02] M. Cryan, L. A. Goldberg, and P. W. Goldberg. Evolutionary trees can be learned in polynomial time. *SIAM J. Comput.*, 31(2):375–397, 2002. short version, Proceedings of the 39th Annual Symposium on Foundations of Computer Science (FOCS 98), pages 436-445, 1998.

[DB07] WF Doolittle and E Bapteste. Pattern pluralism and the tree of life hypothesis. *Proc Natl Acad Sci USA*, 104:2043–2049, 2007.

[DBP05] Frederic Delsuc, Henner Brinkmann, and Herve Philippe. Phylogenomics and the reconstruction of the tree of life. *Nat Rev Genet*, 6(5):361–375, 05 2005.

[DMR06] Constantinos Daskalakis, Elchanan Mossel, and Sébastien Roch. Optimal phylogenetic reconstruction. In *STOC*, pages 159–168, 2006.

[DMR11a] Constantinos Daskalakis, Elchanan Mossel, and Sébastien Roch. Evolutionary trees and the ising model on the bethe lattice: a proof of steel’s conjecture. *Probability Theory and Related Fields*, 149:149–189, 2011. 10.1007/s00440-009-0246-2.

[DMR11b] Constantinos Daskalakis, Elchanan Mossel, and Sébastien Roch. Phylogenies without branch bounds: Contracting the short, pruning the deep. *SIAM J. Discrete Math.*, 25(2):872–893, 2011.

[DR10] Constantinos Daskalakis and Sébastien Roch. Alignment-free phylogenetic reconstruction. In *RECOMB*, pages 123–137, 2010.

[DR13] Constantinos Daskalakis and Sebastien Roch. Alignment-free phylogenetic reconstruction: sample complexity via a branching process analysis. *Ann. Appl. Probab.*, 23(2):693–721, 2013.

[DR16] Constantinos Daskalakis and Sebastien Roch. Species trees from gene trees despite a high rate of lateral genetic transfer: A tight bound (extended abstract). In *Proceedings of the Twenty-Seventh Annual ACM-SIAM Symposium on Discrete Algorithms, SODA 2016*, Arlington, VA, USA, January 10-12, 2016, pages 1621–1630, 2016.

[ESSW99a] P. L. Erdős, M. A. Steel, L. A. Székely, and T. A. Warnow. A few logs suffice to build (almost) all trees (part 1). *Random Struct. Algor.*, 14(2):153–184, 1999.

[ESSW99b] P. L. Erdős, M. A. Steel, L. A. Székely, and T. A. Warnow. A few logs suffice to build (almost) all trees (part 2). *Theor. Comput. Sci.*, 221:77–118, 1999.

[Fel04] J. Felsenstein. *Inferring Phylogenies*. Sinauer, Sunderland, MA, 2004.
[FSH+80] GE Fox, E Stackebrandt, RB Hespell, J Gibson, J Maniloff, TA Dyer, RS Wolfe, WE Balch, RS Tanner, LJ Magrum, LB Zablen, R Blakemore, R Gupta, L Bonen, BJ Lewis, DA Stahl, KR Luehrsen, KN Chen, and CR Woese. The phylogeny of prokaryotes. *Science*, 209(4455):457–463, 1980.

[Gal07] Nicolas Galtier. A model of horizontal gene transfer and the bacterial phylogeny problem. *Systematic Biology*, 56(4):633–642, 2007.

[GD08] N Galtier and V Daubin. Dealing with incongruence in phylogenomic analyses. *Philos Trans R Soc Lond B Biol Sci*, 363:4023–4029, 2008.

[GWK05] F Ge, LS Wang, and J Kim. The cobweb of life revealed by genome-scale estimates of horizontal gene transfer. *PLoS Biol*, 3:e316, 2005.

[HJ98] D.L. Hartl and E.W. Jones. *Genetics: Principles and Analysis*. Life Science Series. Jones and Bartlett Publishers, 1998.

[JNST06] G. Jin, L. Nakhleh, S. Snir, and T. Tuller. Maximum likelihood of phylogenetic networks. *Bioinformatics*, 22(21):2604–11, 2006.

[JNST09] Guohua Jin, Luay Nakhleh, Sagi Snir, and Tamir Tuller. Parsimony score of phylogenetic networks: Hardness results and a linear-time heuristic. *IEEE/ACM Trans. Comput. Biology Bioinform.*, 6(3):495–505, 2009.

[KS01] Junhyong Kim and Benjamin A. Salisbury. A tree obscured by vines: Horizontal gene transfer and the median tree method of estimating species phylogeny. In *Pacific Symposium on Biocomputing*, pages 571–582, 2001.

[KZZ03] Valerie King, Li Zhang, and Yunhong Zhou. On the complexity of distance-based evolutionary tree reconstruction. In *SODA ’03: Proceedings of the fourteenth annual ACM-SIAM symposium on Discrete algorithms*, pages 444–453, Philadelphia, PA, USA, 2003. Society for Industrial and Applied Mathematics.

[Lin92] T. Lindvall. *Lectures on the Coupling Method*. Wiley, New York, 1992.

[LRvH07] Simone Linz, Achim Radtke, and Arndt von Haeseler. A likelihood framework to measure horizontal gene transfer. *Molecular Biology and Evolution*, 24(6):1312–1319, 2007.

[Mad97] Wayne P. Maddison. Gene trees in species trees. *Systematic Biology*, 46(3):523–536, 1997.

[Mos01] E. Mossel. Reconstruction on trees: beating the second eigenvalue. *Ann. Appl. Probab.*, 11(1):285–300, 2001.

[Mos03] E. Mossel. On the impossibility of reconstructing ancestral data and phylogenies. *J. Comput. Biol.*, 10(5):669–678, 2003.

[Mos04] E. Mossel. Phase transitions in phylogeny. *Trans. Amer. Math. Soc.*, 356(6):2379–2404, 2004.

[Mos07] E. Mossel. Distorted metrics on trees and phylogenetic forests. *IEEE/ACM Trans. Comput. Bio. Bioinform.*, 4(1):108–116, 2007.

[MR95] Rajeev Motwani and Prabhakar Raghavan. *Randomized algorithms*. Cambridge University Press, Cambridge, 1995.
[MR05] Elchanan Mossel and Sébastien Roch. Learning nonsingular phylogenies and hidden Markov models. In STOC ’05: Proceedings of the 37th Annual ACM Symposium on Theory of Computing, pages 366–375, New York, 2005. ACM.

[MRS11] Elchanan Mossel, Sébastien Roch, and Allan Sly. On the inference of large phylogenies with long branches: How long is too long? Bulletin of Mathematical Biology, 73:1627–1644, 2011. 10.1007/s11538-010-9584-6.

[Nak13] Luay Nakhleh. Computational approaches to species phylogeny inference and gene tree reconciliation. Trends in ecology & evolution, 28(12):10.1016/j.tree.2013.09.004, 12 2013.

[Per99] Yuval Peres. Probability on trees: an introductory climb. In Lectures on probability theory and statistics (Saint-Flour, 1997), volume 1717 of Lecture Notes in Math., pages 193–280. Springer, Berlin, 1999.

[Roc10] Sébastien Roch. Toward extracting all phylogenetic information from matrices of evolutionary distances. Science, 327(5971):1376–1379, 2010.

[RS12] Sébastien Roch and Sagi Snir. Recovering the tree-like trend of evolution despite extensive lateral genetic transfer: A probabilistic analysis. In RECOMB, pages 224–238, 2012.

[RS13] Sébastien Roch and Sagi Snir. Recovering the treelike trend of evolution despite extensive lateral genetic transfer: A probabilistic analysis. Journal of Computational Biology, 20(2):93–112, 2015/06/08 2013.

[SLHS13] Mike Steel, Simone Linz, Daniel H. Huson, and Michael J. Sanderson. Identifying a species tree subject to random lateral gene transfer. Journal of Theoretical Biology, 322(0):81 – 93, 2013.

[SS02] M. A. Steel and L. A. Székely. Inverting random functions. II. Explicit bounds for discrete maximum likelihood estimation, with applications. SIAM J. Discrete Math., 15(4):562–575 (electronic), 2002.

[SS03] C. Semple and M. Steel. Phylogenetics, volume 22 of Mathematics and its Applications series. Oxford University Press, 2003.

[SS13] Andreas Sand and Mike Steel. The standard lateral gene transfer model is statistically consistent for pectinate four-taxon trees. Journal of Theoretical Biology, 335(0):295 – 298, 2013.

[Suc05] Marc A. Suchard. Stochastic models for horizontal gene transfer. Genetics, 170(1):419–431, 2005.

[ZGC +06] Olga Zhaxybayeva, J. Peter Gogarten, Robert L. Charlebois, W. Ford Doolittle, and R. Thane Papke. Phylogenetic analyses of cyanobacterial genomes: Quantification of horizontal gene transfer events. Genome Research, 16(9):1099–1108, 2006.