Phase transition in the sample complexity of likelihood-based phylogeny inference *

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Abstract

Reconstructing evolutionary trees from molecular sequence data is a fundamental problem in computational biology. Stochastic models of sequence evolution are closely related to spin systems that have been extensively studied in statistical physics and that connection has led to important insights on the theoretical properties of phylogenetic reconstruction algorithms as well as the development of new inference methods. Here, we study maximum likelihood, a classical statistical technique which is perhaps the most widely used in phylogenetic practice because of its superior empirical accuracy.

At the theoretical level, except for its consistency, that is, the guarantee of eventual correct reconstruction as the size of the input data grows, much remains to be understood about the statistical properties of maximum likelihood in this context. In particular, the best bounds on the sample complexity or sequence-length requirement of maximum likelihood, that is, the amount of data required for correct reconstruction, are exponential in the number, n, of tips—far from known lower bounds based on information-theoretic arguments. Here we close the gap by proving a new upper bound on the sequence-length requirement of maximum likelihood that matches up to constants the known lower bound for some standard models of evolution.

More specifically, for the r-state symmetric model of sequence evolution on a binary phylogeny with bounded edge lengths, we show that the sequence-length requirement behaves logarithmically in n when the expected amount of mutation per edge is below what is known as the Kesten-Stigum threshold. In general, the sequence-length requirement is polynomial in n. Our results imply moreover that the maximum likelihood estimator can be computed efficiently on randomly generated data provided sequences are as above.

Our main technical contribution, which may be of independent interest, relates the total variation distance between the leaf state distributions of two trees to a notion of combinatorial distance between the trees. In words we show in a precise quantitative manner that the more different two evolutionary trees are, the easier it is to distinguish their output.

*Keywords: phylogenetic reconstruction, maximum likelihood, sequence-length requirement.

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1 Introduction

Background  Reconstructing evolutionary trees, or phylogenies, from biomolecular data is a fundamental problem in computational biology [SS03, Fel04, DTW05]. Roughly, in the basic form of the problem, sequences from a common gene (or other DNA region) are collected from representative individuals of contemporary species of interest. From that sequence data (which is usually aligned to account for insertions and deletions), a phylogeny depicting the shared history of the species is inferred. At a high level, the idea behind this reconstruction is simple: the closer two species are in the tree of life, the fewer mutations are likely to have accumulated since their respective ancestors diverged; and, hence, the more similarity can be expected between their sequences.

From a formal statistical point of view, one typically assumes that each site in the (aligned) data has evolved independently according to a common Markov model of substitution along the tree of life. The problem then boils down to reconstructing this generating model from i.i.d. samples at the leaves of the tree. Such models are closely related to spin systems that have been extensively studied in statistical physics [Lig85, Geo88] and that connection has led to new insights on the amount of data required for accurately reconstructing phylogenies [Ste01]. More specifically, under broad modeling assumptions, algorithmic upper bounds have been obtained on the sample complexity of the phylogenetic reconstruction problem, together with matching information-theoretic (i.e., applying to any method) lower bounds [Mos03, Mos04a, Roc10, DMR11a, MRS11, MHR13]. In particular it was established that the best achievable sample complexity undergoes a phase transition as the maximum branch length varies. That phase transition is closely related to the well-studied problem of reconstructing the root sequence of a Markov model on a tree given the leaf sequences [Mos04b], a tool which plays a key role in the above results.

The algorithmic results in [Roc10, DMR11a, BT12, MHR13] concern ad hoc methods of inference. On the other hand, little is known about the precise sample complexity of reconstruction methods used by evolutionary biologists in practice (with some exceptions [LC06]). Here we consider maximum likelihood (ML), introduced in phylogenetics in [Fel81], where one computes (or approximates) the tree most likely to have produced the data among a class of allowed models. Likelihood-based methods are perhaps the most widely used and most trusted methods in current phylogenetic practice [Sta06]. In previous theoretical work, upper bounds were derived on the sample complexity of ML that were far from the lower bound [SS02]—in some regimes, doubly exponentially far in the number of species. Here we close the gap by proving a new upper bound on the sample complexity of maximum likelihood that matches up to constants the known information-theoretic lower bound for some standard models of evolution.

Overview of main results and techniques  In order to state our main results more precisely, we briefly describe the model of evolution considered here. (See Section 2 for more details.) The unknown phylogeny $T$ is a weighted binary tree with $n$ leaves labeled by species names, one leaf for each species of interest. Without loss of generality, we assume that the leaf labels are $[n] = \{1, \ldots, n\}$. The weights on the edges (or branches), $\{w_e\}_{e \in E}$ where $E$ is the set of edges of $T$, are assumed to be discretized and bounded between two constants $f < g$. The quantity $w_e$ can be interpreted as the expected number of mutations per site along edge $e$. We denote by $\mathcal{Y}_{f,g}^{(n)}[\frac{1}{r}]$ the set of all such phylogenies, where $\frac{1}{r}$ is the discretization.

Let $\rho$ be the root of the tree, that is, the most recent common ancestor to the species at the leaves (which formally can be chosen arbitrarily as it turns out not to affect the distribution of the data). Let $\mathcal{R}$ be a state space of size $r$. A typical choice is $\mathcal{R} = \{A, G, C, T\}$ and $r = 4$, but we consider more general spaces as well. Define

$$\delta_e = \frac{1}{r} \left(1 - e^{-w_e}\right).$$

In the $r$-state symmetric model, we start at $\rho$ with a sequence of length $k$ chosen uniformly in $\mathcal{R}^k$. Moving
away from the root, each vertex \( v \) in \( T \) is assigned the sequence \( (s^i_u)_{i=1}^k \) of its parent \( u \) randomly “mutated” as follows: letting \( e \) be the edge from \( u \) to \( v \), for each \( i \), with probability \((r-1)\delta_e\) set \( s^i_v \) to a uniform state in \( R - \{s^i_u\} \) (corresponding to a substitution), or otherwise set \( s^i_v = s^i_u \). Let \((s^i_{[n]})_{i=1}^k \in (R^{[n]})^k \) be the sequences at the leaves. Those are the sequences that are observed. We let \( \mu^T_{[n]}(s^i_{[n]}) \) be the probability of observing \( s^i_{[n]} \) under \( T \).

In the phylogenetic reconstruction problem, we are given sequences \((s^i_{[n]})_{i=1}^k\), assumed to have been generated under the \( r \)-state symmetric tree model on an unknown phylogeny \( T \), and our goal is to recover \( T \) (without the root) as a leaf-labeled tree (that is, we care about the locations of the species on the tree). This problem is known to be well-defined in the sense that, under our assumptions, the phylogeny is uniquely identifiable from the distribution of the data at the leaves [Cha96]. A useful proxy to assess the “accuracy” of a reconstruction method is its sample complexity or sequence-length requirement, roughly, the smallest sequence length \( k \) (as a function of \( n \)) such that a perfect reconstruction is guaranteed with probability approaching 1 as \( n \) goes to \( +\infty \). (See Section 2 for a more precise definition.) A smaller sequence-length requirement is an indication of superior statistical performance. We denote by \( k_0(\Psi, n) \) the sequence-length requirement of method \( \Psi \).

Here we analyze the sequence-length requirement of ML which, in our context, we define as

\[
\Psi^\text{ML}_{n,k}((s^i_{[n]})_{i=1}^k) \in \arg\min_{T \in \mathcal{V}^{(n)}_{f,g}([\frac{1}{k}])} \mathcal{L}_T[(s^i_{[n]})_{i=1}^k],
\]

where \( \mathcal{L}_T[(s^i_{[n]})_{i=1}^k] = -\sum_{i=1}^k \ln \mu^T_{[n]}(s^i_{[n]}) \) is the log-likelihood (breaking ties arbitrarily). In words ML selects a phylogeny that maximizes the probability of observing the data. This method is known to be consistent, that is, the reconstructed phylogeny is guaranteed to converge on the true tree as \( k \) goes to \( +\infty \).

The previous best known bound on the sequence-length requirement of ML in this context is \( k_0(\Psi^\text{ML}, n) \leq \exp(Kn) \), for a constant \( K \), as proved in [SS02].

Our first main result is that, for any constant \( f, g, \frac{1}{k} \), the ML sequence-length requirement \( k_0(\Psi^\text{ML}, n) \) grows at most polynomially in \( n \), where the degree of the polynomial depends on \( g \). Such a bound had been previously established for other reconstruction methods, including certain types of distance-matrix methods [ESSW99a], and it was a long-standing open problem to show that a polynomial bound holds for ML as well. Interestingly, our simple proof in fact uses the result of [ESSW99a]. (The argument is detailed in Section 2.) Further, it is known that no method in general achieves a better bound (up to a constant in the degree of the polynomial) [Mos03].

On the other hand, our second—significantly more challenging—result establishes a phase transition on the sequence-length requirement of ML. We show that when the maximum branch length of the true phylogeny is constrained to lie below a given threshold, an improved sequence-length requirement is achieved, namely that

\[
k_0(\Psi^\text{ML}, n) = O(\log n), \quad \text{if } g < g^* := \ln \sqrt{2}.
\]

The same sequence-length requirement has been obtained previously for other methods [Mos04a, DMR11a, Roc10, BT12, MHR13], but as we mentioned above our result is the first that concerns an important method in practice and greatly improves previous bound for ML. It is known further that a sub-logarithmic sequence-length requirement is not possible in general for any method [Mos03]. That can be seen by the following back-of-the-envelope calculation: when \( k = \Theta(\log n) \), the total number of datasets is \( e^{\Theta(n \log n)} \), which is asymptotically of the same order as the number of phylogenies in \( \mathcal{V}^{(n)}_{f,g}([\frac{1}{k}]) \) (see, e.g., [SS03]); and, intuitively, we need at least as many datasets as we have possible phylogenies.

The question of whether the threshold in (1) is tight, however, is not completely resolved (and we do not address this issue here). The quantity \( g^* \) corresponds to what is sometimes known as the Kesten-Stigum
threshold [KS66], which is roughly speaking the threshold at which reconstructing the root state from a “weighted majority” of the leaf states becomes no better than guessing at random as the depth of the (binary) tree diverges. (See, e.g., [EKPS00, Mos04b] for some background on this problem. See also [JM04] for a different characterization of the threshold.) To understand the connection between root state reconstruction and phylogenetic reconstruction, a connection which was first articulated by Steel [Ste01], note that the depth of the phylogeny plays a key role in phylogenetic reconstruction. That is because we only have access to the sequences at the leaves of the tree. When good estimates of internal sequences are available, the phylogeny is “shallower” and reconstructing the deeper parts of the tree is significantly easier, leading to a better sequence-length requirement for some methods.

For \( r = 2 \), no root state inference method has a better threshold than weighted majority [Iof96] and the bound in (1) is known to be tight [Mos04a]. In general, the question is not settled [Mos01, Sly09, MRS11]. In the case \( r = 4 \), the most relevant in the biological context, the threshold \( g^* \) translates into a 22% substitution probability along each edge. That is a significant amount of mutation, which suggests that our result potentially applies to many real-world datasets. By comparison, the percentage sequence divergence between humans and chimpanzees is below 2% [SC05]. (Of course, many factors affect the maximum branch length of a phylogeny, including how densely sampled the species are and which genes (whose mutation rates vary widely) are used.)

In [Mos04a, DMR11a, Roc10, BT12, MHR13], in order to achieve logarithmic sequence-length requirement in the Kesten-Stigum regime, new inference methods that explicitly estimate internal sequences were devised. In ML, by contrast, the internal sequences play a more implicit role in the definition of the likelihood and our analysis of ML proceeds in a very different manner. Our main technical contribution, which may be of independent interest, is a quantitative bound on the total variation distance between the leaf state distributions of two phylogenies as a function of a notion of combinatorial distance between them. In words, the more different are the trees, the more different are the data distributions at their leaves. We prove this new bound by constructing explicit tests that distinguish between the leaf distributions. For general trees, this turns out to present serious difficulties, as sketched in Section 2. The bound on the total variation distance in turn gives a bound on the probability that ML returns an incorrect tree and allows us to perform a union bound over all such trees.

It is worth pointing out that the reconstruction methods of [Mos04a, DMR11a, Roc10, BT12, MHR13] have the advantage of running in polynomial time, while computing the ML phylogeny is in the worst-case NP-hard [Roc06, CT06]. So why care about ML? Of course, worst-case computational complexity results are not necessarily relevant in practice as real data tend to be more structured. Actually, good heuristics for ML have been developed that have achieved considerable practical success in large-scale phylogenetic analyses and are now seen as the standard approach [Sta06, SS14]. A side consequence of our results is that, on randomly generated data of sufficient sequence length, using the methods of [Mos04a, DMR11a, Roc10, BT12, MHR13] we are in fact guaranteed to recover what happens to be the ML phylogeny with high probability in polynomial time. Although this is not per se an algorithmic result in that we do not directly solve the ML problem, it does show that computing the ML phylogeny is easier than previously thought in an average sense and may help explain the success of practical heuristics.

Although the discretization assumption above may not be needed, removing it in the logarithmic regime appears to present significant technical challenges. Note that this assumption is also needed for the results of [DMR11a, Roc10, BT12, MHR13].

Further related work There exists a large literature on the sequence-length requirement of phylogenetic reconstruction methods, stemming mainly from the seminal work of Erdös et al. [ESSW99a] which were the first to highlight the key role of the depth in inferring phylogenies. Sequence-length requirement results—both upper and lower bounds—have been derived for more general models of sequence evolu-
tion [ESSW99b, Mos03, MR06, BCMR06, CTAW11], including models of insertions and deletions [ADHR10, DR13], for partial or forest reconstruction [CGG02, Mos07, DMR11b, TAW11, GMS12], and for reconstructing mixtures of phylogenies [MR12, MR13]. These results have in some cases also inspired successful practical heuristics [HNW99].

The connection between root state reconstruction and phylogenetic reconstruction has also been studied in more general models of evolution where mutation probabilities are not necessarily symmetric [Roc08, Roc10, MRS11]. A good starting point for the extensive literature on root state reconstruction is [Per99, Mos04b].

Some bounds on the total variation distance between leaf distributions that are related to our techniques were previously obtained in the special case of pairs of random trees, which are essentially at maximum combinatorial distance [SS06]. Similar ideas were also used to reconstruct certain mixtures of phylogenies in [MR12].

The sample complexity of maximum likelihood when all internal vertices are also observed was studied in [TATW11].

**Organization** The paper is organized as follows. Basic definitions are provided in Section 2. In Section 2 we also state formally our main results and give a sketch of the proof. The probabilistic aspects of the proof are sketched in Section 3. The combinatorial aspects are illustrated first in a special case in Section 4. The general case is detailed in Section 5. A few useful lemmas can be found in the appendix for ease of reference.

## 2 Definitions, Results, and Proof Sketch

In this section, we introduce formal definitions and state our main results.

### 2.1 Basic Definitions

**Phylogenies** A phylogeny is a graphical representation of the speciation history of a collection of organisms. The leaves correspond to current species (i.e., those that are still living). Each branching indicates a speciation event. Moreover we associate to each edge a positive weight. As we will see below, this weight corresponds roughly to the amount of evolutionary change on the edge. More formally, we make the following definitions. See e.g. [SS03] for more background. Fix a set of leaf labels (or species names) \( X = [n] = \{1, \ldots, n\} \).

**Definition 2.1** (Phylogeny). A weighted binary phylogenetic \( X \)-tree (or phylogeny for short) \( T = (V, E; \phi; w) \) is a tree with vertex set \( V \), edge set \( E \), leaf set \( L \) with \( |L| = n \), edge weights \( w : E \to (0, +\infty) \), and a bijective mapping \( \phi : X \to L \) (that assigns "species names" to the leaves). We assume that the degree of all internal vertices \( V - L \) is exactly 3. We let \( T_1[T] = (V, E; \phi) \) be the leaf-labelled topology of \( T \). We denote by \( T_n \) the set of all leaf-labeled trees on \( n \) leaves with internal degrees 3 and we let \( T = \{T_n\}_{n \geq 1} \).

We restrict ourselves to the following setting introduced in [DMR11a].

**Definition 2.2** (Regular phylogenies). Let \( 0 < \frac{1}{T} \leq f \leq g < +\infty \). We denote by \( Y_{f,g}[\frac{1}{T}] \) the set of phylogenies \( T = (V, E; \phi; w) \) with \( n \) leaves such that \( f \leq w_e \leq g \), \( \forall e \in E \), where moreover \( w_e \) is a multiple of \( \frac{1}{T} \). We also let \( Y_{f,g}[\frac{1}{T}] = \bigcup_{n \geq 1} Y_{f,g}[\frac{1}{T}]^{(n)} \). (We assume for simplicity that \( f \) and \( g \) are themselves multiples of \( \frac{1}{T} \).)
To illustrate our techniques, we also occasionally appeal to the special case of homogeneous phylogenies. For an integer $h \geq 0$ and $n = 2^h$, a homogeneous phylogeny is an $h$-level complete binary tree $T^{(h)} = (V^{(h)}, E^{(h)}; \phi; w)$ where the edge weight function $w$ is identically $g$ and $\phi$ may be any one-to-one labeling of the leaves.

**Substitution model** We use the following standard model of DNA sequence evolution. See e.g. [SS03] for generalizations. Fix some integer $r > 1$.

**Definition 2.3 (r-State Symmetric Model of Substitution).** Let $T = (V, E; \phi; w)$ be a phylogeny and $\mathcal{R} = \{r\}$. Let $\pi = (1/r, \ldots, 1/r)$ be the uniform distribution on $\{r\}$ and let $\delta_e = \frac{1}{r}(1 - e^{-we})$. Consider the following stochastic process. Choose an arbitrary root $\rho \in V$. Denote by $E_\downarrow$ the set $E$ directed away from the root. Pick a state for the root at random according to $\pi$. Moving away from the root toward the leaves, apply the following Markov transition matrix to each edge $e = (u, v)$ independently:

$$(M(e))_{ij} = (e_w Q)_{ij} = \begin{cases} 1 - (r - 1)\delta_e & \text{if } i = j \\ \delta_e & \text{o.w.} \end{cases}$$

where

$$Q_{ij} = \begin{cases} -\frac{1}{r} & \text{if } i = j \\ \frac{1}{r} & \text{o.w.} \end{cases}$$

(Or equivalently run a continuous-time Markov jump process with rate matrix $Q$ started at the state of $u$.) Denote the state so obtained by $s_V = (s_v)_{v \in V}$. In particular, $s_L$ is the state vector at the leaves, which we also denote by $s_X$. The joint distribution of $s_V$ is given by

$$\mu^T_V(s_V) = \pi(s_\rho) \prod_{e = (u, v) \in E_\downarrow} [M(e)]_{s_u s_v}.$$  

For $W \subseteq V$, we denote by $\mu^T_W$ the marginal of $\mu^T_V$ at $W$. We denote by $D[T]$ the probability distribution of $s_V$. (It can be shown that the choice of the root does not affect this distribution. See e.g. [Ste94].) We also let $D[T]$ denote the probability distribution of $s_X := (s_{\phi(a)})_{a \in X}$. More generally we take $k$ independent samples $(s^i_V)_{i=1}^k$ from the model above, that is, $s^i_V, \ldots, s^k_V$ are i.i.d. $D[T]$. We think of $(s^i_V)_{i=1}^k$ as the sequence at node $v \in V$. When considering many samples $(s^i_V)_{i=1}^k$, we drop the superscript to refer to a single sample $s_V$.

The case $r = 4$, known as the Jukes-Cantor (JC) model [JC69], is the most natural choice in the biological context where, typically, $\mathcal{R} = \{A, G, C, T\}$ and the model describes how DNA sequences stochastically evolve by point mutations along an evolutionary tree under the assumption that each site in the sequences evolves independently and identically. For ease of presentation, we restrict ourselves to the case $r = 2$, known as the Cavender-Farris-Neyman (CFN) model [Cav78, Far73, Ney71], but our techniques extend to a general $r$ in a straightforward manner. The CFN model is equivalent to a ferromagnetic Ising model with a free boundary (see e.g. [EKPS00]). We fix $r = 2$. We denote by $E_T, P_T$ the expectation and probability under the CFN model on a phylogeny $T$. We will also use a random cluster representation of the CFN model, which we recall in Lemma 3. It will occasionally be convenient to work on the state space $\{-1, +1\}$. Let $\nu = (1, -1)$. Given samples $(s^i_X)_{i=1}^k$, we define $\sigma_X = (\sigma^i_X)_{i=1}^k$ with $\sigma^i_a = \nu s^i_a$ for all $a, i$.

**Phylogenetic reconstruction.** In the phylogenetic tree reconstruction (PTR) problem, we are given a set of sequences $(s^i_X)_{i=1}^k$ and our goal is to recover the unknown generating tree. An important theoretical criterion in designing a PTR algorithm is the amount of data required for an accurate reconstruction. At
a minimum, a reconstruction algorithm should be consistent, that is, the output should be guaranteed to converge on the true tree as the sequence length $k$ goes to $+\infty$. Beyond consistency, the sequence-length requirement (SLR) of a PTR algorithm is the sequence length required for a guaranteed high-probability reconstruction. Formally:

**Definition 2.4 (Phylogenetic Reconstruction Problem).** A phylogenetic reconstruction algorithm is a collection of maps $\Psi = \{\Psi_{n,k}\}_{n,k \geq 1}$ from sequences $(s^n_i)_{i=1}^k \in ([\mathbb{P}]^m)^k$ to leaf-labeled trees in $\mathbb{T}_n$. Fix $\delta > 0$ (small) and let $k(n)$ be an increasing function of $n$. We say that $\Psi$ solves the phylogenetic reconstruction problem on $\mathbb{Y}_{f,g}[\frac{1}{T}]$ with sequence length $k = k(n)$ if for all $n \geq 1$, and all $T \in \mathbb{Y}_{f,g}[\frac{1}{T}]$, 

$$
\Pr\left[\Psi_{n,k(n)}\left( (s^n_i)_{i=1}^{k(n)} \right) = T \right] \geq 1 - \delta,
$$

where $(s^n_i)_{i=1}^{k(n)}$ are i.i.d. samples from $\mathcal{D}_l[T]$. We let $k_0(\Psi, n)$ be the smallest function $k(n)$ such that the above condition holds (for fixed $f, g, \frac{1}{T}, \delta$).

We call the function $k_0(\Psi, n)$ the sequence-length requirement (SLR) of $\Psi$. For simplicity we emphasize the dependence on $n$. Intuitively the larger the tree, the more data is required to reconstruct it. One can also consider the dependence of $k_0$ on other structural parameters. In the mathematical phylogenetic literature, the SLR has emerged as a key measure to compare the statistical performance of different reconstruction methods. A lower $k_0$ suggests a better statistical performance. Note that, ideally, one would like to compute the probability that a method succeeds given a certain amount of data, but that probability is a complex function of all parameters. Instead the SLR, which can be bounded analytically, is a proxy that measures how effective a method is at extracting phylogenetic signal from molecular data.

**Maximum likelihood estimation** The maximum likelihood (ML) estimator for phylogenetic reconstruction is given (in our setting) by

$$
\Psi_{n,k}^{\text{ML}}((s^i_X)_{i=1}^k) \in \arg \min_{T \in \mathbb{Y}_{f,g}[\frac{1}{T}]} \mathcal{L}_T[(s^i_X)_{i=1}^k],
$$

where $\mathcal{L}_T[(s^i_X)_{i=1}^k] = -\sum_{i=1}^k \ln \mu_T X(s^i_X)$ (breaking ties arbitrarily). In words the ML selects a phylogeny which maximizes the probability of observing the data. Computation of the likelihood on a given phylogeny can be performed efficiently, but solving the maximization problem above over tree space is computationally intractable [Roc06, CT06]. Fast heuristics have been developed and are widely used [GLDG05, Sta06]. Despite the practical importance of ML, much remains to be understood about its statistical properties. Consistency, that is, the convergence of the ML estimate $\hat{T}_k^{\text{ML}}$ on the true tree as the number of sites $k \to \infty$, has been established [Cha96]. But obtaining tight bounds on the SLR of ML has remained an outstanding open problem in mathematical phylogenetics. The best previous known bound, due to [SS02] was that under the CFN model there exists $K > 0$ such that $k_0(\Psi^{\text{ML}}, n) \leq \exp(Kn)$.

### 2.2 Main results

Our main result is the following.

**Theorem 1** (Sequence-length requirement of maximum likelihood). Let $0 < \frac{1}{f} < f < g^* := \ln \sqrt{2}$. Then the sequence-length requirement of maximum likelihood for the phylogenetic tree reconstruction problem on $\mathbb{Y}_{f,g}[\frac{1}{T}]$ is

$$
k_0(\Psi^{\text{ML}}, n) = \begin{cases}
O(\log n), & \text{if } g < g^*; \\
\text{poly}(n), & \text{if } g \geq g^*.
\end{cases}
$$
Combined with the results of [DMR11a], this bound implies that the ML estimator can be computed in polynomial time with high probability as long as \( k \geq k_0(\Psi_{\text{ML}}, n) \). Note that our definition of the ML estimator implicitly assumes that we know (or have bounds on) the parameters \( f, g, \frac{1}{T} \) as the search is restricted over the space \( \mathbb{Y}_{f,g}^{(n)} \left[ \frac{1}{T} \right] \). In practice it is not unnatural to restrict the space of possible models in this way.

2.3 Proof overview

**Known results: identifiability, consistency and the Steel-Székely bound** Before sketching the proof of Theorem 1, we first mention previously known facts about the statistical properties of ML in phylogenetics. Fix \( f, g, \frac{1}{T}, n \) and let \( \mathbb{Y} = \mathbb{Y}_{f,g}^{(n)} \left[ \frac{1}{T} \right] \). Let \( T^0 \in \mathbb{Y} \) be the generating phylogeny and denote by \( s_X = (s_X^i)_{i=1}^k \) a set of \( k \) samples from the corresponding CFN model. Recalling that \( \nu = (1, -1) \), we let \( \sigma_X = (\sigma_X^i)_{i=1}^k \) with \( \sigma_a^i = \nu_{s_a} \) for all \( a, i \). Under our assumptions, the model is known to be identifiable [Cha96], that is,

\[
T^0 \neq T^\# \implies D_l[T^0] \neq D_l[T^\#].
\]

Moreover the ML estimator is known to converge on \( T^0 \) almost surely as \( k \to \infty \) [Cha96]. That fact follows from the law of large numbers by which

\[
\frac{1}{k} \mu_{T^\#}^X (s_X) \to -E_{T^0} [\ln \mu_{X}^{T^\#} (s_X)],
\]

as \( k \to \infty \), identifiability, the positivity of the Kullback-Leibler (KL) divergence, that is,

\[
T^0 \neq T^\# \implies \text{KL}(T^0 \| T^\#) := -E_{T^0} [\ln \mu_{X}^{T^\#} (s_X)] + E_{T^0} [\ln \mu_{X}^{T^0} (s_X)] > 0,
\]

and a compactness argument [Wal49].

Steel and Székely [SS02] also derived along the same lines a quantitative upper bound on the SLR. They used Pinsker’s inequality to lower bound the KL divergence with the total variation distance. And they appealed to concentration inequalities to bound the probability that any leaf vector state frequency is away from its expectation, thereby quantifying the speed of convergence of the log-likelihood. The argument ends up depending inversely on the lowest non-zero state probability, which is exponentially small in \( n \), leading to an exponential SLR. The Steel-Székely bound does not make use of the structure of the phylogenetic problem and, in fact, is derived in a more general setting.

**A polynomial bound** In order to make use of the structure of the problem, we propose a different approach. The basic idea is to design for each incorrect tree \( T^\# \) a statistical test that excludes it from being selected by ML with high probability. We first illustrate this idea by sketching a polynomial bound on the SLR of ML. This proves the polynomial regime of Theorem 1.

In [ESSW99a], a reconstruction algorithm was provided that, for any \( g \), returns the correct phylogeny with probability \( 1 - \exp(-n^{C_2}) \) as long as \( k \geq n^{C_2} \) for a large enough \( C_2 > 0 \). We refer to this algorithm as the ESSW algorithm. Letting \( T^0 \) be the true phylogeny generating the data and \( T^\# \neq T^0 \) be in \( \mathbb{Y} \), denote by \( D_{T^\#} \) the event that the ESSW algorithm reconstructs (incorrectly) \( T^\# \) and by \( M_{T^\#} \) the event that ML prefers \( T^\# \) over \( T^0 \) (including a tie), that is, the set of \( s_X = (s_X^i)_{i=1}^k \) such that \( \mathcal{L}_{T^\#} (s_X) \leq \mathcal{L}_{T^0} (s_X) \) or equivalently

\[
\frac{\mu_{X}^{T^\#} (s_X)}{\mu_{X}^{T^0} (s_X)} \geq 1.
\]

(3)
Then, re-deriving a bound similar to (3.1) in [SS02], we observe that

\[
\Pr_T[R_{T^0}^C] \leq \Pr_T[R_{T^0}^C] + \sum_{\mathbf{s} \in [r]^{nk}} \mathbb{I}\{s' \in R_{T^0}^C\} \Pr_T[R_{T^0}^C = s']
\]

\[
\leq \Pr_T[R_{T^0}^C] + \sum_{\mathbf{s} \in [r]^{nk}} \Pr_T[R_{T^0}^C = s'] \Pr_{\mathcal{X}}[\mathbf{s}]^T \leq \Pr_T[R_{T^0}^C] + \Pr_{\mathcal{X}}[\mathbf{s}]^T
\]

\[
\leq \Pr_T[R_{T^0}^C] + \Pr_{T^0}[D_{T^0}^C] \leq 2e^{-nC_1},
\]

whenever \( k \geq n^{C_2} \), where we used (3). Recall (e.g. [SS03]) that the number of binary trees on \( n \) labeled leaves is \((2n-5)!! = e^{O(n \log n)}\). For each such tree, our discretization assumption implies that there are at most \( (g-f)k + 1 \) choices of branch lengths. Hence, provided we choose \( C_1 \) and \( C_2 \) large enough and taking a union bound over the \( e^{O(n \log n)} \) possible trees \( T^\# \neq T^0 \) in \( \mathcal{Y} \), we obtain: under our assumptions, there exists \( K > 0 \) such that \( k_0(\Psi_{\text{ML}}, n) \leq n^K \).

This bound improves significantly over the Steel-Székely bound. It has interesting computational implications as well. Although ML for phylogenetic reconstruction is NP-hard [Roc06, CT06], our polynomial SLR bound in combination with the computationally efficient ESSW algorithm indicates that the ML estimator can be computed efficiently with high probability when data is generated from a CFN model with polynomial sequence lengths.

**A refined union bound**
Dealing with logarithmic-length sequences is significantly more challenging. As the argument below suggests, certain close-by trees cannot be distinguished using logarithmic-length sequences with exponentially small failure probability. In particular the naive union bound above cannot work in this regime. Instead we use a more refined union bound.

We make two observations. We introduce \( \Delta_{\text{BL}}(T^\#, T^0) \), the blow-up distance between the topologies of \( T^\# \) and \( T^0 \), that is, roughly the smallest number of edges that need to be rearranged to produce \( T^\# \) from \( T^0 \) (see Definition 5.1 for a formal definition). The number of trees at blow-up distance \( D \) from \( T^0 \) is at most \( O(n^{2D}) \) so that it suffices to prove

\[
\Pr_{T^0}[M_{T^\#}] \leq C_1 e^{-C_2k\Delta_{\text{BL}}(T^\#, T^0)},
\]

in order to apply a union bound over blow-up distances, when \( k \) is logarithmic in \( n \). To prove (5), we need to find an appropriate test—as we did before—but now the power of this test must depend on the blow-up distance between \( T^\# \) and \( T^0 \). This is intuitively reasonable as we expect similar trees to be harder to distinguish.

A bound such as (5) may be of independent interest as it naturally relates combinatorial and variational distances between trees. Indeed note that (4) holds for any set \( D_{T^\#} \) so that it suffices to find an event \( A \subseteq [r]^{nk} \) such that

\[
\Pr_{T^0}[A^c] + \Pr_{T^\#}[A] \leq C_1 e^{-C_2k\Delta_{\text{BL}}(T^\#, T^0)},
\]

which implies

\[
\Delta_{TV}^k(T^\#, T^0) \geq \Pr_{T^0}[A] - \Pr_{T^\#}[A] \geq 1 - C_1 e^{-C_2k\Delta_{\text{BL}}(T^\#, T^0)},
\]

where \( \Delta_{TV}^k(T^\#, T^0) \) is the total variation distance between the models generated by \( T^\# \) and \( T^0 \) under \( k \) samples. We summarize this claim, the main technical contribution of the paper, as a lemma. The lemma is proved with Theorem 3.
Lemma 1 (Relating combinatorial and variational distances). For $T^#, T^0 \in \mathbb{Y}_{f,g}[\frac{1}{T}]$ with $g < g^*$,

$$\Delta^k_{TV}(T^#, T^0) \geq 1 - C_1 e^{-C_2 k \Delta_{BL}(T^#, T^0)}.$$

Phase transition: Homogeneous case

We sketch our construction of the test $A$ above in the special case of homogeneous trees. Fix $g, n = 2^h$ and let $HY = HY^{(h)}$. Let $T^0 \in HY$ be the generating phylogeny and denote by $s_X = (s^X_i)_{i=1}^k$ a set of $k$ samples from the corresponding CFN model. In the homogeneous case, it will be more convenient to work with we call the swap distance $\Delta_{SW}(T^#, T^0)$, which is defined, roughly, as the smallest number of same-level swaps of subtrees of $T^#$ in order to obtain $T^0$. (See Section 4 for a formal definition.)

Recall that a cherry is a pair of leaves with a common immediate ancestor. A result of [MR12] shows that if $T^#$ is obtained from $T^0$ by applying a uniformly random permutation of the leaf labels of $T^0$ then, with high probability, there is a positive fraction (independent of $n$) of the cherries in $T^0$ such that the corresponding leaves in $T^#$ are far (at least a large constant graph distance away) from each other. Let $C$ be such a collection of cherries. As a result, it was shown that the total pairwise correlation over $C$ as measured for instance by

$$Z^i = \frac{1}{n} \sum_{(a,b) \in C} \sigma^a_i \sigma^b_i,$$

is concentrated on two well-separated values under $T^0$ and $T^#$, and the event

$$A = \left\{ \frac{1}{k} \sum_{i=1}^k Z^i > z \right\},$$

for a well-chosen value of $z$, satisfies an exponential bound as in (6).

Returning to our context this argument suggests that, if the incorrect tree $T^#$ is far from the generating tree $T^0$ in swap distance, a powerful enough test can be constructed from the cherries of $T^0$. One of our main contributions is to show how to generalize this idea to trees at an arbitrary combinatorial distance. This is non-trivial because $T^#$ and $T^0$ may only differ by deep swap moves, in which case cherries cannot be used in distinguishing tests. Instead, we show how to find deep pairs of test nodes that are close under $T^0$, but somewhat far under $T^#$ (see Proposition 2). To build a corresponding test, we reconstruct the ancestral states at the test nodes and estimate the correlation between the reconstructed values as above (see Proposition 1). Note that the reconstruction phase transition plays a critical role in this argument.

The main challenge is to find such deep test pairs and relate their number to the swap distance. For this purpose, we design a procedure that identifies dense subtrees that are shared by $T^#$ and $T^0$, working recursively from the leaves up (see Claim 4.4) and we prove that this procedure leads to a number of tests that grows linearly in the swap distance (see Claim 4.3). A further issue is to guarantee enough independence between the tests, which we accomplish via a sparsification step (see Claim 4.5). The full argument for homogeneous trees is in Section 4.

General case

In the homogeneous case, we produce a sufficient number of deep test pairs by identifying subtrees that are matching in $T^#$ and $T^0$. As we mentioned above, that can be done recursively starting from the leaves. In the case of general trees, the lack of symmetry makes this task considerably more challenging. One significant new issue that arises is that the matching subtrees found through the same type of procedure may in fact “overlap” in $T^#$, that is, have a non-trivial intersection.

Hence, to construct a linear number of tests in blow-up distance, we proceed in two phases. We first attempt to identify matching subtrees similarly to the homogeneous case. We show that if the overlap
produced is small, then a linear number of tests (see Claim 5.4) can be constructed in a manner similar to the homogeneous case (see Proposition 4), although several new difficulties arise. See Section 5.5 for details.

On the other hand, if the overlap in $T^\#$ is too large, then the first phase will fail. In that case, we show that a sufficient number of deep test pairs can be found around the “boundary of the overlap” in $T^\#$ (see Proposition 5). That construction is detailed in Section 5.6.

3 Distinguishing between leaf distributions

In this section, we detail our main tool for distinguishing between the leaf distributions of different phylogenies. Fix $f, g < g^*, \frac{1}{T}, n$ and let $\mathcal{Y} = \mathcal{Y}^{(n)}_{f,g}[\frac{1}{T}]$. Let $T^0 \in \mathcal{Y}$ be the generating phylogeny and denote by $s_X = (s^i_X)_{i=1}^k$ a set of $k$ i.i.d. samples from the corresponding CFN model. Recalling that $\nu = (1, -1)$, we let $\sigma^i_X = (\sigma^i_X)_{k=1}^0$ with $\sigma^i_a = \nu^i$ for all $a, i$.

As outlined in Section 2.3, our strategy is to construct for each erroneous tree $T^\# \neq T^0$ a statistical test that distinguishes between the two corresponding leaf distributions. The classification error of the test ultimately depends on the combinatorial distance between $T^\#$ and $T^0$. We show in Sections 4 (for homogeneous trees) and 5 (for general trees) how to construct such tests. Here we define formally the type of tests we seek to use and derive bounds on their classification error.

At a high level, the idea is to consider pairs of subtrees that are shared between $T^\#$ and $T^0$ (see Definition 3.3) and that further have the property that the distance between their roots (that is, a distinguished vertex of each subtree) differ in $T^\#$ and $T^0$. To ensure a strong enough signal, we require that the roots are close in either $T^0$ or $T^\#$ and that the subtrees are dense enough to guarantee accurate reconstruction of ancestral states (see Definition 3.4). Another requirement is that the paths connecting the roots of each pair do not intersect the corresponding subtrees (see Definition 3.5); that property ensures that the biases of the ancestral state estimates are conditionally independent given the root states.

3.1 Definitions

We first need several definitions. Let $T = (V, E; \phi; w)$ be a phylogeny in $\mathcal{Y}$ and denote its leaf set by $L$. We will work with a special type of subtrees defined as follows.

**Definition 3.1 (Restricted subtree).** A (connected) subtree $Y$ of $T$ is restricted if there exists $V_R \subseteq V$ such that $Y$ is obtained by keeping only those edges of $T$ lying on the path between two vertices in $V_R$. We typically restrict $T$ to a subset of the leaves (in which case we denote $V_R$ by $L_R$ instead). When $|V_R| = 4$, $Y$ is called a quartet. The topology of a binary quartet on $V_R = \{u, v, x, y\}$ is characterized by the pairs in $V_R$ lying on each side of the internal edge, e.g., we write $uv | xy$ if $\{u, v\}$ and $\{x, y\}$ are on opposite sides. Let $Y$ and $Z$ be restricted subtrees of $T$. We let $Y \cap Z$ (respectively $Y \cup Z$) be the intersection (respectively the union) of the edge sets of $Y$ and $Z$.

We will need to compare restricted subtrees in $T^\#$ and $T^0$. For this purpose, we will use the following metric-based definition. We first recall the notion of a tree metric.

**Definition 3.2 (Tree metric).** A phylogeny $T = (V, E; \phi; w)$ is naturally equipped with a tree metric $d_T : X \times X \to (0, +\infty)$ defined as follows

$$ \forall a, b \in X, \quad d_T(a, b) = \sum_{e \in P_T(\phi(a), \phi(b))} w_e,$$

where $P_T(u, v)$ is the set of edges on the path between $u$ and $v$ in $T$. We will refer to $d_T(a, b)$ as the evolutionary distance between $a$ and $b$. In a slight abuse of notation, we also sometimes use $d_T(u, v)$ to
denote the evolutionary distance between any two vertices \( u, v \) of \( T \) as defined above. Tree metrics satisfy the following four-point condition: \( \forall a_1, a_2, a_3, a_4 \in X, \)

\[
d_T(a_1, a_2) + d_T(a_3, a_4) \leq \max\{d_T(a_1, a_3) + d_T(a_2, a_4), d_T(a_1, a_4) + d_T(a_3, a_2)\}. \tag{7}
\]

In the non-degenerate case, one of the three sums above is strictly smaller than the other two, which are equal. From the four-point condition, it can be shown that to each tree metric corresponds a unique phylogeny (with positive edge weights). See e.g. [SS03].

**Definition 3.3 (Matching subtrees).** Let \( T = (V, E; \phi; w) \) and \( T' = (V', E'; \phi'; w') \) be trees in \( Y \) with \( n \) leaves \( L \) and \( L' \) respectively (and the same leaf label set \( [n] \)). Let \( Y \) and \( Y' \) be subtrees of \( T \) and \( T' \) restricted respectively to leaf sets \( L_R \subseteq L \) and \( L'_R \subseteq L' \). We say that \( Y \) and \( Y' \) are metric-matching or simply matching if: the tree metrics corresponding to \( Y \) and \( Y' \) are identical. Note that, even if \( Y \) and \( Y' \) are metric-matching, their vertex and edge sets may differ. E.g., an edge in \( Y \) may correspond to a (non-trivial) path in \( Y' \), and vice versa. However, thinking of \( Y \) and \( Y' \) as continuous objects, for each vertex \( v \in Y \), we can create a corresponding extra vertex \( v' \) in \( Y' \).

As we mentioned above, we will assign a distinguished vertex to each subtree included in the tests. We think of these as roots. The following definitions apply to such rooted subtrees.

**Definition 3.4 (Dense subtree).** Let \( \ell \) and \( \varphi \leq 2^\ell \) be nonnegative integers. Let \( Y \) be a restricted subtree of \( T \) rooted at \( y \). The \( \ell \)-completion \( [Y]_\ell \) of \( Y \) is obtained by adding complete binary subtrees with \( 0 \)-length edges below the leaves of \( Y \) so that all leaves in \([Y]_\ell \) are at the same graph distance from \( y \) and the height of \([Y]_\ell \) is the smallest integer greater than the height of \( Y \). We say that \( Y \) is \((\ell, \varphi)\)-dense in \( T \) if: the number of vertices on the \((i\ell)\)-th level of \([Y]_\ell \) is at least \((2^\ell - \varphi)^i\) for all \( i \geq 0 \) such that \( i\ell \) is smaller than the height of \([Y]_\ell \).

**Definition 3.5 (Co-hanging subtrees).** Two rooted restricted subtrees \( Y \) and \( Z \) of a tree \( T \) with empty intersection are co-hanging if the path between their roots does not intersect with the edges in their union. The linkage \( Y \oplus Z \) of co-hanging rooted restricted subtrees \( Y \) and \( Z \) is the (unrooted) restricted subtree obtained by adding to \( Y \) and \( Z \) the path joining their roots.

We need one last definition.

**Definition 3.6 (Topped subtree).** Let \( T \) be rooted. Let \( \gamma \in \mathbb{N} \) and \( Y \) be a restricted subtree of \( T \) rooted at \( y \). The \( \gamma \)-topping \([Y]^\gamma \) of \( Y \) is obtained from \( Y \) by adding the \( \gamma \) edges immediately above \( y \) on the path to the root of \( T \) (or the entire path if it is has fewer than \( \gamma \) edges), which we refer to as the hat of \([Y]^\gamma \).

### 3.2 Batteries

In the proof below, we will compare the true phylogeny \( T^0 = (V^0, E^0; \phi^0; w^0) \) to an incorrect phylogeny, which will be denoted by \( T^\# = (V^\#, E^\#; \phi^\#; w^\#) \). Assume that \( T^0 \) and \( T^\# \) are rooted at \( \rho^0 \) and \( \rho^\# \) respectively. The comparison will be based on the following combinatorial definition and the associated statistical test below. A test pair in \( T^0 \) is a pair of vertices (leaf or internal; possibly extra) \((y^0, z^0)\) in \( T^0 \), which we will refer to as test roots, as well as a pair of restricted subtrees \((Y^0, Z^0)\) of \( T^0 \) rooted at \( y^0, z^0 \) respectively, which we will refer to as test subtrees. Similarly we define a test pair in \( T^\# \). We call a test panel two corresponding test pairs in \( T^0 \) and \( T^\# \). See Figure 1 for an illustration.

**Definition 3.7 (Battery of Tests).** Fix nonnegative integers \( \ell \geq 2, 0 \leq \varphi \leq 2^\ell - 1, \Gamma \geq 1 \) and \( \gamma_\ell \geq 1 \). We say that a collection of test panels

\[ \{((y_i^0, z_i^0); (Y_i^0, Z_i^0))\}_{i=1}^\Gamma \text{ in } T^0 \text{ and } \{((y_i^\#, z_i^\#); (Y_i^\#, Z_i^\#))\}_{i=1}^\Gamma \text{ in } T^\# \]

form an \((\ell, \varphi, \Gamma, \gamma_\ell, I)\)-battery if:
Figure 1: A test panel: proximal in $T^0$ and non-proximal in $T^\#$.

1. Cluster requirements

   (a) (Dense subtrees) All test subtrees are $(\ell, \wp)$-dense.

2. Pair requirements

   (a) (Matching subtrees) The subtrees $Y_i^0$ and $Y_i^\#$ are matching for all $i = 1, \ldots, I$, and similarly for $Z_i^0$ and $Z_i^\#$.

   (b) (Co-hanging) For $i = 1, \ldots, I$, we require that $Y_i^0$ and $Z_i^0$ be co-hanging. Similarly for the pairs in $T^\#$.

   (c) (Proximity) For $i = 1, \ldots, I$, if the graph distance between $y_i^0$ and $z_i^0$ is less than $\Gamma$, we say that the corresponding pair is proximal. (If $y_i^0$ or $z_i^0$ is an extra vertex we use the graph distance in $T^0$ to the closest neighbor.) Else, if the graph distance between $y_i^0$ and $z_i^0$ is less than $\gamma_t$, we say that the corresponding pair is semi-proximal. In both proximal and semi-proximal cases, we let

   \[ F_i^0 = Y_i^0 \oplus Z_i^0. \]  

   Else, if the graph distance between $y_i^0$ and $z_i^0$ is greater than $\gamma_t$, in which case we say that the corresponding pair is non-proximal, we let

   \[ F_i^0 = \lceil Y_i^0 \rceil_{\gamma_t} \cup \lceil Z_i^0 \rceil_{\gamma_t}. \]  

We refer to the path between $y_i^0$ and $z_i^0$ as the connecting path of the test pair. We similarly define $F_i^\#$'s from the pairs in $T^\#$.
(d) (Evolutionary distance) For each $i = 1, \ldots, I$, we have
\[ d_{T^0}(y^0_i, z^0_i) \neq d_{T^#}(y^#_i, z^#_i) \]
and at least one of the corresponding pairs is proximal. Further, we let
\[ \alpha_i = \begin{cases} +1, & \text{if } d_{T^0}(y^0_i, z^0_i) < d_{T^#}(y^#_i, z^#_i) \\ -1, & \text{o.w.} \end{cases} \]

3. Global requirements

(a) (Global intersection) The $F^0_i$'s have empty pairwise intersection. Similarly for the $F^#_i$'s.

Tests For a restricted subtree $Y$ rooted at $y$, we denote by $X[Y]$ the leaf labels of $Y$ and we let
\[ \hat{\sigma}_y^j = \begin{cases} 1, & \text{if } \mathbb{P}_Y[\sigma_y = +1 | \sigma^j_{X[Y]}] > \mathbb{P}_Y[\sigma_y = -1 | \sigma^j_{X[Y]}], \\ -1, & \text{o.w.} \end{cases} \]
be the MLE of the state at $y$ on site $j$, given $\sigma^j_{X[Y]}$. Let
\[ \{(y^0_i, z^0_i); (Y^0_i, Z^0_i)\}^I_{i=1} \text{ in } T^0 \text{ and } \{(y^#_i, z^#_i); (Y^#_i, Z^#_i)\}^I_{i=1} \text{ in } T^# \]
form a $(\ell, \varphi, \Gamma, \gamma, I)$-battery with corresponding $\alpha_i$s. The distinguishing statistics of the battery are defined as
\[ \hat{D}^0 = \sum_{i=1}^I \sum_{j=1}^k \alpha_i \hat{\sigma}_y^j \hat{\sigma}_y^j \quad \text{and} \quad \hat{D}^# = \sum_{i=1}^I \sum_{j=1}^k \alpha_i \hat{\sigma}_y^j \hat{\sigma}_y^j \tag{11} \]
Note that, because the subtrees in $T^0$ and $T^#$ are matching, $\hat{D}^0$ and $\hat{D}^#$ are identical as a function of the leaf states, which we denote by $\hat{D}$. However their distributions, in particular their means $D^0 = \mathbb{E}_{T^0}[\hat{D}]$ and $D^# = \mathbb{E}_{T^#}[\hat{D}]$ respectively, differ (as we quantify below). The distinguishing event is then defined as
\[ A = \left\{ \hat{D} - \frac{D^0 + D^#}{2} > 0 \right\}. \]

Properties of batteries We show that the distinguishing event $A$ is likely to occur under $T^0$, but unlikely to occur under $T^#$. The proof is in the next section.

Proposition 1 (Batteries are distinguishing). For any positive integers $\varphi$ and $\Gamma$, there exist constants $\ell = \ell(g, \varphi)$ large enough, $\gamma = \gamma(g, \varphi, \ell, \Gamma, T)$ large enough, and $C = C(g, \varphi, \ell, \Gamma, T, \gamma) > 0$ small enough such that the following holds. If $\{((y^0_i, z^0_i); (Y^0_i, Z^0_i))\}^I_{i=1}$ in $T^0$ and $\{((y^#_i, z^#_i); (Y^#_i, Z^#_i))\}^I_{i=1}$ in $T^#$ form a $(\ell, \varphi, \Gamma, \gamma, I)$-battery with corresponding $\alpha_i$s, $D$, $D^0$, $D^#$, and $A$, then
\[ \max\{\mathbb{P}_{T^0}[A^c], \mathbb{P}_{T^#}[A]\} \leq \exp(-CkI), \]
for all $I$ and $k$. 

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3.3 Proof of Proposition 1

We give a proof of Proposition 1. The proof has several steps:

1. We bound the accuracy of the ancestral state estimator (10) using Lemma 2.
2. We show that the distinguishing statistics (11) have well-separated expectations. That follows from the fact that by assumption the evolutionary distances between the roots of the corresponding subtrees differ between $T^\#$ and $T^0$. The accuracy of the ancestral state estimation also guarantees that the signal is strong enough at the leaves.
3. Finally, in the more delicate step of the argument, we establish that the distinguishing statistics (11) are concentrated around their respective means. Proving concentration is complicated by the fact that the terms in the sums (11) are not independent. That is the result of the non-proximal pairs having connecting paths that may intersect with other test subtrees. We decompose this step into two cases:

(a) When the number of non-proximal pairs is small enough, we show that their contribution is negligible.

(b) When the number of non-proximal pairs is not small, we show that the corresponding terms are “almost independent” of the other terms by bounding the probability that their hat is closed.

Proof of Proposition 1. Accuracy of ancestral reconstruction. Let $Y$ be any subtree in the battery and let $y$ be its root. To obtain a bound on the probability of erroneous ancestral reconstruction through Lemma 2, it suffices to bound the denominator in (44) for the $\ell$-completion $\lfloor Y \rfloor_\ell$. Choose a unit flow $\Psi$ such that the flow through each vertex on level $i\ell$ of $\lfloor Y \rfloor_\ell$ splits evenly among its descendant vertices on level $(i+1)\ell$. Then, letting $E(\lfloor Y \rfloor_\ell)$ denote the edges of $\lfloor Y \rfloor_\ell$ and recalling that $R_y(e) = (1 - \theta^2_e) \Theta_{y,x}^{-2}$ with $0 \leq (1 - \theta^2_e) \leq 1$,

$$
\sum_{e=(x',x)\in E(\lfloor Y \rfloor_\ell)} R_y(e) \Psi(e)^2 \leq \sum_{e=(x',x)\in E(\lfloor Y \rfloor_\ell)} \Theta_{y,x}^{-2} \Psi(e)^2
$$

$$
\leq \sum_{i=0}^{n/2\ell} \sum_{j=1}^{\ell} 2^\ell j \left( e^{-(\ell i+j)g} \right)^2
$$

$$
\times \left( \frac{1}{(2^\ell - \varphi)^i \max\{1, 2^{(\ell-i)} - \varphi\}} \right)^2
$$

$$
\leq \sum_{i=0}^{n/2\ell} 2^\ell e^{2\ell(i+1)} \left( \frac{1}{(2^\ell - \varphi)^i} \right)^2
$$

$$
\times \left[ \sum_{j=1}^{\ell} 2^j e^{2jg} \left( \frac{1}{\max\{1, 2^{(\ell-j)} - \varphi\}} \right)^2 \right],
$$

where, in the second inequality, the quantity $\max\{1, 2^{(\ell-j)} - \varphi\}$ is a lower bound on the number of descendants on level $(i+1)\ell$ of a vertex at graph distance $j$ below level $i\ell$. The term in square bracket on the last line is bounded by a positive constant $0 < K_{\ell,\varphi,g} < +\infty$ depending only on $\ell, \varphi, g$. Recall that $g < g^* = \ln \sqrt{2}$ and let $g' = \frac{g^* + g}{2}$. Choose $\ell$ large enough (depending only on $g$ and $\varphi$) such that

$$
\frac{2^\ell}{(2^\ell - \varphi)^2} \leq \frac{1}{e^{2\ell g'}},
$$
which is possible because $g' < g^*$ and $e^{2g^*} = 2$. Then

$$
\sum_{e=\langle x', x \rangle \in \mathcal{E}(\langle Y \rangle)} R_g(e) \Psi(e)^2 \leq K_{\ell, q, g} \sum_{i=0}^{+\infty} e^{2\ell_i (g-g')}
= \frac{K_{\ell, q, g}}{1 - e^{-2\ell (g'-g)}}
= \frac{K_{\ell, q, g}}{1 - e^{-\ell (g^*-g)}} < +\infty.
$$

Hence by Lemma 2 the probability of correct ancestral reconstruction is bounded away from 1/2 from below. Let $\beta_{g, \varphi}$, depending only on $g$ and $\varphi$ (and implicitly on $\ell$), such that

$$
P_Y[\hat{\sigma}_y = \sigma_y] \equiv \frac{1 + e^{-\beta_Y}}{2} \geq 1 + e^{-\beta_{g, \varphi}},
$$

where the first equality is a definition.

*Separation of expectations.* Let $\langle (y, z); (Y, Z) \rangle$ be a test pair in the battery with corresponding tree $T$ (equal to either $T^0$ or $T^\#$). Then, from (12) and the Markov property, we have in the proximal case

$$
- \ln \mathbb{E}_T[\hat{\sigma}_y \hat{\sigma}_z] = - \ln [\mathbb{E}_T[\mathbb{E}_T[\hat{\sigma}_y \hat{\sigma}_z | \sigma_y, \sigma_z]]]
= - \ln [\mathbb{E}_T[\hat{\sigma}_y | \sigma_y] \mathbb{E}_T[\hat{\sigma}_z | \sigma_z]]
= - \ln [\mathbb{E}_T[\beta_Y \sigma_y \beta_Z \sigma_z]]
= \beta_Y + \beta_Z + d_T(y, z).
$$

The last equality follows from

$$
\mathbb{E}_T[\sigma_y \sigma_z] = \mathbb{E}_T[\mathbb{E}_T[\sigma_y \sigma_z | \sigma_y]]
= \mathbb{E}_T[\sigma_y \mathbb{E}_T[\sigma_z | \sigma_y]]
= \mathbb{E}_T[\sigma_y e^{-d_T(y, z)} \sigma_y]
= e^{-d_T(y, z)} \mathbb{E}_T[\sigma_y^2]
= e^{-d_T(y, z)},
$$

because $\nu$ is an eigenvector of $e^{d_T(y, z) Q}$ with eigenvalue $e^{-d_T(y, z)}$ and $\sum_{i \in \mathcal{R}} \pi_i \nu_i^2 = 1$.

Further in the proximal case,

$$
- \ln \mathbb{E}_T[\hat{\sigma}_y \hat{\sigma}_z] = \beta_Y + \beta_Z + d_T(y, z)
\leq 2\beta_{g, \varphi} + g\Gamma
\equiv \chi_{g, \varphi, \Gamma}.
$$

Moreover, by the pair requirements of the battery,

$$
|d_T^0(y_i^0, z_i^0) - d_T^\#(y_i^\#, z_i^\#)| \geq \frac{1}{Y}.
$$

The expectation of $\tilde{D}$ under $T^0$ is

$$
\frac{D^0 - D^0 + D^\#}{2} = \frac{D^0 - D^\#}{2}
= \frac{1}{2} \sum_{i=1}^{I} \sum_{j=1}^{k} \alpha_i \left( \mathbb{E}_{T^0}[\hat{\sigma}_y^i \hat{\sigma}_z^i] - \mathbb{E}_{T^\#}[\hat{\sigma}_y^{\#} \hat{\sigma}_z^{\#}] \right).
$$

15
Under the assumptions on the battery each term in the sum, whether it corresponds to a proximal-proximal, semi-proximal-proximal, or non-proximal-proximal case, is at least
\[ D_\delta \equiv e^{-\lambda_{g,v,v}} (1 - e^{-\frac{1}{\gamma}}), \]
by (13), (14), (15), and the definition of \( \alpha_i \). Hence,
\[ D^0 - D^0 + D^\# = \frac{D^0 - D^\#}{2} \geq \frac{1}{2} D_\delta k I. \] (16)

Below we will also need the following bound in the non-proximal case. Assume that the test pair is non-proximal in \( T \) and consider the \( \gamma_t \)-toppings \( [Y]^\gamma_t \) and \( [Z]^\gamma_t \). Note that at least one of \( [Y]^\gamma_t \) and \( [Z]^\gamma_t \) has a hat of length \( \gamma_t \) as otherwise \( Y \) and \( Z \) would be connected through the root at distance at most \( 2\gamma_t \), contradicting the non-proximal assumption. We refer to the corresponding hat as the hat of the pair. If both toppings have long enough hats, choose the lowest one of the two so that the hat is necessarily part of the connecting path. The probability that all edges in this hat are open under the random cluster representation of the model, which we refer to as an open hat, is at most \( e^{-f\gamma_t} \). If at least one such edge is closed, in which case we say the hat is closed, \( \hat{\sigma}_y \) and \( \hat{\sigma}_z \) are independent. Hence, we have in the non-proximal case
\[ -\ln E_T[\hat{\sigma}_y \hat{\sigma}_z] \geq -\ln \left( (e^{-f\gamma_t})(1) + (1)(0) \right) \geq f\gamma_t. \] (17)

**Concentration.** Note that, because non-proximal connecting paths may intersect with each other or with other test subtrees, the terms in the sum \( \tilde{D} \) are not necessarily independent. Hence we cannot apply the concentration result in Lemma 4 directly to \( \tilde{D} \). Instead we argue by dealing with the non-proximal pairs with an open hat separately. A related argument is used in [MR12].

Consider \( \tilde{D} \) on \( T^0 \). (The argument is the same on \( T^\# \).) Let \( T^0_{np} \) be the set of non-proximal pairs in \( T^0 \) and let \( T^0_p \) be the set of pairs that are either semi-proximal or proximal. We also let
\[ J^0_{np} = \left\{ (i,j) : i \in I^0_{np}, j \in \{1, \ldots, k\} \right\}, \]
and
\[ J^0_p = \left\{ (i,j) : i \in I^0_p, j \in \{1, \ldots, k\} \right\}. \]
The analysis is divided into two cases depending on the size of \( T^0_{np} \). Fix \( 0 < \varepsilon < 1 \) small (to be determined below):

1. **Small \( T^0_{np} \).** We consider first the case where
\[ |T^0_{np}| < \varepsilon I. \]

We define the following sum
\[ \tilde{D} = \sum_{(i,j) \in J^0_p} \alpha_i \hat{\sigma}_y^i \hat{\sigma}_z^j - |J^0_{np}|, \]
that is, we set the terms in \( J^0_{np} \) to their worst-case value, \(-1\), which implies \( \tilde{D} \geq \tilde{D} \).

The remaining terms in the sum are independent. Indeed, for all \((i,j) \in J^0_p\), the term \( \hat{\sigma}_y^i \hat{\sigma}_z^j \) is independent of the state \( \sigma^{j}_{x_0^i} \) at the root \( x_0^i \) of \( J^0_i \) by the random cluster representation. Moreover, we claim that the set of all such roots separates the \( J^0_i \)'s in \( T^0_p \), that is, a path between any two of them
must go through one of these roots. This follows from the fact that any such path must enter one of the \( F_i \)'s from above (otherwise there would be a loop) and therefore must go through its root. This proves mutual independence.

The event
\[
A^c = \left\{ \tilde{D} - \frac{D^0 + D^#}{2} \leq 0 \right\},
\]
implies the event
\[
\tilde{D} \leq \frac{D^0 + D^#}{2},
\]
or, after rearranging,
\[
\tilde{D} - \mathbb{E}_{T^0}[\tilde{D}] \leq -\frac{D^0 - D^#}{2} + \{D^0 - \mathbb{E}_{T^0}[\tilde{D}]\},
\]
which in turn implies
\[
\tilde{D} - \mathbb{E}_{T^0}[\tilde{D}] \leq -\frac{D^0 - D^#}{2} kI + 2\varepsilon kI,
\]
where we used the fact that the \( F_i \)-terms cancel out in the expression in curly brackets in (18). Choose \( \varepsilon \) small enough so that the RHS is less than \(-\frac{D^0 - D^#}{2} kI\). Then, by Lemma 4,
\[
\mathbb{P}_{T^0}[A^c] \leq 2 \exp \left( -\frac{\left(\frac{D^0 - D^#}{2} kI\right)^2}{2(2)^2(2)(kI)} \right)
= \exp (-\Omega(kI)).
\] (19)

2. **Large \( T_{np}^0 \)**. Consider now the case where
\[
|T_{np}^0| \geq \varepsilon I.
\]
Let \([J_{np}^0]_c\) be the random set corresponding to those pairs in \( J_{np}^0 \) with a closed hat. By the argument above (17),
\[
\mathbb{E}_{T^0}[|[J_{np}^0]_c|] \geq (1 - e^{-f\gamma t})|J_{np}^0|.
\] (20)

Hence, by Lemma 4, letting \( 0 < \varepsilon' < 1 - e^{-f\gamma t} \) (determined below)
\[
\mathbb{P}_{T^0} \left[ |[J_{np}^0]_c| < \mathbb{E}_{T^0}[|[J_{np}^0]_c|] - \varepsilon'|J_{np}^0| \right] \leq 2 \exp \left( -\frac{\left(\frac{\varepsilon'|J_{np}^0|}{2} \right)^2}{2(1)^2|J_{np}^0|} \right)
= \exp (-\Omega(\varepsilon'^2 |J_{np}^0|))
= \exp (-\Omega(\varepsilon'^2 \varepsilon kI)).
\]

We condition on the event
\[
C = \{ |[J_{np}^0]_c| \geq \mathbb{E}_{T^0}[|[J_{np}^0]_c|] - \varepsilon'|J_{np}^0| \}.
\]

Let \([J_{np}^0]_o\) be the random set corresponding to those pairs in \( J_{np}^0 \) with an open hat. We consider the following sum
\[
\tilde{D} = \sum_{(i,j) \in J_{np}^0 \cup [J_{np}^0]_c} \alpha_i \sigma_j^i \hat{\sigma}_j^i - |[J_{np}^0]_o|,
\]
that is, we set the terms with open hats to their worst-case value \(-1\) which implies \(\hat{D} \geq \tilde{D}\).

The remaining terms in the sum are conditionally independent given \([\mathcal{J}_{np}^0]_c\). Note in particular that conditioning on \(C\) does not affect ancestral reconstruction on the latter terms because non-proximal hats do not intersect with test subtrees. Then independence follows from an argument similar to that in the previous paragraph. Considering only the proximal and semi-proximal test subtrees and their connecting paths as well as the non-proximal test subtrees whose hat is closed, we claim that the roots of the former and the hats of the latter form a separating set in the sense that any path between two of these subtrees must go through one of the roots or an entire hat. Indeed, a path between any two of these test subtrees must enter one of them from above. Moreover if one of the two subtrees is non-proximal but the path does not visit its entire hat, then the other test subtree must also be entered from above (as the path must deviate downwards from the hat) and its entire hat be visited if non-proximal (otherwise the two hats would intersect). This proves mutual independence.

Given \(C\), the event

\[
A^c = \left\{ \hat{D} - \frac{D^0 + D^#}{2} \leq 0 \right\},
\]

implies the event

\[
\tilde{D} \leq \frac{D^0 + D^#}{2},
\]

or, after rearranging,

\[
\hat{D} - \mathbb{E}_{T^0}[\hat{D} | [\mathcal{J}_{np}^0]_c, C] \leq -\frac{D^0 - D^#}{2} + \{D^0 - \mathbb{E}_{T^0}[\hat{D} | [\mathcal{J}_{np}^0]_c, C]\}. \tag{21}
\]

From \(C\) and (20),

\[
|[\mathcal{J}_{np}^0]_c| = |\mathcal{J}_{np}^0| - |[\mathcal{J}_{np}^0]_c|
\]

\[
\leq |\mathcal{J}_{np}^0| - \mathbb{E}_{T^0}[|[\mathcal{J}_{np}^0]_c|] + \varepsilon' |\mathcal{J}_{np}^0|
\]

\[
\leq (e^{-f \gamma t} + \varepsilon') |\mathcal{J}_{np}^0|
\]

\[
\leq (e^{-f \gamma t} + \varepsilon') kI.
\]

From (16), that implies

\[
\hat{D} - \mathbb{E}_{T^0}[\hat{D} | [\mathcal{J}_{np}^0]_c, C] \leq -\frac{D^0}{2} kI + (e^{-f \gamma t} + \varepsilon') kI,
\]

where we used that, in (21), the \(\mathcal{J}_{np}^0\)-terms cancel out in the expression in curly brackets, the \(\mathcal{J}_{np}^0\)-terms in \(D^0\) are negative and the \([\mathcal{J}_{np}^0]_c\)-terms in the expectation are 0 by independence. Choose \(\varepsilon'\) small enough and \(\gamma_t\) large enough so that the RHS is less than \(-\frac{D^0}{3} kI\). Then, by Lemma 4,

\[
\mathbb{P}_{T^0}[A^c] = \mathbb{P}_{T^0}[A^c | C] \mathbb{P}_{T^0}[C] + \mathbb{P}_{T^0}[A^c | C^c] \mathbb{P}_{T^0}[C^c]
\]

\[
\leq \mathbb{E}_{T^0}[\mathbb{P}_{T^0}[A^c | [\mathcal{J}_{np}^0]_c, C] | C] + \mathbb{P}_{T^0}[C^c]
\]

\[
\leq 2 \exp \left( -\frac{D^0}{3} kI \right) + \exp \left( -\Omega((\varepsilon')^2 kI) \right)
\]

\[
= \exp \left( -\Omega(kI) \right). \tag{22}
\]

The result follows from (22) and (19), and a similar argument for \(T^#\).
4 Homogeneous trees

We first detail our techniques for constructing batteries of tests on a special case, homogeneous trees. Formally:

**Definition 4.1** (Homogeneous phylogenies). For an integer \( h \geq 0 \) and \( n = 2^h \), we denote by \( \mathbb{H}Y_g^{(h)} \) the subset of \( \mathbb{H}Y_g \) comprised of all \( h \)-level complete binary trees \( T_{\phi,w}^{(h)} = (V^{(h)}, E^{(h)}; \phi; w) \) where the edge weight function \( w \) is identically \( g \) and \( \phi \) may be any one-to-one labeling of the leaves. We denote by \( \rho^{(h)} \) the natural root of \( T_{\phi,w}^{(h)} \). For \( 0 \leq h' \leq h \), we let \( L_{h'} \) be the vertices on level \( h - h' \) (from the root). In particular, \( L_0 = L^{(h)} \) denotes the leaves of the tree and \( L_{h'}^{(h)} = \{ \rho^{(h)} \} \) denotes the root.

Fix \( g, n = 2^h \) and let \( \mathbb{H}Y = \mathbb{H}Y_g^{(h)} \) be the set of homogeneous phylogenies on \( h \) levels with branch lengths \( g \). Let \( T^0 \in \mathbb{H}Y \) be the generating phylogeny and denote by \( s_X = (s_X^i)_{i=1}^k \) a set of \( k \) i.i.d. samples from the corresponding CFN model. We first need an appropriate notion of distance between homogeneous trees.

Note that standard tree operations, such as subtree-prune-regraft or nearest-neighbor interchange [SS03], may not result in homogeneous trees. It will be more convenient to work with the following definition. We say that two homogeneous trees \( T \) and \( T' \) are equivalent, denoted by \( T \sim T' \), if \( \forall a, b \in [n], d_T(a, b) = d_{T'}(a, b) \), that is, if they agree as tree metrics.

**Definition 4.2** (Swap distance). We call a swap the operation of choosing two (non-sibling) vertices \( u \) and \( v \) on the same level of a homogeneous tree and exchanging the subtrees rooted at \( u \) and \( v \). The swap distance \( \Delta_{SW}(T, T') \) between \( T \) and \( T' \) in \( \mathbb{H}Y \) is the smallest number of swaps needed to transform \( T \) into \( T' \) (up to \( \sim \)). Because a swap operation is invertible, we have \( \Delta_{SW}(T', T) = \Delta_{SW}(T, T') \). By simply re-ordering the leaves, it holds that \( \Delta_{SW}(T, T') \leq n - 1 \).

We need a bound on the size of the neighborhood around a tree. Since for each swap operation, we choose one of \( 2n - 2 \) vertices, then choose one of at most \( n - 2 \) non-sibling vertices on the same level, we have:

**Claim 4.1** (Neighborhood size: Swap distance). Let \( T \) be a phylogeny in \( \mathbb{H}Y \). The number of phylogenies at swap distance \( \Delta \) of \( T \) is at most \( (2n^2)^\Delta \).

In the following subsections, we prove the existence of a sufficiently large battery of distinguishing tests.

**Proposition 2** (Existence of batteries). Let \( \varphi = 1, \ell = \ell(g, \varphi) \) as in Proposition 1, \( \Gamma = 2\ell \), and \( \gamma_t \geq \Gamma \) and \( C \) as in Proposition 1. For all \( T^0 \neq T^0 \in \mathbb{H}Y \), there exists a \((\ell, \varphi, \Gamma, \gamma_t, I)\)-battery

\[
\{((y_i^0, z_i^0); (Y_i^0, Z_i^0))\}_{i=1}^I \text{ (in } T^0) \text{ and } \{((y_i^#, z_i^#); (Y_i^#, Z_i^#))\}_{i=1}^I \text{ (in } T^#)\),
\]

with

\[
I \geq \frac{\Delta_{SW}(T^0, T^#)}{C_S(1 + 2^2\gamma_t + 2)},
\]

where \( C_S \) is a constant (defined in Claim 4.3 below).

The formal proof of this proposition can be found in Section 4.3.

From Propositions 1 and 2 and Claim 4.1, we obtain our main theorem in this special case.

**Theorem 2** (Sequence-length requirement of ML: Homogeneous trees). For all \( \delta > 0 \), there exists \( \kappa > 0 \) depending on \( \delta \) and \( g \) such that the following holds. For all \( h \geq 2, n = 2^h \) and generating phylogeny \( T^0 \in \mathbb{H}Y_g \), if \( s_X = (s_X^i)_{i=1}^k \) is a set of \( k = \kappa \log n \) i.i.d. samples from the corresponding CFN model, then the probability that MLE fails to return \( T^0 \) is at most \( \delta \).
Proof of Theorem 2. For $T^* \neq T^0$ in $\mathbb{H}^{(h)}_g$, let $M_{T^*}$ be the event that the MLE prefers $T^*$ over $T^0$ (including a tie), that is, the set of $s_X = (s_{X_i})_{i=1}^k$ such that $\mathcal{L}_{T^*}(s_X) \leq \mathcal{L}_{T^0}(s_X)$ or equivalently

$$\frac{\mu_{X}^T(s_X)}{\mu_{X}^{T_0}(s_X)} \geq 1. \quad (23)$$

Combining Propositions 1 and 2, for all $T^* \neq T^0 \in \mathbb{H}^{(h)}_g$, there exists an event $A_{T^*}$ such that

$$\max\{\mathbb{P}_{T^0}[A_{T^*}] , \mathbb{P}_{T^0}[A_{T^*}^c] \} \leq e^{-C_1 k \Delta_{SW}(T^0, T^*)}, \quad (24)$$

where $C_1$ depends only on $g$. Then

$$\mathbb{P}_{T^0}[\exists T^* \neq T^0, M_{T^*}] \leq \sum_{T^* \neq T^0} \mathbb{P}_{T^0}[M_{T^*}] \leq \sum_{T^* \neq T^0} [\mathbb{P}_{T^0}[A_{T^*}] + \mathbb{P}_{T^0}[A_{T^*}^c, M_{T^*}]]. \quad (25)$$

For each $T^* \neq T^0$, by (24),

$$\mathbb{P}_{T^0}[A_{T^*}] \leq e^{-C_1 k \Delta_{SW}(T^0, T^*)},$$

and, by (23),

$$\mathbb{P}_{T^0}[A_{T^*}^c, M_{T^*}] \leq \sum_{s' \in \mathbb{R}^{nk}} 1\{s' \in M_{T^*}\} 1\{s' \in A_{T^*}^c\} \mu_{X}^{T_0}(s') \leq \sum_{s' \in \mathbb{R}^{nk}} \frac{\mu_{X}^{T}(s')}{\mu_{X}^{T_0}(s')} 1\{s' \in A_{T^*}^c\} \mu_{X}^{T_0}(s') \leq \mathbb{P}_{T^0}[A_{T^*}^c] \leq e^{-C_1 k \Delta_{SW}(T^0, T^*)}.$$

By Claim 4.1, plugging back into (25),

$$\mathbb{P}_{T^0}[\exists T^* \neq T^0, M_{T^*}] \leq \sum_{T^* \neq T^0} [\mathbb{P}_{T^0}[A_{T^*}] + \mathbb{P}_{T^0}[A_{T^*}^c, M_{T^*}]] \leq \sum_{\Delta=1}^{n-2} (2n^2)^\Delta [2e^{-C_1 k \Delta}] \leq \sum_{\Delta=1}^{\infty} \frac{e^{-(C_1 \kappa \log n - 2 \log n - \log 2) \Delta}}{1 - e^{-(C_1 \kappa \log n - 2 \log n - \log 2)}} \leq \frac{1}{e^{(C_1 \kappa - 2) \log n - \log 2} - 1} \leq \delta,$$

for $\kappa$ large enough, depending only on $g$ and $\delta$, for all $n \geq 2$. \qed
4.1 Finding matching subtrees

We now describe a procedure to construct a battery of distinguishing tests on homogeneous trees. To be clear, the procedure is not carried out on data. It takes as input the true (unknown) generating phylogeny $T^0$ and an alternative tree $T^\# \neq T^0$. It merely serves to prove the existence of a distinguishing statistic that, in turn, implies a bound on the failure probability of maximum likelihood as detailed in the proof of Theorem 2. In essence, the procedure attempts to build maximal matching subtrees between $T^0$ and $T^\#$ and pair them up appropriately to construct distinguishing tests.

Definition 4.3 ($\ell$-vertices). For a fixed positive integer $\ell$, we call $\ell$-vertices those vertices in $T^0$ whose graph distance from the root is a multiple of $\ell$. The sets of all $\ell$-vertices at the same distance from the root are called $\ell$-levels. For an $\ell$-vertex $x$, its descendant $\ell$-vertices on the next $\ell$-level (that is, farther from the root) are called the $\ell$-children of $x$, which we also refer to as a family of $\ell$-siblings.

Let $\varphi = 1$ and $\ell = \ell(g, \varphi)$ be as in Proposition 1. Assume for simplicity that the total number of levels $h$ in $T^0$ is a multiple of $\ell$. Extending the analysis to general $h$ is straightforward.

Procedure Our goal is to color each $\ell$-vertex $x$ with the following interpretation:

- Green $G$: indicating a matching subtree rooted at $x$ that can be used to reconstruct ancestral states reliably on both $T^0$ and $T^\#$ using the same function of the leaf states.
- Red $R$: indicating the presence among the $\ell$-children of $x$ of a pair of matching subtrees that can be used in a distinguishing test as their pairwise distance differs in $T^0$ and $T^\#$.
- Yellow $Y$: none of the above.

We call $G$-vertices (respectively $G$-children) those $\ell$-vertices (respectively $\ell$-children) that are colored $G$, and similarly for the other colors. Before describing the coloring procedure in details, we need a definition.

Definition 4.4 ($G$-cluster). Let $x$ be a $G$-vertex. Assume that each $\ell$-vertex below $x$ in $T^0$ has been colored $G$, $R$, or $Y$ and that the leaves have been colored $G$. The $G$-cluster rooted at $x$ is the restricted subtree of $T^0$ containing all vertices and edges (not necessarily $\ell$-vertices) lying on at least one path between $x$ and a leaf below $x$ that traverses only $\ell$-vertices colored $G$.

We now describe the coloring procedure. Below, when counting the $\ell$-children of an $\ell$-vertex $x$ with a specified property, each leaf among the $\ell$-children of $x$ counts as $2^{\ell-d}$ vertices if $d$ is the graph distance between $x$ and that leaf.

1. Initialization
   (a) All leaves of $T^0$ are colored $G$.

2. For each $\ell$-vertex $x$ in the $\ell$-level furthest from the root that has yet to be colored, do:
   (a) Vertex $x$ is colored $G$ if:
      - at most one of its $\ell$-children is non-$G$ and:
      - the resulting $G$-cluster rooted at $x$ and the corresponding restricted subtree in $T^\#$, that is, the subtree of $T^\#$ restricted to the same leaf set, are matching.
   (b) Else, vertex $x$ is colored $R$ if:
• at most one of its \( \ell \)-children is non-\( G \);
• but, if \( x \) were colored \( G \), the resulting \( G \)-cluster rooted at \( x \) and the corresponding restricted subtree in \( T^\# \) would not be matching.

(c) Else, vertex \( x \) is colored \( Y \). In particular, at least two \( \ell \)-children of \( x \) are non-\( G \).

As explained above, we are interested in \( R \)-vertices, from which tests can be constructed. We prove that the number of \( R \)-vertices scales linearly in the swap distance. More precisely, we show that

\[
\#R \geq 2^{-\ell - 2} \Delta_{SW}(T^0, T^\#).
\]

**Relating combinatorial distance and the number of matching subtrees** We relate the swap distance between \( T^0 \) and \( T^\# \) to the number of \( R \)-vertices in the procedure above. Let \( \#G \) be the number of \( G \)-vertices in \( T^0 \) in the construction, and similarly for the other colors. For an \( \ell \)-vertex \( x \) in \( T^0 \), we let \( T^0_x \) be the subtree of \( T^0 \) rooted at \( x \) and we let \( V_\ell(T^0_x) \) be the set of \( \ell \)-vertices in \( T^0_x \). We denote by \( d^G_{T^0} \) the graph distance on \( T^0 \). We first bound the number of \( Y \)-vertices.

**Claim 4.2** (Bounding the number of yellow vertices). We have

\[
\#Y \leq \#R.
\]

**Proof.** From our construction, each \( Y \)-vertex in \( T^0 \) has at least two non-\( G \)-children. Hence, intuitively, one can think of the \( Y \)-vertices as forming the internal vertices of a forest of multifurcating trees whose leaves are \( R \)-vertices. The inequality follows.

Formally, if \( x \) is a \( Y \)-vertex, from the observation above we have

\[
\sum_{y \in V_\ell(T^0_x)} 2^{-d^G_{T^0}(x,y)/\ell} \mathbb{1}\{y \text{ is a } R\text{-vertex}\} \geq 1,
\]

by induction on the \( \ell \)-levels starting with the level farthest away from the root. Similarly if \( y \) is an \( R \)-vertex, we have

\[
\sum_{x \in V_\ell(T^0_y)} 2^{-d^G_{T^0}(x,y)/\ell} \mathbb{1}\{x \text{ is a } Y\text{-vertex}\} < 1,
\]

where the inequality follows from the fact that the sum is over a path from \( x \) to the root of \( T^0 \). Summing (26) over \( Y \)-vertices \( x \) and (27) over \( R \)-vertices \( y \) gives the same quantity on the LHS, so that the RHS gives the inequality.

We can now relate the swap distance to the output of the procedure.

**Claim 4.3** (Relating swaps and \( \#R \)). We have

\[
\Delta_{SW}(T^0, T^\#) \leq C_S \#R,
\]

where \( C_S = 2^{\ell + 2} \).

**Proof.** Pick a lowest non-\( G \)-vertex \( u \) in \( T^0 \). Being lowest, all \( \ell \)-children of \( u \) must be colored \( G \). In fact, all \( \ell \)-vertices on the level below \( u \) must be colored \( G \). Make \( u \) a \( G \)-vertex by transforming the subtree below \( u \) in \( T^\# \) to match the corresponding subtree in \( T^0 \). This takes at most \( 2^{\ell + 1} \) swaps.

Repeat until \( T^0 \) and \( T^\# \) match. The inequality then follows from Claim 4.2.
4.2 Constructing a battery of tests

We now construct a battery of tests from the $R$-vertices. The basic idea is that each $R$-vertex has two $G$-children which satisfy many of the requirements of a battery and therefore can potentially be used as a test pair. In particular, they are the roots of dense subtrees that are matching with their corresponding restricted subtrees in $T^\#$ and their evolutionary distance differs in $T^0$ and $T^\#$. Note that we also have a number of $R$-vertices that scales linearly in the swap distance by Claim 4.3. However one issue to address is the global requirement of the battery. In words, we need to ensure that the test pairs do not intersect. We achieve this by sparsifying the battery. A similar argument was employed in [MR12].

In this section, $T^0$ and $T^\#$ are fixed. To simplify notation, we let $\Delta = \Delta_{SW}(T^0, T^\#)$. Fix $\phi = 1$. Choose $\ell = \ell(g, \phi)$ as in Proposition 1. Then take $\Gamma = 2\ell$, and set $\gamma_t \geq \Gamma$ and $C$ as in Proposition 1. In the rest of this subsection, we build a $(\ell, \phi, \Gamma, \gamma_t, I)$-battery

$$\{(\ell, \phi, \Gamma, \gamma_t, I)\}-battery$$

with corresponding $\alpha_i$s. We number the $R$-vertices $i = 1, \ldots, I'$ and we build one test panel for each $R$-vertex. Here $I' \geq I$ as we will later need to reject some of the test panels to avoid unwanted correlations.

**Co-hanging pairs in $T^\#$.** We first construct test panels that satisfy the pair and cluster requirements of the battery. Let $x^0_i$ be an $R$-vertex in $T^0$ and let $x^\#_i$ be the corresponding vertex in $T^\#$. Because $x^0_i$ is colored $R$, by construction it has at least $2^\ell - 1$ $G$-children, but its $G$-children are connected in different ways in $T^\#$. In particular, at least one pair of $G$-children $(y^0_i, z^0_i)$ must be at a different evolutionary distance in $T^0$ than the corresponding pair $(y^\#_i, z^\#_i)$ in $T^\#$. We use these pairs as our test panel.

**Claim 4.4 (Test panels).** For each $R$-vertex $x^0_i$ we can find a test pair of $G$-children $(y^0_i, z^0_i)$ of $x^0_i$, with corresponding test pair $(y^\#_i, z^\#_i)$ in $T^\#$, such that the test panel satisfy the cluster and pair requirements of a battery.

**Proof.** By construction, the test subtrees, that is, the $G$-clusters rooted at the test vertices, are $(\ell, 1)$-dense. The test subtrees are also matching, co-hanging and their roots are at different evolutionary distances in $T^0$ and $T^\#$. Finally, the test pair in $T^0$ is proximal as

$$d_{T^0}(y^0_i, z^0_i) \leq 2\ell \leq \Gamma.$$ 

\[\Box\]

**Sparsification in $T^\#$.** It remains to satisfy the global requirements of the battery. Note that by construction the test subtrees are non-intersecting in both $T^0$ and $T^\#$. However we must also ensure that proximal/semi-proximal connecting paths and non-proximal hats do not intersect with each other or with test subtrees from other test panels. By construction, this is automatically satisfied in $T^0$ where all test pairs are proximal. To satisfy this requirement in $T^\#$, we make the collection of test pairs sparser by rejecting a fraction of them.

**Claim 4.5 (Sparsification in $T^\#$).** Let $\mathcal{H}' = \{(y^0_i, z^0_i); (y^\#_i, z^\#_i)\}_{i=1}^{I'}$ be the test panels constructed in Claim 4.4. We can find a subset $\mathcal{H} \subseteq \mathcal{H}'$ of size

$$|\mathcal{H}| = I \geq \frac{1}{1 + 2^{2\gamma_t + 2}I'} \geq \frac{\Delta}{C_S(1 + 2^{2\gamma_t + 2})}$$

such that the test panels in $\mathcal{H}$ satisfy all global requirements of a battery.
Proof. We sparsify the set $H'$ of test pairs as follows. Let $\{(Y^0_i, Z^0_i); (Y^#_i, Z^#_i)\}_{i=1}^I'$ be the test subtrees corresponding to $H'$. Start with test panel $((y^0_1, z^0_1); (y^#_1, z^#_1))$. Remove from $H'$ all test panels $i \neq 1$ such that

$$\min\{d^g_{T^#}(v, w) : v \in \{y^#_1, z^#_1\}, w \in V(Y^#_i) \cup \mathcal{V}(Z^#_i)\} \leq 2\gamma_t.$$  \hfill (28)

Because there are at most $2 \cdot 2^{2\gamma_t+1}$ vertices in $T^#$ satisfying the above condition and that the test subtrees are non-overlapping in $T^#$, we remove at most $2^{2\gamma_t+2}$ test panels from $H'$.

Let $i$ be the smallest index remaining in $H'$. Proceed as above and then repeat until all indices in $H'$ have been selected or rejected.

At the end of the procedure, there are at least

$$\frac{1}{1 + 2^{2\gamma_t+2}} I'$$

test panels remaining, the set of which we denote by $H$. Recalling that $\gamma_t \geq \Gamma$, note that, in $H$, the connecting paths of proximal/semi-proximal pairs and the hats of non-proximal pairs cannot intersect with each other or with any of the test subtree rooted at test vertices in $H$ by (39).

4.3 Proof of Proposition 2

It remains to prove Proposition 2. Recall that $\varphi = 1$, $\ell = \ell(g, \varphi)$ is chosen as in Proposition 1, $\Gamma = 2\ell$, and $\gamma_t \geq \Gamma$ and $C$ are also chosen as in Proposition 1.

By Claim 4.3, the number of $R$-vertices is at least $\frac{1}{C_S} \Delta_{SW}(T^0, T^#)$. By Claim 4.4, for each $R$-vertex, we can construct a test panel satisfying the pair and cluster requirements of the battery. By Claim 4.5, we can further choose a fraction $\frac{1}{1 + 2^{2\gamma_t+2}}$ of these test panels that also satisfy the global requirement of the battery. To sum up, we have built a $(\ell, \varphi, \Gamma, \gamma_t, I)$-battery

$$\{((Y^0_i, Z^0_i); (Y^#_i, Z^#_i))\}_{i=1}^I \text{ (in } T^0) \text{ and } \{(y^#_i, z^#_i); (Y^#_i, Z^#_i)\}_{i=1}^I \text{ (in } T^#)$$

with

$$I \geq \frac{\Delta}{C_S(1 + 2^{2\gamma_t+2})}.$$ 

That concludes the proof of Proposition 2.

5 General trees

We now prove our main result in the case of general trees. Once again, we use the tests introduced in Section 3. We also use a procedure similar to that in the homogeneous case to construct dense subtrees shared by $T^#$ and $T^0$. However, as described in the next subsections, a number of new issues arise, mainly the possibility of overlapping subtrees and non-co-hanging pairs. Fix $f, g < g^*, \frac{1}{T}$ and let $\Upsilon = \Upsilon_f^{(n)}[\frac{1}{T}].$

5.1 Blow-up distance

We first need an appropriate notion of distance between general trees. Although standard definitions exist [SS03], the following definition (related to tree bisection and reconnection [AS01]) will be particularly convenient for our purposes.
Definition 5.1 (Blow-up distance). A B-blowup operation consists of removing a subset of B edges from a phylogeny (as well as the non-leaf, isolated, adjacent vertices) and forming a new phylogeny by adding B new (weighted) edges to the resulting subtrees. The new edges must be adjacent to existing vertices in the resulting subtrees or adjacent to vertices of other new edges. The blowup distance $\Delta_{BL}(T, T')$ between phylogenies $T$ and $T'$ is defined as the smallest $B$ such that there is a B-blowup operation transforming $T$ into $T'$ (with the same edge weights). Because the blowup operation is invertible, we have $\Delta_{BL}(T, T') = \Delta_{BL}(T', T)$.

We will need a bound on the size of the neighborhood around a tree.

Claim 5.1 (Neighborhood size: Blowup distance). Let $T$ be a phylogeny in $\mathcal{Y}$. The number of phylogenies at blowup distance $\Delta$ of $T$ is at most $(12g\Upsilon n^2)^\Delta$.

Proof. There are $2n - 3$ edges in $T$ so there are at most $(2n - 3)^\Delta$ choices for the first half of the transformation. At this point there are at most $2\Delta$ vertices where new edges can be attached. Vertices of degree 1 can take 2 new edges, those of degree 2 can take 1. Counting such vertices with multiplicity, adding a new edge can increase by at most 1 the number of choices where edges can be attached. Indeed the multiplicity of at least one vertex is decreased by 1 and a new vertex of multiplicity at most 2 may be created. So there are at most $(3\Delta g\Upsilon)^\Delta$ choices for the second half of the transformation, including the choice of edge weights. Since clearly the blowup distance is $\leq 2n - 3$, there are at most

$$(2n - 3)^\Delta (3\Delta g\Upsilon)^\Delta \leq (3g\Upsilon(2n - 3)^2)^\Delta \leq (12g\Upsilon n^2)^\Delta,$$

choices. $\square$

5.2 Main steps of the proof

In the following subsections, we prove the existence of a sufficiently large battery of distinguishing tests.

Proposition 3 (Existence of batteries). Let $\varphi = 5$, $\ell = \ell(g, \varphi)$ as in Proposition 1,

$$\Gamma = \max \left\{ (6 + 4\Upsilon g)\ell, 6g\Upsilon \log_2 \left( \frac{4g\Upsilon}{1 - 1/\sqrt{2}} \right) + 2\ell g\Upsilon + 4 \right\},$$

and $\gamma_t \geq \Gamma$, a multiple of $\ell$, and $C$ as in Proposition 1. For all $T^\# \neq T^0 \in \mathcal{Y}$, there exists a $(\ell, \varphi, \Gamma, \gamma_t, I)$-battery

$$\{(y_i^0, z_i^0); (Y_i^0, Z_i^0))\}_{i=1}^I \text{ (in } T^0) \text{ and } \{(y_i^#, z_i^#); (Y_i^#, Z_i^#))\}_{i=1}^I \text{ (in } T^#),$$

with

$$I \geq \frac{\Delta_{BL}(T^0, T^#)}{20C_O(1 + 2^{6\gamma_t + C_w + 2})},$$

where

$$C_w = 3g\Upsilon \log_2 \left( \frac{4g\Upsilon}{1 - 1/\sqrt{2}} \right) + 2\ell g + 2,$$

and $C_O$ is a constant (defined in Claim 5.4 below).

Proof. This follows from Propositions 4 and 5 below. $\square$

From Propositions 1 and 3 we obtain of our main bound in the general case.
This proves Lemma 1 in Section 2. By Claim 5.1, plugging back into (31),
\[
\Pr[T^\# \neq T^0, M_{T^\#}] \leq \sum_{T^\# \neq T^0} \Pr[T^0, M_{T^\#}] \\
\leq \sum_{T^\# \neq T^0} [\Pr[T^0, M_{T^\#}] + \Pr[T^0, A_{T^\#}^c, M_{T^\#}]].
\]
For each $T^\# \neq T^0$, by (30),
\[
\Pr[T^0, A_{T^\#}] \leq e^{-C_1 k \Delta_{BL}(T^0, T^\#)},
\]
and, by (29),
\[
\Pr[T^0, A_{T^\#}^c, M_{T^\#}] \leq \sum_{s' \in [\nu]^{2n+1}} 1\{s' \in M_{T^\#}\} 1\{s' \in A_{T^\#}^c\} \mu_X^{T^0}(s') \\
\leq \sum_{s' \in [\nu]^{2n+1}} \frac{\mu_X^{T^\#}(s')}{\mu_X^{T^0}(s')} 1\{s' \in A_{T^\#}^c\} \mu_X^{T^0}(s') \\
\leq \Pr[T^\# \neq T^0, A_{T^\#}] \\
\leq e^{-C_1 k \Delta_{BL}(T^0, T^\#)}.
\]
This proves Lemma 1 in Section 2. By Claim 5.1, plugging back into (31),
\[
\Pr[T^0, T^\# \neq T^0, M_{T^\#}] \leq \sum_{T^\# \neq T^0} [\Pr[T^0, A_{T^\#}] + \Pr[T^0, A_{T^\#}^c, M_{T^\#}]] \\
\leq 2n-3 \sum_{\Delta=1}^{+\infty} (12\nu n^2)^\Delta [2e^{-C_1 k \Delta}] \\
\leq \sum_{\Delta=1}^{+\infty} e^{-(C_1 \kappa \log n - 2 \log n - \log(12\nu \eta))\Delta} \\
\leq \frac{e^{-(C_1 \kappa \log n - 2 \log n - \log(12\nu \eta))}}{1 - e^{-(C_1 \kappa \log n - 2 \log n - \log(12\nu \eta))}} \\
\leq \frac{1}{e^{(C_1 \kappa - 2) \log n - \log(12\nu \eta)} - 1} \\
\leq \delta,
\]
for $\kappa$ large enough, depending only on $g$, $\Upsilon$ and $\delta$, for all $n \geq 2$. \qed
Finally:

Proof of Theorem 1. Combining Theorems ?? and 3 immediately gives Theorem 1. 

5.3 Finding matching subtrees

We now describe our procedure to construct a battery of distinguishing tests for general trees. As in the homogeneous case, the procedure attempts to build dense, maximal subtrees shared by $T^0$ and $T^#$ and pair them up appropriately to construct distinguishing tests. For general trees, however, care must be taken to deal with possible overlaps in $T^0$ and $T^#$. Such overlaps produce unwanted dependencies between the test pairs. See Figure 2 for an illustration.

As a result, we proceed in two stages:

1. First, pairs of matching subtrees are constructed, similarly to the homogeneous case.

2. Second, if the overlap between the tests is too large, new distinguishing tests are constructed along the “boundary of the overlap.”

The first stage is described below. Analysis of the size of the overlap is presented in Section 5.4. The more delicate second stage is described in Sections 5.5 and 5.6.

We root $T^0$ arbitrarily.

Definition 5.2 ($\ell$-vertices). For a fixed positive integer $\ell$, we call $\ell$-vertices those vertices in $T^0$ whose graph distance from the root is a multiple of $\ell$. The sets of all $\ell$-vertices at the same distance from the root are called $\ell$-levels. For an $\ell$-vertex $x$, its descendant $\ell$-vertices on the next $\ell$-level (that is, farther from the root)
are called the $\ell$-children of $x$, which we also refer to as a family of $\ell$-siblings. For simplicity, the leaves of $T^0$ are also considered $\ell$-vertices irrespective of their distance from the root and they belong to the $\ell$-level immediately below them.

Our goal is to color each $\ell$-vertex $x$ with the following interpretation:

- **Green $G$:** indicating a matching subtree rooted at $x$ that can be used to reconstruct ancestral states reliably on both $T^0$ and $T^\#$ using the same function of the leaf states.
- **Red $R$:** indicating the presence among the $\ell$-children of $x$ of a pair of matching subtrees that can potentially be used in a distinguishing test because their pairwise distance differs in $T^0$ and $T^\#$.
- **Yellow $Y$:** none of the above.

As before, we call $G$-vertices (respectively $G$-children) those $\ell$-vertices (respectively $\ell$-children) that are colored $G$, and similarly for the other colors. Before describing the coloring procedure in details, we need a definition.

**Definition 5.3 (G-cluster).** Let $x$ be a $G$-vertex. Assume that each $\ell$-vertex below $x$ in $T^0$ has been colored $G$, $R$, or $Y$ and that the leaves have been colored $G$. The $G$-cluster rooted at $x$ is the restricted subtree of $T^0$ containing all vertices and edges (not necessarily $\ell$-vertices) lying on at least one path between $x$ and a leaf below $x$ that traverses only $\ell$-vertices colored $G$.

We now describe the coloring procedure. Below, when counting the $\ell$-children of an $\ell$-vertex $x$ with a specified property, each leaf among the $\ell$-children of $x$ counts as $2^{\ell-d}$ vertices if $d$ is the graph distance between $x$ and that leaf.

1. **Initialization**

   (a) Root $T^0$ at an arbitrary vertex. (Note that $T^\#$ remains unrooted for this part of the proof as we are only interested in metric-matching.)

   (b) All leaves of $T^0$ are colored $G$.

2. For each $\ell$-vertex $x$ in the $\ell$-level furthest from the root that has yet to be colored, do:

   (a) Vertex $x$ is colored $G$ if:
   - at most one of its $\ell$-children is non-$G$ and;
   - the resulting $G$-cluster rooted at $x$ and the corresponding restricted subtree in $T^\#$, that is, the subtree of $T^\#$ restricted to the same leaf set, are matching.

   (b) Else, vertex $x$ is colored $R$ if:
   - at most one of its $\ell$-children is non-$G$;
   - the $G$-clusters rooted at the $G$-children of $x$ have non-intersecting matching subtrees in $T^\#$;
   - but, if $x$ were colored $G$, the resulting $G$-cluster rooted at $x$ and the corresponding matching subtree in $T^\#$ would not be matching.

   (c) Else, vertex $x$ is colored $Y$. In particular, at least two $\ell$-children of $x$ are non-$G$. 
5.4 Relating combinatorial distance, the number of matching subtrees and the overlap size

Let \( \#G \) be the number of \( G \)-vertices in \( T^0 \) in the construction, and similarly for the other colors. For an \( \ell \)-vertex \( x \) in \( T^0 \), we let \( T^0_x \) be the subtree of \( T^0 \) rooted at \( x \) and we let \( V_\ell(T^0_x) \) be the set of \( \ell \)-vertices in \( T^0_x \). We denote by \( d^G_{T^0} \) the graph distance on \( T^0 \).

Unlike the homogeneous case, observe that it is possible for \( G \)-clusters to “overlap” in \( T^# \), that is, pairwise intersect. We define the overlap formally as follows.

**Definition 5.4 (Overlap).** An edge \( e^# \) in \( T^# \) is in the overlap if it belongs to the matching restricted subtrees (the collection of which we denote by \( \{M_i\}_i \)) of at least two distinct maximal \( G \)-clusters in \( T^0 \) (the collection of which we denote by \( \{G_i\}_i \)). For each \( i \), the edge \( e^# \) is on a path of \( M_i \) corresponding to an edge \( e^0 \) in \( G_i \). We also say that \( e^0 \) is in the overlap. Let \( O^# \) (respectively \( O^0 \)) denote the overlap, as a set of edges, in \( T^# \) (respectively \( T^0 \)).

The following bound allows us to work with the overlap in either \( T^0 \) or \( T^# \), whichever is more convenient depending on the context. Notice that it is not immediately clear that \( O^0 \) and \( O^# \) are roughly the same size because, by definition, each edge in \( O^# \) corresponds to several edges in \( O^0 \).

**Claim 5.2 (Overlaps in \( T^0 \) and \( T^# \)).** We have

\[
|O^0| = \Theta \left( |O^#| \right),
\]

where the constants depend on \( f, g, \frac{1}{T}, \ell \).

**Proof.** Intuitively the result follows from the fact that the boundary of the overlap dominates its size in both trees, that edges in \( O^0 \) close to the boundary in their respective \( G \)-cluster are also close to the boundary in \( O^# \), but that edges close to the boundary in \( O^# \) cannot correspond to more than a constant number of edges in \( O^0 \) close to the boundary in their respective \( G \)-cluster. Indeed the latter must be near vertices in their \( G \)-cluster outside of the overlap, of which there are only a constant number at a constant distance from the former.

Formally let \( e^# \) be an edge in \( O^# \). There is an edge \( e^0 \) (in fact at least two) in a \( G \)-cluster in \( T^0 \) whose corresponding path in \( T^# \) includes \( e^# \). Note that \( e^0 \) has weight at most \( g \) and therefore can be identified in this way with at most \( g \times |V_\ell| \) edges in \( O^# \). That is, for every edge in \( O^0 \) there are at most \( g \times |V_\ell| \) edges in \( O^# \), or

\[
|O^0| \geq \frac{1}{g \times |V_\ell|} |O^#|.
\]

For the other direction, root \( T^# \) at an arbitrary vertex \( \rho^# \). Let \( G \) be a maximal \( G \)-cluster in \( T^0 \) and re-root \( G \) consistently with the rooting in \( T^# \). (Note that there is no global rooting in \( T^0 \) consistent with the rooting in \( T^# \), but that will not matter.) We say that a vertex in \( G \) is in the overlap if it is adjacent to an edge in \( O^0 \). Let \( V^G_x \) and \( V^G_y \) be the vertices in \( G \) and the vertices in the overlap in \( G \) respectively. Letting \( V^G_x \) (respectively \( V^G_y \)) be the vertices in \( V^G \) (respectively \( V^G \)) below vertex \( x \) (including \( x \)), we say that \( x \) is \( G \)-overlap-shallow if

\[
\sum_{y \in V^G_y} 2^{-\frac{d^G_y(x,y)}{2}} < \frac{2}{1 - 1/\sqrt{2}}.
\]

Because by the sum of a geometric series

\[
\sum_{x \in V^G} \sum_{y \in V^G_y} 2^{-\frac{d^G_y(x,y)}{2}} = \sum_{y \in V^G} \sum_{x \in V^G_x} 2^{-\frac{d^G_y(x,y)}{2}} \leq \sum_{y \in V^G} 2^{-\frac{1}{2}} = \frac{|V^G|}{1 - 1/\sqrt{2}},
\]

29
the number of $G$-overlap-shallow vertices in $W^G$ is at least
\[
\left(1 - \frac{1 - 1/\sqrt{2}}{2} \frac{1}{1 - 1/\sqrt{2}}\right) |W|^G = \frac{|W|^G}{2}.
\] (32)

In particular, the number of edges in $G$ in the overlap is at most twice the number of $G$-overlap-shallow vertices in $W^G$.

If $x$ is $G$-overlap-shallow, then there must be a witness, that is, a vertex in $V^G \setminus W^G$ or a leaf in $V^G$ at graph distance at most $C$ below $x$, for a constant $C$ depending only on $\ell$. Indeed, because a $G$-cluster is $(\ell, 1)$-dense (that is, nearly bifurcating), the sum $\sum_{y \in V^G} 2^{-d_{G,T}^G(x,y)}$ increases unboundedly with the distance to the closest witness.

Let $x_0$ be $G$-overlap-shallow with witness $y_0$ and let $x^#$ and $y^#$ be the corresponding (possibly extra) vertices in $T^#$. Note that, in $T^#$, the graph distance between $x^#$ and $y^#$ is at most $C g \Upsilon$. Note further that a witness, not being adjacent to an edge in the overlap in $T^#$ (including the leaf case), belongs only to one $G$-cluster. Hence there can only be $2^{C g \Upsilon}$ distinct maximal $G$-clusters containing a vertex corresponding to $x^#$ that is $G$-overlap-shallow. The vertex $x_0^0$ is adjacent to an edge $e_0^0$ in $T^0$ whose corresponding path in $T^#$ contains an edge $e^#$ in $O^#$. Since there are at most $2^g \Upsilon + 1$ vertices in $T^#$ at evolutionary distance $g$ from $e^#$, for each edge in $O^#$ there are at most $2 \cdot 2 \cdot 2^g \Upsilon + 1 \cdot 2^{C g \Upsilon}$ edges in the overlap in $O^0$, or
\[
|O|^# \geq \frac{1}{4} 2^{C g \Upsilon + 2^g \Upsilon + 1},
\]
where one factor of 2 accounts for passing between edges and vertices in $T^#$ and the other comes from (32). That concludes the proof.

We now relate the blow-up distance between $T^0$ and $T^#$ to the number of $R$-vertices, from which tests can potentially be constructed, and the size of the overlap. We first bound the number of yellow vertices.

**Claim 5.3** (Bounding the number of yellow vertices). Assume $\ell \geq 1$. We have
\[
\#_Y \leq \#_R.
\]

*Proof.* From our construction, each $Y$-vertex in $T^0$ has at least two non-$G$-children. Hence, intuitively, one can think of the $Y$-vertices as forming the internal vertices of a forest of multifurcating trees whose leaves are $R$-vertices. The inequality follows.

Formally, if $x$ is a $Y$-vertex, from the observation above we have
\[
\sum_{y \in V_\ell(T^0)} 2^{-d_{G,T}^G(x,y)} \frac{1}{\ell} \{y \text{ is a } R\text{-vertex}\} \geq 1,
\] (33)
by induction on the $\ell$-levels starting with the level farthest away from the root. Similarly if $y$ is an $R$-vertex, we have
\[
\sum_{x : y \in V_\ell(T^0)} 2^{-d_{G,T}^G(x,y)} \frac{1}{\ell} \{x \text{ is a } Y\text{-vertex}\} < 1,
\] (34)
where the inequality follows from the fact that the sum is over a path from $x$ to the root of $T^0$. Summing (33) over $Y$-vertices $x$ and (34) over $R$-vertices $y$ gives the same quantity on the LHS, so that the RHS gives the inequality.

\[
\square
\]
Claim 5.4 (Relating blowup, \#R, and overlap). There is a constant \(0 < C_O < +\infty\), depending on \(\ell\), \(g\) and \(\Upsilon\), such that

\[
\Delta_{\text{BL}}(T^0, T^\#) \leq C_O \left( \#R + |O^\#| \right).
\]

Proof. First remove all edges in \(T^0\) that are not in a maximal G-cluster. Counting all edges (of which there are at most \(2^{\ell+1} - 2\)) between a non-G-vertex and its \(\ell\)-children and the edge above each such vertex if its parent \(\ell\)-vertex is colored G, we need to remove at most

\[
(2^{\ell+1} - 1)(\#R + \#Y) \leq 2(2^{\ell+1} - 1)\#R,
\]

edges, where the inequality follows from Claim 5.3.

Next replace every degree-2 vertex produced after the first step with a single edge. Each such replacement (of which there are at most \(2^{\ell+1} + 1\) for each non-G-vertex; one for its parent and one for each of its G-children) requires 3 operations, bringing the total number of operations so far to at most

\[2 \cdot 3(2^{\ell+1} + 1) + 2(2^{\ell+1} - 1)\#R \leq 8(2^{\ell+1} + 1)\#R,\]

where we used Claim 5.3 again. We will say that the new single edges are in the overlap if either of the edges they are replacing are in the overlap themselves.

At this point, every vertex remaining in \(T^0\) corresponds to a (non-extra) vertex in \(T^\#\) and every edge remaining in \(T^0\) corresponds to a path in \(T^\#\) with at most \(2g\Upsilon\) edges. Finally remove all edges in the overlap.

Note that the total number of edges in \(T^0\) and \(T^\#\) is the same. Hence if we were to replace every remaining edge in \(T^0\) corresponding to a non-trivial path in \(T^\#\) with one of the corresponding edges in \(T^\#\) (which would take two operations), we would need to add back at most \(8(2^{\ell+1} + 1)\#R + |O^0|\) edges to produce \(T^\#\). The extra operations above bring the total number of operations to at most

\[24(2^{\ell+1} + 1)\#R + 3 |O^0| \leq 24(2^{\ell+1} + 1)(\#R + |O^0|)\]

From Claim 5.2, the constant \(C_O\) in the statement can therefore be taken as a function of \(\ell\), \(g\), and \(\Upsilon\). \(\Box\)

Our next goal is to construct batteries with a number of tests scaling linearly in the blowup distance between \(T^0\) and \(T^\#\). Using Claim 5.4, we first divide the analysis into two cases depending on the values of \(\#R\) and \(|O^\#|\).

- **Large overlap.** If

\[|O^\#| \geq \frac{1}{10} \frac{\Delta_{\text{BL}}(T^0, T^\#)}{C_O},\]

we say that we are in the large overlap case. We will show in Section 5.6 that a linear (in the blowup distance) number of tests can be built “around the periphery of the overlap.”

- **Many R-vertices.** By Claim 5.4, if (35) fails, then

\[\#R \geq \frac{9}{10} \frac{\Delta_{\text{BL}}(T^0, T^\#)}{C_O},\]

in which case we say that we are in the many-R case. In that case, we proceed similarly to the homogeneous case and construct a distinguishing test for a linear fraction of R-vertices. See Section 5.5.
5.5 Constructing a battery of tests: Many-R case

We now construct a battery of tests in the many-R case. This case is similar to the homogeneous case (although many new difficulties arise from the lack of symmetry of general trees). The basic idea is that each R-vertex has two G-children which satisfy many of the requirements of a battery and therefore can potentially be used as a test pair. In particular, they are the roots of dense subtrees that are matching with their corresponding restricted subtrees in \( T^\# \) and their evolutionary distance differs in \( T^0 \) and \( T^\# \). Note that, in the many-R case, we also have a number of R-vertices that scales linearly in the blowup distance.

Like in the homogeneous case, we enforce the global requirement of the battery, that is, we make sure that the test pairs do not intersect, via a sparsification argument. Unlike in the homogeneous case, there are other issues to address to construct a battery of tests, including the overlap of G-clusters and the possibility of non-co-hanging pairs in \( T^\# \).

In this section, \( T^0 \) and \( T^\# \) are fixed. To simplify notation, we let \( \Delta = \Delta_{BL}(T^0, T^\#) \). Fix \( \wp = 1 \). Choose \( \ell = \ell(g, \wp) \) as in Proposition 1. Then take

\[
\Gamma = (6 + 4\Upsilon g)\ell,
\]

and set \( \gamma_t \geq \Gamma \), a multiple of \( \ell \), and \( C \) as in Proposition 1.

**Non-overlapping G-clusters.** To build a battery, the test subtrees must be non-intersecting in \( T^\# \). (By construction, the test subtrees are non-intersecting in \( T^0 \).) We proceed as follows. Re-color those R-vertices that have at least one G-child who is the root of a G-cluster that intersects with another G-cluster in \( T^\# \). (The other G-cluster may be rooted at a G-child of a different \( \ell \)-vertex.) Intuitively, if too many R-vertices are lost in this recoloring step, then the overlap must be large. Indeed, we prove the following.

**Claim 5.5 (Re-coloring).** In the many-R case, after re-coloring, we have

\[
\#_R \geq \frac{\Delta}{2 C_O}.
\]

**Proof.** Assume maximal G-cluster \( G_i \) intersects with another (distinct) G-cluster in \( T^\# \) and let \( M_i \) be the matching subtree corresponding to \( G_i \) in \( T^\# \). Consider a shortest path (in graph distance, say) between a leaf in \( M_i \) and the overlap in \( T^\# \), and let \( v_i \) be the vertex in \( T^\# \) where this path enters the overlap. Because 1) \( T^\# \) is bifurcating and 2) at least one edge adjacent to \( v_i \) must be in \( O^\# \), it follows that \( v_i \) can arise as the entrance vertex to the overlap for at most two G-clusters. Hence the number of maximal G-clusters intersecting with another (distinct) G-cluster is at most

\[
2 \cdot 2 \left| O^\# \right| \leq \frac{\Delta}{10} C_O,
\]

where we took into account that the number of vertices in the overlap is at most twice the number of edges in the overlap. That implies that the number of recolored \( \ell \)-vertices is at most \( 4 \frac{\Delta}{10} C_O \). After recoloring we therefore have

\[
\#_R \geq \frac{9 \Delta}{10 C_O} - \frac{4 \Delta}{10 C_O} = \frac{\Delta}{2 C_O},
\]

by our assumptions. \( \square \)

In the rest of this subsection, we build a \((\ell, \wp, \Gamma, \gamma_t, I)\)-battery

\[
\{(y^0_i, z^0_i); (Y^0_i, Z^0_i)\}_{i=1}^I \text{ (in } T^0) \text{ and } \{(y^\#_i, z^\#_i); (Y^\#_i, Z^\#_i)\}_{i=1}^I \text{ (in } T^\#)\]
with corresponding $\alpha_i$s. We number the $\mathbb{R}$-vertices $i = 1, \ldots, I'$ and we build one test panel for each $\mathbb{R}$-vertex. Here $I' \geq I$ as we will later need to reject some of the test panels to avoid unwanted correlations. We root $T^\#$ at an arbitrary vertex $\rho^\#$. (Note that $T^0$ was rooted previously and that whether or not the rootings of $T^0$ and $T^\#$ are consistent will not matter.)

Co-hanging pairs in $T^\#$. Let $x_i^0$ be an $\mathbb{R}$-vertex (after recoloring) in $T^0$ and let $x_i^\#$ be the corresponding vertex in $T^\#$. (Note that $x_i^\#$ may in fact be an extra vertex of degree 2.) Because $x_i^0$ is colored $\mathbb{R}$, by construction it has at least $2^\ell - 1 \mathbb{G}$-children, but its $\mathbb{G}$-children are connected in different way in $T^\#$. There are two cases:

1. All pairs of $\mathbb{G}$-children of $x_i^0$ are the roots of co-hanging matching subtrees in $T^\#$, in which case at least one pair $(y_i^0, z_i^0)$ must be at a different evolutionary distance in $T^0$ than the corresponding pair $(y_i^\#, z_i^\#)$ in $T^\#$. We use these pairs as our test panel with the following caveat. If the test subtrees are not rooted consistently in $T^0$ and $T^\#$, we move each test vertex to one of its $\mathbb{G}$-children where the rooting is consistent. This can always be done as there is at most one $\mathbb{G}$-child (as an extra vertex) between a test vertex and the root of $T^\#$. All other choices lead to a consistent rooting.

2. Otherwise at least one pair $(\tilde{y}_i^0, \tilde{z}_i^0)$ of $\mathbb{G}$-children of $x_i^0$, with corresponding pair $(\tilde{y}_i^\#, \tilde{z}_i^\#)$, has a connecting path in $T^\#$ that intersects with the corresponding matching test subtrees $\tilde{Y}_i^\#$ or $\tilde{Z}_i^\#$ (or both). We show next how to construct a test panel in this case.

Claim 5.6 (Co-hanging pairs). In the many-$\mathbb{R}$ case, after recoloring, for each remaining $\mathbb{R}$-vertex $x_i^0$ we can find a test pair of $\mathbb{G}$-vertices $(y_i^0, z_i^0)$ below $x_i^0$, with corresponding test pair $(y_i^\#, z_i^\#)$ in $T^\#$, such that the test panel satisfy the cluster and pair requirements of a battery.

Proof. The argument above settles the first case. Indeed by construction the test subtrees, that is, the $\mathbb{G}$-clusters rooted at the test vertices, are $(\ell, 1)$-dense. The test subtrees are also matching, co-hanging and their roots are at different evolutionary distances in $T^0$ and $T^\#$ by (36). Finally, the test pair in $T^0$ is proximal as, after re-rooting,

$$d_{T^0}(y_i^0, z_i^0) \leq 3\ell \leq \Gamma.$$ 

For the second case, we use the same notation as above. Because $T^\#$ has no cycle, the path between $\tilde{y}_i^\#$ and $\tilde{z}_i^\#$ must be of the following form: there is a vertex $\tilde{v}$ in $\tilde{Y}_i^\#$ (possibly equal to $\tilde{y}_i^\#$) and a vertex $\tilde{w}$ in $\tilde{Z}_i^\#$ (possibly equal to $\tilde{z}_i^\#$) such that the path between $\tilde{y}_i^\#$ and $\tilde{z}_i^\#$ 1) intersects with $\tilde{Y}_i^\#$ between $\tilde{y}_i^\#$ and $\tilde{v}$, 2) does not intersect with either $\tilde{Y}_i^\#$ or $\tilde{Z}_i^\#$ between $\tilde{v}$ and $\tilde{w}$, and 3) intersects with $\tilde{Z}_i^\#$ between $\tilde{w}$ and $\tilde{z}_i^\#$. We consider two subcases:

1. $\tilde{y}_i^\#, \tilde{z}_i^\#$ are “far.” Suppose first that

$$d_{T^\#}(\tilde{y}_i^\#, \tilde{z}_i^\#) > 2g\ell.$$ 

If $\tilde{v} \neq \tilde{y}_i^\#$, let $y_i^0$ be a $\mathbb{G}$-child of $\tilde{y}_i^0$ which is not in the subtree containing $\tilde{v}$ (as an extra vertex) with the following caveat. We choose $y_i^0$ so that the test subtree rooted at $y_i^0$ and the test subtree rooted at the corresponding (possibly extra) vertex $y_i^\#$ in $T^\#$ are rooted consistently. This can always be done as there is at most one $\mathbb{G}$-child (as an extra vertex) between a vertex and the root of $T^\#$. All other choices (of which there are at least $2^\ell / 2$) lead to a consistent rooting. Similarly, we define $z_i^0$ and
Then

\[
\begin{align*}
    d_{T_0}(y_i^0, z_i^0) &= d_{T_0}(y_i^0, \tilde{y}_i^0) + d_{T_0}(\tilde{y}_i^0, z_i^0) + d_{T_0}(z_i^0, z_i^0) \\
    &\leq d_{T_0}(y_i^0, \tilde{y}_i^0) + 2g\ell + d_{T_0}(z_i^0, z_i^0) \\
    &< d_{T^*}(y_i^#, \tilde{y}_i^#) + d_{T^*}(\tilde{y}_i^#, z_i^#) + d_{T^*}(z_i^#, z_i^#) \\
    &= d_{T^*}(y_i^#, z_i^#),
\end{align*}
\]

(36)

where we used that \(\tilde{y}_i^0, z_i^0\) are \(\ell\)-siblings, so that \(d_{T_0}(y_i^0, z_i^0) \neq d_{T^*}(y_i^#, z_i^#)\). Moreover note that the subtrees rooted at \(y_i^#\) and \(z_i^#\) are co-hanging in \(T^#\). Hence the pairs \((y_i^0, z_i^0)\) and \((y_i^#, z_i^#)\) satisfy the cluster and pair requirements of the battery. Indeed by construction the test subtrees are \((\ell, 1)\)-dense. The test subtrees are also matching, co-hanging and their roots are at different evolutionary distances in \(T^0\) and \(T^#\) by (36). Finally, the test pair in \(T^0\) is proximal as

\[
d_{T^0}(y_i^0, z_i^0) \leq 3\ell \leq \Gamma.
\]

2. \(\tilde{y}_i^#, z_i^#\) are “close.” Assume instead that

\[
d_{T^*}(\tilde{y}_i^#, z_i^#) \leq 2g\ell.
\]

(37)

If \(d_{T_0}(y_i^0, z_i^0) \neq d_{T^*}(\tilde{y}_i^#, z_i^#)\), we can proceed as above and let \(y_i^0\) be a \(G\)-child of \(\tilde{y}_i^0\) which is not in the subtree containing \(\tilde{v}\) (as an extra vertex), and similarly for \(z_i^0\), with corresponding vertices \(y_i^#\) and \(z_i^#\) in \(T^#\). As above we choose \(G\)-children such that the rooting is consistent in \(T^0\) and \(T^#\).

If \(d_{T_0}(y_i^0, z_i^0) = d_{T^*}(y_i^#, z_i^#)\), let \(y_i^0\) be the closest \(G\)-vertex below \(\tilde{v}\) (as an extra vertex) resulting in a consistent rooting and let \(z_i^0\) be defined similarly. Such vertices exist within graph distance at most \(2\ell\) of \(\tilde{v}\) and \(\tilde{w}\). Let \(y_i^#\) and \(z_i^#\) be the corresponding vertices in \(T^#\). Then,

\[
\begin{align*}
    d_{T^*}(y_i^#, z_i^#) &= d_{T^*}(y_i^#, \tilde{v}) + d_{T^*}(\tilde{v}, \tilde{w}) + d_{T^*}(\tilde{w}, z_i^#) \\
    &< d_{T_0}(y_i^0, y_i^0) + d_{T_0}(\tilde{y}_i^0, z_i^0) + d_{T_0}(z_i^0, z_i^0) \\
    &= d_{T_0}(y_i^0, z_i^0),
\end{align*}
\]

(38)

where the inequality holds term by term. Hence \(d_{T_0}(y_i^0, z_i^0) \neq d_{T^*}(y_i^#, z_i^#)\). Moreover note that the subtrees rooted at \(y_i^#\) and \(z_i^#\) are co-hanging in \(T^#\). Also, from (37) and the choice of \(y_i^#, z_i^#\),

\[
\begin{align*}
    d_{T^0}(y_i^0, z_i^0) &= d_{T^0}(y_i^0, \tilde{y}_i^0) + d_{T^0}(\tilde{y}_i^0, z_i^0) + d_{T^0}(z_i^0, z_i^0) \\
    &\leq (2\ell + 2\Upsilon g\ell) + 2\ell + (2\ell + 2\Upsilon g\ell) \\
    &= (6 + 4\Upsilon g)\ell \\
    &\leq \Gamma.
\end{align*}
\]

Hence the pairs \((y_i^0, z_i^0)\) and \((y_i^#, z_i^#)\) satisfy the cluster and pair requirements of the battery. Indeed by construction the test subtrees are \((\ell, 1)\)-dense. The test subtrees are also matching, co-hanging and their roots are at different evolutionary distances in \(T^0\) and \(T^#\) by (38).

\[\square\]
Sparsification in $T^\#$. It remains to satisfy the global requirements of the battery. Note that by construction the test subtrees are non-intersecting in both $T^0$ and $T^\#$. However we must also ensure that proximal/semi-proximal connecting paths and non-proximal hats do not intersect with each other or with test subtrees from other test panels. By construction, this is automatically satisfied in $T^0$ where all test pairs are proximal. To satisfy this requirement in $T^\#$, we make the collection of test pairs sparser by rejecting an appropriate fraction of them.

Claim 5.7 (Sparsification in $T^\#$). Let $\mathcal{H}' = \{(y_i^0, z_i^0); (y_i^\#, z_i^\#)\}_{i=1}^I$ be the test panels constructed in Claim 5.6. We can find a subset $\mathcal{H} \subseteq \mathcal{H}'$ of size

$$|\mathcal{H}| = I \geq \frac{1}{1 + 2^{2\gamma_t+2}} I' \geq \frac{\Delta}{2C_O(1 + 2^{2\gamma_t+2})}$$

such that the test panels in $\mathcal{H}$ satisfy all global requirements of a battery.

Proof. We sparsify the set $\mathcal{H}'$ of test pairs as follows. Let $\{(Y_i^0, Z_i^0); (Y_i^\#, Z_i^\#)\}_{i=1}^I$ be the test subtrees corresponding to $\mathcal{H}'$. Start with test panel $((y_1^0, z_1^0); (y_1^\#, z_1^\#))$. Remove from $\mathcal{H}'$ all test panels $i \neq 1$ such that

$$\min\{d_{T^\#}(v, w) : v \in \{y_1^\#, z_1^\#\}, w \in V(Y_i^\#) \cup V(Z_i^\#)\} \leq 2\gamma_t.$$ (39)

Because there are at most $2 \cdot 2^{2\gamma_t+1}$ vertices in $T^\#$ satisfying the above condition and that the test subtrees are non-overlapping in $T^\#$ by the remark above Claim 5.5, we remove at most $2^{2\gamma_t+2}$ test panels from $\mathcal{H}'$.

Let $i$ be the smallest index remaining in $\mathcal{H}'$. Proceed as above and then repeat until all indices in $\mathcal{H}'$ have been selected or rejected.

At the end of the procedure, there are at least

$$\frac{1}{1 + 2^{2\gamma_t+2}} I'$$

test panels remaining, the set of which we denote by $\mathcal{H}$. Recalling that $\gamma_t \geq \Gamma$, note that, in $\mathcal{H}$, the connecting paths of proximal/semi-proximal pairs and the hats of non-proximal pairs cannot intersect with each other or with any of the test subtree rooted at test vertices in $\mathcal{H}$ by (39).

Summary of many-\$r\$ case. We have proved the following in the many-\$r\$ case. Recall that $\varphi = 1$, $\ell = \ell(g, \varphi)$ is chosen as in Proposition 1, $\Gamma = (6 + 4Y g)\ell$, and $\gamma_t \geq \Gamma$, a multiple of $\ell$, and $C$ are chosen as in Proposition 1.

Proposition 4 (Battery in the many-\$r\$ case). In the many-\$r\$ case, we can build a $(\ell, \varphi, \Gamma, \gamma_t, I)$-battery

$$\{((y_i^0, z_i^0); (Y_i^0, Z_i^0))\}_{i=1}^I \text{ (in } T^0\text{)}$$

and

$$\{((y_i^\#, z_i^\#); (Y_i^\#, Z_i^\#))\}_{i=1}^I \text{ (in } T^\#\text{)}$$

with

$$I \geq \frac{\Delta}{2C_O(1 + 2^{2\gamma_t+2})}.$$  

Proof. The result follows from Claims 5.5, 5.6, and 5.7. □
5.6 Constructing a battery of tests: Large overlap case

We now construct a battery of tests in the large overlap case. By assumption we have,

\[ |O^\#| \geq \frac{1}{10} \frac{\Delta_{BL}(T^0, T^\#)}{C_O}. \]

Moreover, by the proof of Claim 5.2, a significant fraction of the vertices in the overlap are in fact shallow, that is, they are close to the boundary of the overlap. To build a battery in this case, we show that a test pair can be found near each shallow vertex. As in the many-R case, we need to deal with a number of issues, including the overlap of \( G \)-clusters, the possibility of non-co-hanging pairs, and the proximity of the matching subtrees.

In this section, \( T^0 \) and \( T^\# \) are fixed. To simplify notation, we let \( \Delta = \Delta_{BL}(T^0, T^\#) \). Recall that \( T^0 \) is rooted. We also root \( T^\# \) arbitrarily. (Note that the roots of \( T^0 \) and \( T^\# \) are not consistent with each other, in the sense that the \( G \)-clusters and their matching subtrees are not necessarily rooted in the same way.) Recall that a vertex \( v^\# \) in \( T^\# \) is in the overlap if it is adjacent to an edge \( e^\# \in O^\# \). We also say that \( v^\# \) is in a \( G \)-cluster \( G \) if \( v^\# \) lies on the matching subtree corresponding to \( G \). (Recall that edges of \( T^0 \) in \( G \) correspond to paths of the matching subtree in \( T^\# \).)

Fix \( \wp = 5 \). Choose \( \ell = \ell(g, \wp) \) as in Proposition 1. Then take

\[ \Gamma = 6g\Upsilon \log_2 \left( \frac{4g\Upsilon}{1 - 1/\sqrt{2}} \right) + 2\ell g\Upsilon + 4, \]

and set \( \gamma_t \geq \Gamma \), a multiple of \( \ell \), and \( C \) as in Proposition 1.

Test pairs near the boundary of the overlap. Let \( v^\# \) in \( T^\# \) be in the overlap. Intuitively, vertex \( v^\# \) can be used to construct a test pair for the following two reasons:

1. It corresponds to (at least) two distinct vertices \( v^0_i, v^0_j \) in \( T^0 \), and the evolutionary distance between these vertices differs in \( T^0 \) (where it is \( > 0 \)) and in \( T^\# \) (where it is \( 0 \)).

2. It is in the \( G \)-clusters including \( v^0_i \) and \( v^0_j \) above, and therefore its sequence can be reconstructed using the same estimator on both \( T^0 \) and \( T^\# \).

However, to avoid unwanted correlations between the ancestral reconstructions on \( T^\# \), one must be careful to construct appropriate co-hanging test subtrees that further satisfy all requirements of a battery. For this purpose, it turns out to be easier to work with those \( v^\# \in O^\# \) that are \#-overlap-shallow, defined as follows. Let \( V^\# \) be the vertices of \( T^\# \) in a \( G \)-cluster. Let \( W^\#_x \) be those vertices in \( V^\# \) that are also in the overlap. Letting \( W^\#_x \) (respectively \( V^\#_x \)) be the vertices in \( W^\# \) (respectively \( V^\# \)) below vertex \( x \) (including \( x \)), we say that \( x \) is \#-overlap-shallow if

\[
\sum_{y \in W^\#_x} 2^{\frac{d^\#_{T^\#}(x, y)}{2g\Upsilon}} < \frac{2g\Upsilon}{1 - 1/\sqrt{2}}.
\]

Arguing as in the proof of Claim 5.2, we have:

Claim 5.8 (Size of the overlap boundary). At least half of the vertices in \( W^\# \) are \#-overlap-shallow.

Let \( v^\# \) be \#-overlap-shallow. We construct a test pair nearby \( v^\# \) as follows. Let \( G_i \) and \( G_j \) be \( G \)-clusters overlapping at \( v^\# \), that is, \( v^\# \) is in both \( G_i \) and \( G_j \). In the proof of Claim 5.2, we argued that an inequality of
the form (40) implies the existence of a close witness, that is, a leaf or vertex not in the overlap at a constant graph distance below \( x \). By restricting the sum in (40) to those vertices \( y \) that are both in \( G_i \) (or \( G_j \)) and on only one side below \( x = v^\# \) (that is, below one of the immediate children of \( v^\# \)), we can in fact find four (distinct) witnesses \( \tilde{y}_i^\#, \tilde{y}_j^\#, \tilde{z}_i^\#, \text{ and } \tilde{z}_j^\# \) at constant graph distance \( C' = C'(g, \Upsilon) \) from \( v^\# \). The four witnesses satisfy the following properties:

- They are not in the overlap. (Note that leaves in particular are not in the overlap.)
- For \( \ell = i, j, \tilde{y}_i^\# \text{ and } \tilde{z}_i^\# \) are in \( G_i \).
- For \( x = y, z, \tilde{x}_i^\# \text{ and } \tilde{x}_j^\# \) are on the same side below \( v^\# \).

Let \( \tilde{y}_i^0, \tilde{y}_j^0, \tilde{z}_i^0, \text{ and } \tilde{z}_j^0 \) be the corresponding (possibly extra) vertices in \( T^0 \). By construction, the topology of \( T^0 \) restricted to \( \{ \tilde{y}_i^0, \tilde{y}_j^0, \tilde{z}_i^0, \tilde{z}_j^0 \} \) is \( \tilde{y}_i^0 \tilde{z}_i^0 \tilde{y}_j^0 \tilde{z}_j^0 \) because \( G \)-clusters in \( T^0 \) are not overlapping. (Refer to Definition 3.1 for quartet topology notation.) It differs from the topology of \( T^\# \) restricted to \( \{ \tilde{y}_i^\#, \tilde{y}_j^\#, \tilde{z}_i^\#, \tilde{z}_j^\# \} \), which is \( \tilde{y}_i^\# \tilde{z}_i^\# \tilde{y}_j^\# \tilde{z}_j^\# \) by construction. Note that

\[
d_{T^0}(\tilde{y}_i^0, \tilde{z}_i^0) = d_{T^\#}(\tilde{y}_i^\#, \tilde{z}_i^\#)
\]

for \( \ell = i, j \) by definition of the matching subtree of \( G_i \). Moreover, by the four-point condition (7) in the non-degenerate case,

\[
d_{T^0}(\tilde{y}_i^0, \tilde{y}_j^0) + d_{T^0}(\tilde{z}_i^0, \tilde{z}_j^0) > d_{T^0}(\tilde{y}_i^0, \tilde{z}_i^0) + d_{T^0}(\tilde{y}_j^0, \tilde{z}_j^0),
\]

and

\[
d_{T^\#}(\tilde{y}_i^\#, \tilde{z}_i^\#) + d_{T^\#}(\tilde{y}_j^\#, \tilde{z}_j^\#) > d_{T^\#}(\tilde{y}_i^\#, \tilde{y}_j^\#) + d_{T^\#}(\tilde{z}_i^\#, \tilde{z}_j^\#),
\]

which, with (41), implies

\[
d_{T^0}(\tilde{y}_i^0, \tilde{y}_j^0) + d_{T^0}(\tilde{z}_i^0, \tilde{z}_j^0) > d_{T^\#}(\tilde{y}_i^\#, \tilde{y}_j^\#) + d_{T^\#}(\tilde{z}_i^\#, \tilde{z}_j^\#).
\]

Hence one of the following must hold

\[
d_{T^0}(\tilde{y}_i^0, \tilde{y}_j^0) > d_{T^\#}(\tilde{y}_i^\#, \tilde{y}_j^\#) \quad \text{or} \quad d_{T^0}(\tilde{z}_i^0, \tilde{z}_j^0) > d_{T^\#}(\tilde{z}_i^\#, \tilde{z}_j^\#).
\]

Without loss of generality, assume that \( d_{T^0}(\tilde{y}_i^0, \tilde{y}_j^0) > d_{T^\#}(\tilde{y}_i^\#, \tilde{y}_j^\#) \).

To bound \( d_{T^\#}(\tilde{y}_i^\#, \tilde{y}_j^\#) \), we need an explicit bound on \( C' \).

**Claim 5.9 (Distance to witnesses).** We have

\[
C' \leq 3g\Upsilon \log_2 \left( \frac{4g\Upsilon}{1 - 1/\sqrt{2}} \right),
\]

for \( \ell \) large enough (depending on \( g, \Upsilon \)).

**Proof.** Let \( x \in \mathcal{W}^\# \) and let \( \tilde{x} \) be a child of \( x \). Assume all vertices in \( \mathcal{V}_x^\# \) within graph distance \( C' - 1 \) are in \( \mathcal{W}_x^\# \). Note that the subtree of \( T^\# \) spanned by \( \mathcal{V}_x^\# \) is not necessarily bifurcating. However, because 1) all vertices in \( \mathcal{V}_x^\# \) are in a \( G \)-cluster, 2) every \( \ell \) levels of a \( G \)-cluster below an \( \ell \)-vertex has at most one vertex of \( T^0 \) missing, and 3) every edge in a \( G \)-cluster of \( T^0 \) corresponds to at most \( g\Upsilon \) edges in \( T^\# \), we have that within graph distance \( C' \) of \( x \) there is at least

\[
\frac{1}{2}(2^{\ell} - 1)C'_x.
\]
vertices in $W_x^\#$ below $\bar{x}$, where we counted only the furthest vertices within this ball. Hence the sum in (40) restricted to vertices below $\bar{x}$ satisfies
\[
\sum_{y \in W_x^\#} 2^{-d_{2gT}(x,y)} \geq \frac{1}{2} (2^\ell - 1) \frac{c'_T}{2gT} 2^{-c'_T} \geq \frac{1}{2} 2^\ell \frac{c'_T}{2gT} > \frac{2g\Upsilon}{1 - 1/\sqrt{2}},
\]
for $\ell$ large enough (depending on $g$, $\Upsilon$), if
\[
C' > 3g\Upsilon \log_2 \left( \frac{4g\Upsilon}{1 - 1/\sqrt{2}} \right).
\]

\textbf{Co-hanging pairs.} Note that the roots of $T^0$ and $T^\#$ may not be consistent, in the sense that the $G$-clusters and their matching subtrees may not be rooted at corresponding vertices. However we can make it so that the test subtrees are rooted consistently.

For every test panel constructed above, using the same notation, we proceed as follows. If $\bar{y}_i^0$ is on the path between the root of $G_i$ in $T^0$ and the (possibly extra) vertex corresponding to the root of the matching subtree in $T^\#$, we move $\bar{y}_i^0$ over to one of its immediate children such that the corresponding vertex $\bar{y}_i^0$ is not on this path unless $\bar{y}_i^0$ is a descendant of that vertex. In that case, we instead move $\bar{y}_i^0$ over to the child of its other immediate child such that the corresponding vertex $\bar{y}_i^0$ is not on the path above. The reason we need these two cases is that we seek to preserve the inequality
\[
d_{T^0}(\bar{y}_i^0, \bar{y}_j^0) > d_{T^\#}(\bar{y}_i^0, \bar{y}_j^0).
\]
In both cases, the two sides of the inequality increase by the same amount, at most $2g$. We do the same on $G_j$.

At this point, 1) the $G$-cluster of $T^0$ rooted at $\bar{y}_i^0$ and the matching subtree rooted at $\bar{y}_i^0$ are rooted consistently (and similarly for $\bar{y}_j^0$ and $\bar{y}_j^0$) and 2) the $G$-clusters rooted at $\bar{y}_i^0$ and $\bar{y}_j^0$ are co-hanging (and similarly for the matching subtrees in $T^\#$).

Let $y_i^0$ be a closest $G$-vertex below $\bar{y}_i^0$ on $G_i$ and similarly for $y_j^0$. Let $y_i^\#$ and $y_j^\#$ be the corresponding vertices in $T^\#$. Then the test subtrees (that is the $G$-clusters) $Y_i^0$, $\bar{Y}_i^0$ and $\bar{Y}_j^\#$ rooted respectively at $y_i^0$, $y_j^0$ are co-hanging. In particular, they are non-intersecting by construction. Indeed, $(\bar{Y}_i^0, \bar{Y}_j^0)$ belong to different $G$-clusters in $T^0$ and $(\bar{Y}_i^\#, \bar{Y}_j^\#)$ are on different sides below $\nu^\#$ in $T^\#$.

Moreover, by Claim 5.9, we have
\[
d_{T^\#}(y_i^\#, y_j^\#) \leq 6g\Upsilon \log_2 \left( \frac{4g\Upsilon}{1 - 1/\sqrt{2}} \right) + 2fg\Upsilon + 4 \leq \Gamma,
\]
so that the test pair $(y_i^\#, y_j^\#)$ is proximal. We also have
\[
d_{T^0}(y_i^0, y_j^0) > d_{T^\#}(y_i^\#, y_j^\#),
\]
because $d_{T^0}(\bar{y}_i^0, \bar{y}_j^0) > d_{T^\#}(\bar{y}_i^0, \bar{y}_j^0)$, $d_{T^0}(\bar{y}_i^0, y_i^0) = d_{T^\#}(\bar{y}_i^0, y_i^0)$, for $\nu = i, j$, and $y_i^0$ is below $\bar{y}_i^0$ for $* = 0, \#$ and $\nu = i, j$.  

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**Sparsification.** It remains to satisfy the global requirements of the battery. Unlike the many-$\Gamma$ case, we need to make the collection of test pairs sparser in both $T^#$ and $T^0$. Indeed, although there is no overlap in $T^0$, in constructing the tests we may have used the same maximal $G$-cluster repeatedly. Hence there is in fact no guarantee that the test subtrees are not overlapping in $T^0$. In $T^#$, test subtrees may also be overlapping, whether or not they belong to the same $G$-cluster. Moreover, although the test subtrees are co-hanging and proximal in $T^#$, we must ensure that the connecting paths do not intersect with other test subtrees or their connecting paths.

Let
\[ C_w = 3gY \log_2 \left( \frac{4gY}{1 - 1/\sqrt{2}} \right) + 2\ell g + 2. \]

Let \( \{(y_i^0, y_j^0); (y_i^#, y_j^#)\}_{(i,j) \in H'} \) be the test panels constructed above, where by Claim 5.8,
\[ |H'| \geq \frac{1}{10} \cdot \frac{1}{2} \cdot \frac{\Delta}{C_C} = \frac{\Delta}{20C_C}. \]

Let \( \{(Y_i^0, Y_j^0); (Y_i^#, Y_j^#)\}_{(i,j) \in H'} \) be the test panels corresponding to \( H' \).

**Claim 5.10 (Sparsification).** There is a subset \( H \subseteq H' \) of size
\[ |H| \geq \frac{1}{1 + 2^6\gamma t + C_w + 4} |H'| \geq \frac{\Delta}{20C_C(1 + 2^6\gamma t + C_w + 4)} \]
and \((\ell, 5)\)-dense modified test subtrees \( \{(Y_i^0, Y_j^0); (Y_i^#, Y_j^#)\}_{(i,j) \in H} \) such that the test panels in \( H \) satisfy the requirements of a battery.

**Proof.** We proceed in two phases. First we choose a subset of test panels such that the test vertices in different panels are far away from each other. Then we cleave subtrees of the $G$-clusters rooted at the test vertices to ensure that proximal/semi-proximal connecting paths and non-proximal hats do not intersect with test subtrees.

Start with an arbitrary test panel \( \{(y_i^0, y_j^0); (y_i^#, y_j^#)\} \) in \( H' \). Remove from \( H' \) all test panels \( (i', j') \) such that
\[ \min\{d^#_{T^#}(v, w) : v \in \{y_i^0, y_j^0\}, w \in \{y_i^#, y_j^#\}\} \leq 6\gamma t, \quad (42) \]
or
\[ \min\{d^#_{T^0}(v, w) : v \in \{y_i^0, y_j^0\}, w \in \{y_i^#, y_j^#\}\} \leq 6\gamma t. \quad (43) \]

There are at most \( 2 \cdot 2^6\gamma t + 1 \) vertices within graph distance \( 2\gamma t \) of a test pair. Note, however, that some vertices may be used as a test vertex multiple times. Nevertheless we claim that each vertex can be used at most a constant number of times. Indeed, consider a vertex \( y_i^0 \) in \( T^0 \) with corresponding vertex \( y_i^# \) in \( T^# \).

Because each test panel is obtained from a \#-overlap-shallow vertex within graph distance \( C_w \) in \( T^# \) and that each such \#-overlap-shallow vertex produces exactly one test panel, \( y_i^0 \) can arise in this way at most \( 2^{C_w + 1} \) times. Therefore we remove at most \( 2^{6\gamma t + C_w + 3} \) test pairs in \( T^0 \). The same argument applies to test vertices in \( T^# \).

Hence the total number of test panels removed is at most \( 2^{6\gamma t + C_w + 4} \).

Pick a remaining test pair in \( H' \). Proceed as above and then repeat until all pairs in \( H' \) have been picked or removed. At the end of the procedure, there are at least
\[ \frac{1}{1 + 2^6\gamma t + C_w + 4} |H'| \]
test panels remaining, the set of which we denote by \( H \). Recalling that \( \gamma t \geq \Gamma \), in \( H \), the connecting paths of proximal/semi-proximal pairs and the hats of non-proximal pairs cannot intersect with each other.
by (42) and (43) as it would imply the existence of test vertices in different panels at graph distance less than $2\gamma_t \leq 6\gamma_t$.

For each $(i, j) \in \mathcal{H}$, it remains to define the corresponding test subtrees $((Y_i^0, Y_j^0); (Y_i^{\#}, Y_j^{\#}))$. Let $((Y_i^0, Y_j^0); (Y_i^{\#}, Y_j^{\#}))$ be as above and note that, since we may have re-used the same $\mathbb{G}$-clusters multiple times, these subtrees may not satisfy the global requirements of a battery as they may intersect with each other or with connecting paths and hats. We modify $Y_i^0$ as follows, and proceed similarly for $Y_j^0$. For each $(i', j') \in \mathcal{H}$ not equal to $(i, j)$ and each subtree $Z \in \{Y_{i'}, Y_{j'}^0\}$, if $Z$ has its root below the root of $Y_i^0$, remove from $Y_i^0$ all those nodes in $Z$ as well as all descendants of the vertices on the upward path of length $2\gamma_t$ starting at the root of $Z$. Note that the latter path cannot reach $y_i^0$ because both $y_i^0$ and $y_j^0$ are at graph distance at least $6\gamma_t$ from $y_i^0$ from the construction of $\mathcal{H}$. We let $Y_i^0$ be the remaining subtree in $T^0$ and $Y_i^{\#}$, its matching subtree in $T^\#$.

We claim that the resulting restricted subtrees $(Y_i^0, Y_j^0)$ are $(\ell, 3)$-dense. Note first that the subtrees in $(Y_i^0, Y_j^0)_{(i,j) \in \mathcal{H}}$ are $(\ell, 1)$-dense as they were obtained from the procedure in Section 5.3. Moreover, because 1) the roots of the removed subtrees are at graph distance at most $2\gamma_t$ from a $\ell$-vertex in $(y_i^0, y_j^0)_{(i,j) \in \mathcal{H}}$, 2) test vertices in different pairs are at graph distance at least $6\gamma_t$ from each other, and 3) $\gamma_t$ is a multiple of $\ell$, if we remove a subtree rooted at a $\mathbb{G}$-child of a $\mathbb{G}$-vertex in $(Y_i^0, Y_j^0)$ we cannot remove more than one other subtree rooted at another $\mathbb{G}$-child of the same $\mathbb{G}$-vertex as that would imply the existence of two test vertices in different pairs at graph distance less than

$$2(2\gamma_t) + 2g\ell < 6\gamma_t,$$

in $T^0$, a contradiction.

We then proceed similarly in $T^\#$. The resulting restricted subtrees

$$\{(Y_i^0, Y_j^0); (Y_i^{\#}, Y_j^{\#})\}_{(i,j) \in \mathcal{H}},$$

are then $(\ell, 5)$-dense (in fact, $(\ell, 4)$-dense as there are no non-proximal pairs in $T^\#$).

\[ \square \]

**Summary of the large overlap case.** We have proved the following in the large overlap case. Recall that $\varphi = 5$, $\ell = \ell(g, \varphi)$ is chosen as in Proposition 1,

$$\Gamma = 6g \Upsilon \log_2 \left( \frac{4g \Upsilon}{1 - 1/\sqrt{2}} \right) + 2g \Upsilon + 4,$$

and $\gamma_t \geq \Gamma$, a multiple of $\ell$, and $C$ are chosen as in Proposition 1.

**Proposition 5** (Battery in the large overlap case). In the large overlap case, we can build a $(\ell, \varphi, \Gamma, \gamma_t, I)$-battery

$$\{(y_i^0, z_i^0); (Y_i^0, Z_i^0)\}_{i=1}^I \text{ (in } T^0 \text{)} \text{ and } \{(y_i^\#, z_i^\#); (Y_i^\#, Z_i^\#)\}_{i=1}^I \text{ (in } T^\# \text{)}$$

with

$$I \geq \frac{\Delta}{20C^2 \sigma (1 + 2^6 \gamma + C^w + 4)}.$$

**Proof.** The result follows from Claim 5.10. \[ \square \]
Acknowledgments

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A  Preliminary lemmas

In this section, we collect a few useful lemmas.

A.1 Ancestral reconstruction

An important part of our construction involves reconstructing ancestral states. We will use the following lemma from [EKPS00] which we typically apply to a rooted subtree. Let $T = (V, E; \phi; w) \in Y$ rooted at $\rho$. Let $e = (x, y) \in E$ and assume that $x$ is closest to $\rho$ (in topological distance). We define $P(\rho, e) = P(\rho, y)$, $|e|_{\rho} = |P(\rho, e)|$, and $R_{\rho}(e) = (1 - \theta_{e}^{2}) \Theta_{\rho,y}^{-2}$, where $\Theta_{\rho,y} = e - d_{T}(\rho, y)$ and $\theta_{e} = e - w_{e}$.

Lemma 2 (Ancestral reconstruction [EKPS00]). For any unit flow $\Psi$ from $\rho$ to $[n]$.

$$\mathbb{E}_{T} \left[ |P_{T}[\sigma_{\rho} = +1| \sigma_{X}] - P_{T}[\sigma_{\rho} = -1| \sigma_{X}] | \right] \geq \frac{1}{1 + \sum_{e \in E} R_{\rho}(e)\Psi(e)^{2}},$$

(44)

where the LHS is the difference between the probability of correct and incorrect reconstruction using MLE. (See [EKPS00, Equation (14), Lemma 5.1 and Theorem 1.2˚].)

A.2 Random cluster representation

We use a convenient percolation-based representation of the CFN model known as the random cluster model (see e.g. [Gri06]). Let $T = (V, E; \phi; w) \in Y$ with corresponding $\delta_{e} \in E$. (See Example ??.)

Lemma 3 (Random cluster representation). Run a percolation process on $T$ where edge $e$ is open with probability $1 - 2\delta_{e}$. Then associate to each open connected component a state according to the uniform distribution on $\{+1, -1\}$. The state vector on the vertices so obtained $(\sigma_{v})_{v \in V}$ has the same distribution as the corresponding CFN model.

A.3 Concentration inequalities

Recall the following standard concentration inequalities (see e.g. [MR95]):

Lemma 4 (Azuma-Hoeffding Inequality). Suppose $Z = (Z_{1}, \ldots, Z_{m})$ are independent random variables taking values in a set $S$, and $h : S^{m} \to \mathbb{R}$ is any $t$-Lipschitz function: $|h(z) - h(z')| \leq t$ whenever $z, z' \in S^{m}$ differ at just one coordinate. Then, $\forall \zeta > 0$,

$$\mathbb{P} \left[ |h(Z) - \mathbb{E}[h(Z)] | \geq \zeta \right] \leq 2 \exp \left( -\frac{\zeta^{2}}{2t^{2}m} \right).$$

Lemma 5 (Chernoff bounds). Let $Z_{1}, \ldots, Z_{m}$ be independent Poisson trials such that, for $1 \leq i \leq m$,

$$\mathbb{P}[Z_{i} = 1] = p_{i} \text{ where } 0 < p_{i} < 1.$$

Then, for $Z = \sum_{i=1}^{m} Z_{i}$, $M = \mathbb{E}[Z] = \sum_{i=1}^{m} p_{i}$, $0 < \delta_{-} \leq 1$, and $\delta_{+} > 2e - 1$,

$$\mathbb{P}[Z < (1 - \delta_{-})M] < e^{-M\delta^{2}/2},$$

and

$$\mathbb{P}[Z > (1 + \delta_{+})M] < 2^{-(1+\delta_{+})M}.$$