Efficient and consistent inference of ancestral sequences in an evolutionary model with insertions and deletions under dense taxon sampling

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Abstract

In evolutionary biology, the speciation history of living organisms is represented graphically by a phylogeny, that is, a rooted tree whose leaves correspond to current species and branchings indicate past speciation events. Phylogenies are commonly estimated from molecular sequences, such as DNA sequences, collected from the species of interest. At a high level, the idea behind this inference is simple: the further apart in the Tree of Life are two species, the greater is the number of mutations to have accumulated in their genomes since their most recent common ancestor. In order to obtain accurate estimates in phylogenetic analyses, it is standard practice to employ statistical approaches based on stochastic models of sequence evolution on a tree. For tractability, such models necessarily make simplifying assumptions about the evolutionary mechanisms involved. In particular, commonly omitted are insertions and deletions of nucleotides—also known as indels.

Properly accounting for indels in statistical phylogenetic analyses remains a major challenge in computational evolutionary biology. Here we consider the problem of reconstructing ancestral sequences on a known phylogeny in a model of sequence evolution incorporating nucleotide substitutions, insertions and deletions, specifically the classical TKF91 process. We focus on the case of dense phylogenies of bounded height, which we refer to as the taxon-rich setting, where statistical consistency is achievable. We give the first polynomial-time ancestral reconstruction algorithm with provable guarantees under constant rates of mutation. Our algorithm succeeds when the phylogeny satisfies the “big bang” condition, a necessary and sufficient condition for statistical consistency in this context.

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1 Introduction

**Background** In evolutionary biology, the speciation history of living organisms is represented graphically by a phylogeny, that is, a rooted tree whose leaves correspond to current species and branchings indicate past speciation events. Phylogenies are commonly estimated from molecular sequences, such as DNA sequences, collected from the species of interest. At a high level, the idea behind this inference is simple: the further apart in the Tree of Life are two species, the greater is the number of mutations to have accumulated in their genomes since their most recent common ancestor. In order to obtain accurate estimates in phylogenetic analyses, it is standard practice to employ statistical approaches based on stochastic models of sequence evolution on a tree. For tractability, such models necessarily make simplifying assumptions about the evolutionary mechanisms involved. In particular, commonly omitted are insertions and deletions of nucleotides—also known as indels. Properly accounting for indels in statistical phylogenetic analyses remains a major challenge in computational evolutionary biology.

Here we consider the related problem of reconstructing ancestral sequences on a known phylogeny in a model of sequence evolution incorporating nucleotide substitutions as well as indels. The model we consider, often referred to as the TKF91 process, was introduced in the seminal work of Thorne et al. [TKF91] on the multiple sequence alignment problem (see also [TKF92]). Much is known about ancestral sequence reconstruction (ASR) in substitution-only models. See, e.g., [EKPS00, Mos01, Sly09] and references therein, as well as [Lib07] for applications in biology. In the presence of indels, however, the only previous ASR result was obtained in [ADHR12] for vanishingly small indel rates in a simplified version of the TKF91 process. (In related work, Daskalakis and Roch [DR13] devised the first polynomial-time phylogenetic tree reconstruction algorithm for sequences in the presence of indels.) The results in [ADHR12] concern what is known as “solvability”; roughly, a sequence is inferred that exhibits a correlation with the true root sequence bounded away from 0 uniformly in the depth of the tree. The ASR problem in the presence of indels is also related to the trace reconstruction problem. See, e.g., [M +09] and references therein.

**Our results** A desirable property of a reconstruction method is statistical consistency, which roughly says that the reconstruction is correct with probability tending to one as the amount of data increases. It is known [EKPS00] that this is typically not information-theoretically achievable in the standard setting of the ASR problem. Here, however, we consider the taxon-rich context, in which we have a sequence of trees with uniformly bounded heights and growing number of leaves. Building on the work of Gascuel and Steel [GS10], a necessary and sufficient condition for consistent ancestral reconstruction was derived in [FR17, Theorem 1] in this context. In the current paper, we establish statistical consistency for the ASR problem in the TKF91 process in the taxon-rich context.

In fact, an ASR statistical consistency result for the TKF91 process in the taxon-rich context is already implied by the general results of [FR17]. However, the estimator in [FR17] is not useful from a computational point of view. Indeed it relies on the computation of total variation distances between leaf distributions for different root states—and we are not aware of a tractable way to do these computations in TKF models. The main contribution here is the design of an estimator which is not only consistent but also computationally efficient. We obtain this estimator by first
estimating the length of the ancestral sequence, then estimating the sequence itself conditioned on the sequence length. The latter is achieved by deriving explicit formulas to invert the mapping from the root sequence to the distribution of the leaf sequences. (In statistics, this is known as an identifiability result.)

Outline In Section 2, we first recall the definition of the TKF91 process and our key assumptions on the sequence of trees. We then describe our new estimator and state the main results. In Section 3, we give some intuition behind the definition of our estimator by giving a constructive proof of root-state identifiability for the TKF91 model. The proofs of the main results are given in Section B. Some basic properties of the TKF91 process are derived in Section A.

2 Definitions and main results

Before stating our main results, we begin by describing the TKF91 model of Thorne, Kishino and Felsenstein [TKF91], which incorporates both substitutions and insertions/deletions (or indels for short) in the evolution of a DNA sequence on a phylogeny. For simplicity, we follow Thorne et al. and use the F81 model [Fel81] for the substitution component of the model, although our results can be extended beyond this simple model. For ease of reference, a number of useful properties of the TKF91 model are derived in Section A.

2.1 TKF91 process

We first describe the Markovian dynamics on a single edge of the phylogeny. Conforming with the original definition of the model [TKF91], we use an “immortal link” as a stand-in for the empty sequence.

Definition 1 (TKF91 sequence evolution model on an edge). The TKF91 edge process is a Markov process \( \mathcal{I} = (\mathcal{I}_t)_{t \geq 0} \) on the space \( S \) of DNA sequences together with an immortal link “\( \bullet \)”, that is,

\[ S := "\bullet" \otimes \bigcup_{M \geq 0} \{A,T,C,G\}^M, \tag{1} \]

where the notation above indicates that all sequences begin with the immortal link (and can otherwise be empty). We also refer to the positions of a sequence (including nucleotides and the immortal link) as sites. Let \( (\nu, \lambda, \mu) \in (0, \infty)^3 \) with \( \lambda < \mu \) and \( (\pi_A, \pi_T, \pi_C, \pi_G) \in [0, \infty)^4 \) with \( \pi_A + \pi_T + \pi_C + \pi_G = 1 \) be given parameters. The continuous-time Markovian dynamic is described as follows: if the current state is the sequence \( \bar{x} \), then the following events occur independently:

- **(Substitution)** Each nucleotide (but not the immortal link) is substituted independently at rate \( \nu > 0 \). When a substitution occurs, the corresponding nucleotide is replaced by \( A, T, C \) and \( G \) with probabilities \( \pi_A, \pi_T, \pi_C \) and \( \pi_G \) respectively.

- **(Deletion)** Each nucleotide (but not the immortal link) is removed independently at rate \( \mu > 0 \).
Each site gives birth to a new nucleotide independently at rate $\lambda > 0$. When a birth occurs, a nucleotide is added immediately to the right of its parent site. The newborn site has nucleotide $A$, $T$, $C$ and $G$ with probabilities $\pi_A$, $\pi_T$, $\pi_C$ and $\pi_G$ respectively.

The length of a sequence $\vec{x} = (\bullet, x_1, x_2, \ldots, x_M)$ is defined as the number of nucleotides in $\vec{x}$ and is denoted by $|\vec{x}| = M$ (with the immortal link alone corresponding to $M = 0$). When $M \geq 1$ we omit the immortal link for simplicity and write $\vec{x} = (x_1, x_2, \ldots, x_M)$.

The TKF91 process is reversible [TKF91]. Suppose furthermore that $0 < \lambda < \mu$, an assumption we make throughout. Then it has a stationary distribution $\Pi$, given by

$$
\Pi(\vec{x}) = \left(1 - \frac{\lambda}{\mu}\right) \left(\frac{\lambda}{\mu}\right)^M \prod_{i=1}^{M} \pi_{x_i}
$$

for each $\vec{x} = (x_1, x_2, \ldots, x_M) \in \{A, T, C, G\}^M$ where $M \geq 1$, and $\Pi(" \bullet ") = \left(1 - \frac{1}{\mu}\right)$. In words, under $\Pi$, the sequence length is geometrically distributed and, conditioned on the sequence length, all sites are independent with distribution $(\pi_{\sigma})_{\sigma \in \{A, T, C, G\}}$.

We run the TKF91 model on a tree. Let $T = (V, E, \rho, \ell)$ be a phylogeny (or, simply, tree), that is, a finite, edge-weighted, rooted tree, where $V$ is the set of vertices, $E$ is the set of edges oriented away from the root $\rho$, and $\ell : E \to (0, +\infty)$ is a positive edge-weighting function. We denote by $\partial T$ the leaf set of $T$. No assumption is made on the degree of the vertices. We think of $T$ as a continuous object, where each edge $e$ is a line segment of length $\ell(e)$ and whose elements $\gamma \in e$ we refer to as points. We let $\Gamma_T$ be the set of points of $T$. We consider the following stochastic process indexed by the points of $T$.

**Definition 2 (TKF91 sequence evolution model on a tree).** The root is assigned a state $\vec{X}_\rho \in S$, which is drawn from the stationary distribution $\Pi$ of the TKF91 edge process. The state is then evolved down the tree according to the following recursive process. Moving away from the root, along each edge $e = (u, v) \in E$, conditionally on the state $\vec{X}_u$, we run the TKF91 edge process as described in Definition 1 started at $\vec{X}_u$ for an amount of time $\ell(u, v)$. We denote by $\vec{X}_\gamma$ the resulting state at $\gamma \in e$. We call the process $(\vec{X}_\gamma)_{\gamma \in \Gamma_T}$ a TKF91 process on tree $T$.

Our main interest is in the following statistical problem.

### 2.2 Root reconstruction and the big bang condition

In the root reconstruction problem, we seek to estimate the root state $\vec{X}_\rho$ based on the leaf states $\vec{X}_{\partial T} = \{\vec{X}_v : v \in \partial T\}$ of a TKF91 process on a known tree $T$. More formally, we look here for a consistent estimator, as defined next. Fix mutation parameters $(\nu, \lambda, \mu) \in (0, \infty)^3$ with $\lambda < \mu$ and $(\pi_A, \pi_T, \pi_C, \pi_G) \in [0, \infty)^4$ and let $\{T^k = (V^k, E^k, \rho^k, \ell^k)\}_{k \geq 1}$ be a sequence of trees with $|\partial T^k| \to +\infty$. Let $\vec{X}^k = (\vec{X}_\gamma)_{\gamma \in \Gamma_T}$ be a TKF91 process on $T^k$. 


**Definition 3** (Consistent root estimator). A sequence of root estimators

\[ F_k : S^\partial T_k \rightarrow S, \]

is said to be consistent for \( \{T^k\}_k \) if

\[ \lim \inf_{k \rightarrow +\infty} \mathbb{P} \left[ F_k \left( X^k_{\partial T_k} \right) = X^k_{\rho_k} \right] = 1. \]

One important remark: the mutation parameters and the sequence of trees are assumed to be known; that is, the estimators \( F_k \) may depend on them. On the other hand, the leaf sequences \( X^k_{\partial T_k} \) are the only components of the process \( \lambda^k \) that are actually observed.

As shown in [FR17], in general a sequence of consistent estimators may fail to exist. Building upon the work of Gascuel and Steel [GS10], necessary and sufficient conditions for consistent root reconstruction are derived in [FR17, Theorem 1] in the context of bounded-height, nested tree sequences with a growing number of leaves, which we refer to as the taxon-rich setting. These conditions have a combinatorial component (the big bang condition) and a stochastic component (initial-state identifiability, to which we come back in Section 3). To state the combinatorial condition formally, we need a few more definitions:

- **(Nested trees)** Let \( T = (V, E, \rho, \ell) \) be a tree. For a subset of leaves \( L \subset \partial T \), the restriction of \( T \) to \( L \) is the tree obtained from \( T \) by keeping only those points on a path between the root \( \rho \) and a leaf \( u \in L \). We say that \( \{T^k\}_k \) is a nested sequence if for all \( k > 1 \), \( T^{k-1} \) is a restriction of \( T^k \). Without loss of generality, we assume that \( |\partial T^k| = k \), so that \( T^k \) is obtained by adding a leaf edge to \( T^{k-1} \). (More general sequences can be obtained as subsequences.) In a slight abuse of notation, we denote by \( \ell \) the edge-weight function for all \( k \). For \( \gamma \in \Gamma_T \), we denote by \( \ell_{\gamma} \) the length of the unique path from the root \( \rho \) to \( \gamma \). We refer to \( \ell_{\gamma} \) as the distance from \( \gamma \) to the root.

- **(Bounded height)** We further say that \( \{T^k\}_k \) has uniformly bounded height if

\[ h^* := \sup_k h^k < +\infty, \]  

where \( h^k := \max\{\ell_x : x \in \partial T^k\} \) is the height of \( T^k \).

- **(Big bang)** For a tree \( T = (V, E, \rho, \ell) \), let

\[ T(s) = \{\gamma \in \Gamma_T : \ell_{\gamma} \leq s\} \]

denote the tree obtained by truncating \( T \) at distance \( s \) from the root. We refer to \( T(s) \) as a truncation of \( T \). (See the left side of Figure 1 for an illustration.) We say that a sequence of trees \( \{T^k\}_k \) satisfies the big bang condition if: for all \( s \in (0, +\infty) \), we have \( |\partial T^k(s)| \rightarrow +\infty \) as \( k \rightarrow +\infty \). (See Figure 2 for an illustration.)

Finally we are ready to state our main combinatorial assumption.

**Assumption 1** (Taxon-rich setting: big bang condition). We assume that \( \{T^k\}_k \) is a nested sequence of trees with common root \( \rho \), has uniformly bounded height, and satisfies the big bang condition.

In words, the big bang condition ensures the existence of a large number of leaves that are “almost conditionally independent” given the root state, which can be shown to be necessary for consistency [FR17].
2.3 Main results

In our main result, we devise and analyze a sequence of computationally efficient and statistically consistent root estimators for the TKF91 model under Assumption 1. We first describe the root reconstruction algorithm.

**Root reconstruction algorithm** The **input data** are the mutation parameters \((\nu, \lambda, \mu) \in (0, \infty)^3\) and \((\pi_A, \pi_T, \pi_C, \pi_G) \in [0, \infty)^4\) and, for \(k \geq 1\), the tree \(T^k\) together with the leaf states \(\{\bar{X}_v : v \in \partial T^k\}\). Our root reconstruction algorithm has three main steps: to control correlations among leaves, we follow [FR17] and extract a “well-spread” restriction of \(T^k\) (Step 1); then, using only the leaf states on this restriction, we estimate the root sequence length (Step 2) and finally the root sequence itself (Step 3). Motivation behind the construction of the estimator will be given in the Section 3.

We let \((s_k)_k\) be an arbitrary sequence such that \(s_k > 0\) and \(s_k \downarrow 0\) as \(k \to +\infty\). We also fix \(0 \leq t_1 < t_2 < \cdots < \infty\) (e.g., \(t_j = j\) will do). We need the following functions which arise naturally in the TKF91 process (see Section A for details)

\[
\eta(t) = \frac{\mu - \mu e^{(\lambda-\mu)t}}{\mu - \lambda e^{(\lambda-\mu)t}},
\]
\[
\phi(t) = \frac{1 - \gamma\eta(t)}{1 - \eta(t)},
\]
\[
\psi(t) = (1 - \gamma\eta(t))^2 e^{-(\mu+\nu)t},
\]
where $\gamma = \lambda/\mu$. For simplicity, we write
\[ \eta_j = \eta(h^* + t_j), \phi_j = \phi(h^* + t_j) \text{ and } \psi_j = \psi(h^* + t_j). \]

Finally, we use the notation $[[x]]$ for the unique integer such that $[[x]] - 1/2 \leq x < [[x]] + 1/2$.

**Root estimator**

- **Step 1: Restriction**
  - Fix $s := s_k$ and denote $\partial T_k(s) = \{z_1, \ldots, z_m\}$.
  - For each $z_i$, pick an arbitrary leaf $x_i \in \partial T_{[z_i]}^k$ in the subtree $T_{[z_i]}^k$ of $T^k$ rooted at $z_i$.
  - Set $\tilde{T}^k,s$ to be the restriction of $T^k$ to $\{x_1, \ldots, x_m\}$.

- **Step 2: Length estimator**
  - Compute the root sequence-length estimator
  \[ M^{k,*} = \left[ \frac{1}{|\partial T^k,s|} \sum_{v \in \partial \tilde{T}^k,s} (|\tilde{X}_v| e^{(\mu - \lambda)\ell_v} + \frac{\lambda}{\mu} - \frac{\lambda}{\mu} (1 - e^{(\mu - \lambda)\ell_v})) \right]. \]

- **Step 3: Sequence estimator**
  - Compute the conditional frequency estimator
  \[ f^k,s_\sigma(t_j) = \frac{1}{|\partial T^k,s|} \sum_{v \in \partial \tilde{T}^k,s} p^\sigma_{\tilde{X}_v}(t_j + h^* - \ell_v) \]
  \[ \text{for } 1 \leq j \leq M^{k,*} \text{ and } \sigma \in \{A, T, C, G\}, \]
  \[ p^\sigma_{\tilde{X}}(t) = \pi_{\sigma} \phi(t) \left[ 1 - (\eta(t))^{1/|\tilde{x}|} \right] + \psi(t) \sum_{i=1}^{|\tilde{x}|} 1_{\{x_i=\sigma\}} (\eta(t))^{i-1} + \pi_{\sigma} \gamma \eta(t), \]
  \[ \text{when } \tilde{x} = (x_1, x_2, \ldots, x_M). \]
  - Set $U$ to be the $M^{k,*} \times 4$ matrix with entries
  \[ U_{j,\sigma} = f^k,s_\sigma(t_j) - \pi_{\sigma} \phi_j \left[ 1 - \eta_j^{M^{k,*}} \right] - \pi_{\sigma} \gamma \eta_j, \]
  set $\Psi$ to be the $M^{k,*} \times M^{k,*}$ diagonal matrix whose diagonal entries are $\{\psi_j\}_{j=1}^{M^{k,*}}$; and set $V := V_{1,\ldots,t_{M^{k,*}}}$ to be the $M^{k,*} \times M^{k,*}$ Vandermonde matrix
  \[ V_{1,\ldots,t_{M^{k,*}}} = \begin{pmatrix} 1 & \eta_1 & \eta_1^2 & \cdots & \eta_1^{M^{k,*}-1} \\ 1 & \eta_2 & \eta_2^2 & \cdots & \eta_2^{M^{k,*}-1} \\ \vdots \\ 1 & \eta_{M^{k,*}} & \eta_{M^{k,*}}^2 & \cdots & \eta_{M^{k,*}}^{M^{k,*}-1} \end{pmatrix}. \]
  - Define $F_k\left(\tilde{X}_{\partial T^k}\right)$ to be a sequence in $\{A, T, C, G\}^{M^{k,*}}$ such that the $i$-th site satisfies
  \[ \left[ F_k\left(\tilde{X}_{\partial T^k}\right) \right]_i \in \arg \max \{ (V^{-1}\Psi^{-1}U)_{i,\sigma} : \sigma \in \{A, T, C, G\} \} . \]
  If there is more than one choice, pick one uniformly at random.
Statement of results Finally, our main claim is Theorem 1 below, which asserts that the root estimator we just described provides a consistent root estimator in the sense of Definition 3. Recall the sequence space $S$ defined in (1).

**Theorem 1** (Consistent root reconstruction). Suppose $\{T^k\}_k$ satisfies Assumption 1. Then $\{F_k\}_k$ defined in (5) is a sequence of consistent root estimators for $\{T^k\}_k$.

Our main novel contribution lies in Step 3 above, which is based on the derivation of explicit formulas to invert the mapping from the root sequence to the distribution of the leaf sequences. (In statistics, this is known as an identifiability result.) See Section 3 for an overview.

We also derive a quantitative error bound.

**Theorem 2** (Error bound). Suppose $\{T^k\}_k$ satisfies Assumption 1 and $\{F_k\}_k$ are the root estimators described in (5). Then, for any $\epsilon \in (0, \infty)$, there exist positive constants $\{C_i\}_{i=1}^3$ such that

$$P\Pi \left[ F_k(\vec{X}_{\partial T^k}) \neq \vec{X}_\rho \right] \leq \epsilon + C_1 \exp \left( -C_2 |\partial T^k(s)| \right) + C_3 s$$

for all $s \in (0, h^*/2]$ and $k \geq 1$.

3 **Key ideas in the construction of the root estimator**

In the more general context of continuous-time countable-space Markov chains on bounded-height nested trees [FR17], consistent root estimators were shown to exist under the big bang condition of Assumption 1 when, in addition, the edge process satisfies initial-state identifiability, i.e., the state of the process at time 0 is uniquely determined by the distribution of the state at any time $t > 0$. (In fact, these conditions are essentially necessary; see [FR17] for details.) Moreover, reversibility of the TKF91 process together with an observation of [FR17] implies that the TKF91 process does indeed satisfy initial-state identifiability.

The root estimators implicit in [FR17], however, are not useful from an algorithmic point of view. They rely on the computation of the total variation distance between the leaf distribution conditioned on different root states—and we are not aware of a tractable way to do these computations in the TKF91 model. In our main contribution, we give explicit, computationally efficient root estimators that are consistent under Assumption 1. The estimators are defined in Section 2.3.

In this section, we motivate these estimators by giving an alternative, constructive proof of initial-state identifiability in the TKF91 process. At a high level, Theorems 1 and 2 are then established along the following lines: the big bang condition ensures the existence of a large number of leaves whose states are almost independent conditioned on the root state, and concentration arguments imply that the sample version of the inversion formula derived in Lemma 1 below is close to the root state. See Section B for details.

Let $E_M[|I_t|]$ be the expected length of the TKF91 edge process at time $t$ starting from a sequence of length $M$, and $p^\sigma_\sigma(t)$ be the probability of observing the nucleotide $\sigma \in \{A, T, C, G\}$ as the first nucleotide of a sequence at time $t$, under the TKF91 edge process with initial state $\vec{x}$.

**Lemma 1** (Key lemma: a constructive proof of initial-state identifiability). For any $t^* \geq 0$, the following mappings are one-to-one and have explicit expressions for their inverses:
(i) the mapping \( \Phi^{(1)}_t : \mathbb{Z}_+ \to \mathbb{R}_+ \) defined by

\[
\Phi^{(1)}_t(M) = \mathbb{E}_M[|I_t^*|],
\]

(ii) the mappings \( \Phi^{(2)}_{t^* + t_1, \ldots, t^* + t_M} : \{A, T, C, G\}^M \to [0, 1]^M \) defined by

\[
\Phi^{(2)}_{t^* + t_1, \ldots, t^* + t_M}(\vec{x}) = (p^\sigma_{\vec{x}}(t^* + t_j))_{\sigma \in \{A,T,C,G\}, 1 \leq j \leq M},
\]

for any \( \vec{x} \) with \( |\vec{x}| = M \geq 1 \) and any \( 0 \leq t_1 < t_2 < \cdots < t_M < \infty \).

**Proof.** (i) The sequence length of the TKF91 edge process is a well-studied stochastic process known as a continuous-time linear birth-death-immigration process \((|I_t^*|)_{t \geq 0}\). (We give more details on this process in Section A.) The expected sequence length, in particular, is known to satisfy the following differential equation

\[
\frac{d}{dt}\mathbb{E}_M[|I_t^*|] = -(\mu - \lambda)\mathbb{E}_M[|I_t^*|] + \lambda,
\]

with initial condition \( \mathbb{E}_M[|I_0^*|] = M \), whose solution is given by

\[
\mathbb{E}_M[|I_t^*|] = M\beta_t + \frac{\gamma(1 - \beta_t)}{1 - \gamma},
\]

where \( \beta_t = e^{-(\mu - \lambda)t} \) and \( \gamma = \frac{\lambda}{\mu} \). Solving (8) for \( M \), we see that \( \Phi^{(1)}_t \) is injective with inverse

\[
(\Phi^{(1)}_t)^{-1}(z) = \frac{1}{\beta_t} \left( z - \frac{\gamma(1 - \beta_t)}{1 - \gamma} \right).
\]

(ii) For \( \Phi^{(2)} \), we make the following claim regarding the probability of observing \( \sigma \) as the first nucleotide of a sequence at time \( t \) under the TKF91 edge process starting at \( \vec{x} \) with \( |\vec{x}| \geq 1 \), which we denote by \( \mathbb{P}_{\vec{x}}(I_t = [\sigma \cdots]) \). Recall the definition of \( p^\sigma_{\vec{x}}(t) \) in (4).

**Claim 1 (Probability of first nucleotide).** We have

\[
\mathbb{P}_{\vec{x}}(I_t = [\sigma \cdots]) = p^\sigma_{\vec{x}}(t),
\]

for all nucleotide \( \sigma \in \{A, T, C, G\} \), sequence \( \vec{x} \in S \) and time \( t \in (0, \infty) \).

**Proof.** We use some notation of [TKF91], where a nucleotide is also referred to as a “normal link” and a generic such nucleotide is denoted “\( \star \)”. We define

\[
\begin{align*}
p_k &:= p_k(t) := \mathbb{P}_\star(\text{normal link “\( \star \)” survives and has } k \text{ descendants including itself}), \\
p'_k &:= p'_k(t) := \mathbb{P}_\star(\text{normal link “\( \star \)” dies and has } k \text{ descendants}), \\
p''_k &:= p''_k(t) := \mathbb{P}_\bullet(\text{immortal link “\( \bullet \)” has } k \text{ descendants including itself}).
\end{align*}
\]
We decompose the event \( \mathcal{I}_t = [\sigma \cdots] \) according to whether the first nucleotide is the descendant of the immortal link "•" or the descendant of \( v_i \) for \( 1 \leq i \leq |v| \). That is,

\[
\mathbb{P}_{v} (\mathcal{I}_t = [\sigma \cdots]) = \sum_{i=1}^{|v|} \mathbb{P}_{v} (\mathcal{I}_t = [\sigma \cdots], \text{first nucleotide descends from } v_i) \\
+ \mathbb{P}_{v} (\mathcal{I}_t = [\sigma \cdots], \text{first nucleotide descends from immortal link "•"}).
\]

We now compute each term on the RHS. The last term

\[
\mathbb{P}_{v} (\mathcal{I}_t = [\sigma \cdots], \text{first nucleotide descends from immortal link "•"}) \\
= \pi_\sigma \sum_{k=2}^\infty p_k'' = \pi_\sigma (1 - \gamma \eta) \sum_{k=2}^\infty (\gamma \eta)^{k-1} = \pi_\sigma \gamma \eta,
\]

where the first equality is obtained by further decomposing the event according to the number of descendants of the ancestor of the first nucleotide. Similarly, for \( 1 \leq i \leq |v| \), we have

\[
\mathbb{P}_{v} (\mathcal{I}_t = [\sigma \cdots], \text{first nucleotide descends from } v_i) \\
= p_i'' (p'_0)^{i-1} \left[ f_{v_i,\sigma} \sum_{k=1}^\infty p_k + \pi_\sigma \sum_{k=1}^\infty p'_k \right] \\
= p_i'' (p'_0)^{i-1} \left[ f_{v_i,\sigma} e^{-\mu t} (1 - \gamma \eta) + \pi_\sigma (1 - e^{-\mu t} - \eta) \right],
\]

where

\[
f_{ij} := f_{ij}(t) = \pi_j (1 - e^{-\mu t}) + e^{-\mu t} 1_{i=j}
\]
is the transition probabilities that a nucleotide is of type \( j \) after time \( t \), given that it is of type \( i \) initially. In the first equality (13), the term \( f_{v_i,\sigma} p_k \) is the probability that, during \([0, t]\), \( v_i \) survives and has \( k \) descendants including itself (and the first nucleotide of the sequence is \( \sigma \)); the term \( \pi_\sigma p'_k \) is the probability that \( v_i \) dies and has \( k \) descendants (and the first nucleotide of the sequence is \( \sigma \)).

From (11), (12) and (13) we have

\[
\mathbb{P}_{v} (\mathcal{I}_t = [\sigma \cdots]) = \sum_{i=1}^{|v|} p_i'' (p'_0)^{i-1} \left[ f_{v_i,\sigma} e^{-\mu t} (1 - \gamma \eta) + \pi_\sigma (1 - e^{-\mu t} - \eta) \right] + \pi_\sigma \gamma \eta
\]

\[
= p_1'' e^{-\mu t} (1 - \gamma \eta) \left[ \sum_{i=1}^{|v|} (p'_0)^{i-1} f_{v_i,\sigma} \right] + p_1'' (1 - e^{-\mu t} - \eta) \pi_\sigma \sum_{i=1}^{|v|} (p'_0)^{i-1} + \pi_\sigma \gamma \eta
\]
which is exactly (10) upon further writing
\[
\sum_{i=1}^{\lvert \vec{v} \rvert} (p'_0)^{i-1} f_{v_i} = \pi_\sigma (1 - e^{-st}) \frac{1 - (p'_0)^{\lvert \vec{v} \rvert}}{1 - p'_0} + e^{-st} \sum_{i=1}^{\lvert \vec{v} \rvert} 1_{v_i = \sigma} (p'_0)^{i-1}.
\]

The proof is complete. \[\square\]

We therefore have
\[
p'^\sigma_\vec{x}(t^* + t_j) = \pi_\sigma \phi_j \left[ 1 - \eta_j^M \right] + \psi_j \sum_{i=1}^M 1_{\{x_i = \sigma\}} \eta_j^{i-1} + \pi_\sigma \gamma \eta_j,
\]

for all \( \sigma \in \{A, T, C, G\} \) and \( 1 \leq j \leq M \), where \( M = \lvert \vec{x} \rvert \). We then solve (14) for \( \vec{x} = (x_i) \in \{A, T, C, G\}^M \). System (14) is equivalent to the matrix equation
\[
H = \Psi V \chi^{\vec{x}}
\]

where \( \Psi \) and \( V \) are the \( M \times M \) matrices defined in Section 2.3, and

1. \( \chi^{\vec{x}} \) is the \( M \times 4 \) matrix whose entries are \( 1_{\{x_j = \sigma\}} \), and
2. \( H \) is the \( M \times 4 \) matrix with entries
\[
H_{j,\sigma} = p'^\sigma_\vec{x}(t^* + t_j) - \pi_\sigma \phi_j \left[ 1 - \eta_j^M \right] - \pi_\sigma \gamma \eta_j.
\]

It is well-known that the Vandermonde matrix \( V \) is invertible (see, e.g., [Gau62, Theorem 1]), so we can solve the system (15) to obtain
\[
\chi^{\vec{x}} = V^{-1} \Psi^{-1} H.
\]

Sequence \( \vec{x} \in \{A, T, C, G\}^M \) is uniquely determined by \( \chi^{\vec{x}} \). Hence, from (16), we get an explicit inverse for the mappings \( \Phi^{(2)}_{h^*+t_1, \ldots, h^*+t_M} \) defined in (7). \[\square\]

Heuristically, Steps 2 and 3 in the root estimator defined in Section 2.3 are the sample versions of the inverses of \( \Phi^{(1)}_{h^*} \) and \( \Phi^{(2)}_{h^*+t_1, \ldots, h^*+t_M} \). That is, we replace the expectation \( E_{\vec{x}|[\mathcal{I}_{h^*}]} \) and probabilities \( (p'^\sigma_\vec{x}(h^* + t_j))_{\sigma \in \{A, T, C, G\}, 1 \leq j \leq M} \) with their corresponding empirical averages. There is one further detail. The leaves of the tree are in fact at different distances from the root, rather than all at distance \( h^* \). Hence we take the empirical averages of the conditional expectation of the quantities at time \( h^* \) given the values observed at the leaves. For this, we can use again the formulas (8) and (10).
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[TKF92] Jeffrey L Thorne, Hirohisa Kishino, and Joseph Felsenstein. Inchng toward reality: an improved likelihood model of sequence evolution. *Journal of molecular evolution*, 34(1):3–16, 1992.
A Some properties of the TKF91 length process

Recall the TKF91 edge process $I = (I_t)_{t \geq 0}$ in Definition 1, which has parameters $(\nu, \lambda, \mu) \in (0, \infty)^3$ with $\lambda < \mu$ and $(\pi_A, \pi_T, \pi_C, \pi_G) \in [0, \infty)^4$. The sequence length of the TKF91 edge process is a continuous-time linear birth-death-immigration process $|I_t|$ with infinitesimal generator $Q_{i,i+1} = \lambda_0 + i \lambda$ (for $i \in \mathbb{Z}_+$), $Q_{i,i-1} = i \mu$ (for $i \geq 1$) and $Q_{i,j} = 0$ otherwise. This is a well-studied process for which explicit forms for the transition density $p_{ij}(t)$ and probability generating functions $G_i(z, t) = \sum_{j=0}^{\infty} p_{ij}(t) z^j$ are known. See, for instance, [And91, Section 3.2] or [KT81, Chapter 4] for more details. This process was also analyzed in [Tha06] in the related context of phylogeny estimation.

We collect here a few properties that will be useful in our analysis. The probability generating function is given by

$$G_i(z, t) = \left[ \frac{1 - \beta - z(\gamma - \beta)}{1 - \beta \gamma - \gamma z(1 - \beta)} \right]^i \left[ \frac{1 - \gamma}{1 - \beta \gamma - \gamma z(1 - \beta)} \right]^\delta$$

for $i \in \mathbb{Z}_+$ and $t > 0$, where

$$\beta = \beta_t = e^{-(\mu - \lambda)t}, \quad \gamma = \frac{\lambda}{\mu}, \quad \delta = \frac{\lambda_0}{\lambda}.$$

We only consider the case $\lambda_0 = \lambda$ (i.e. $\delta = 1$) in this paper. Fix $t \geq 0$ and let $\varphi_i(\theta) = E_i[e^{\theta |I_t|}]$ be the characteristic function of $|I_t|$ starting at $i$. Then for $\lambda \neq \mu$ (i.e. $\gamma \neq 1$),

$$\varphi_i(\theta) = G_i(e^\theta, t) = \left[ \frac{1 - \beta - e^\theta(\gamma - \beta)}{1 - \beta \gamma - \gamma e^\theta(1 - \beta)} \right]^i \left[ \frac{1 - \gamma}{1 - \beta \gamma - \gamma e^\theta(1 - \beta)} \right]$$

$$= (1 - \gamma) \frac{A^i}{B^{i+1}}, \quad (17)$$

where

$$A = 1 - \beta - e^\theta(\gamma - \beta) \quad \text{and} \quad B = 1 - \beta \gamma - \gamma e^\theta(1 - \beta).$$

Differentiating with respect to $\theta$ gives

$$\varphi_i'(\theta) = (1 - \gamma) \frac{A^{i-1} e^\theta \left\{ (\beta - \gamma) B - (i + 1) \gamma (\beta - 1) A \right\}}{B^{i+2}}$$

$$= (1 - \gamma) \frac{A^{i-1} e^\theta \left\{ \beta (1 - \gamma)^2 i + \gamma (1 - \beta)^2 + e^\theta (\gamma - \beta) \gamma (\beta - 1) \right\}}{B^{i+2}}$$

$$= \frac{A^{i-1}}{B^{i+2}} (Ce^\theta + De^{2\theta}), \quad (18)$$

where

$$C = (1 - \gamma)[\beta (1 - \gamma)^2 i + \gamma (1 - \beta)^2] \quad \text{and} \quad D = (1 - \gamma)(\gamma - \beta) \gamma (\beta - 1).$$

Differentiating with respect to $\theta$ once more gives

$$\varphi_i''(\theta) = \frac{A^{i-2} e^\theta}{B^{i+3}} \left\{ BA(C + 2De^\theta) + (Ce^\theta + De^{2\theta}) \left[ (i - 1)B(\beta - \gamma) + (i + 2)A\gamma (1 - \beta) \right] \right\}$$

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The expected value and the second moment are given by

\[ \mathbb{E}_i[|I_t|] = \phi'_i(0) = i\beta + \frac{\gamma(1 - \beta)}{1 - \gamma} = i\beta + \frac{\lambda}{\lambda - \mu}(\beta - 1) \]

and

\[ \mathbb{E}_i[|I_t|^2] = \phi''_i(0) = i^2\beta^2 + i\frac{\beta(3\gamma + 1)(1 - \beta)}{1 - \gamma} + \frac{(1 - \beta)\gamma[1 + (1 - 2\beta)\gamma]}{(1 - \gamma)^2} \]

From these we also have the variance

\[ \text{Var}_i(|I_t|) = \mathbb{E}_i[|I_t|^2] - (\mathbb{E}_i[|I_t|])^2 \]

\[ = i^2\beta^2 + i\frac{\beta(3\gamma + 1)(1 - \beta)}{1 - \gamma} + \frac{(1 - \beta)\gamma[1 + (1 - 2\beta)\gamma]}{(1 - \gamma)^2} - \left(i\beta + \frac{\gamma(1 - \beta)}{1 - \gamma}\right)^2 \]

\[ = i\frac{\beta(1 - \beta)(1 + 3\gamma - 2\beta)}{1 - \gamma} + \frac{\gamma(1 - \beta)(1 - \beta \gamma)}{(1 - \gamma)^2}. \]  

(19)

Consider the function

\[ \psi_i(\theta) = \frac{\phi'_i(0) - \phi'_i(\theta)}{\phi'_i(\theta)} = i\beta + \frac{\gamma(1 - \beta)}{1 - \gamma} - \frac{Ce^\theta + De^{2\theta}}{(1 - \gamma)AB} \]

\[ = \left(\beta - \frac{C_1 e^\theta}{(1 - \gamma)AB}\right)i + \frac{\gamma(1 - \beta)}{1 - \gamma} - \frac{C_2 e^\theta + De^{2\theta}}{(1 - \gamma)AB} \]

\[ = \left(\beta - \frac{\beta(1 - \gamma)^2 e^\theta}{AB}\right)i + \frac{\gamma(1 - \beta)}{1 - \gamma} - \gamma(1 - \beta)^2 e^\theta + (\gamma - \beta)\gamma(\beta - 1)e^{2\theta} \]

\[ = F(\theta)i + G(\theta) \]

where we wrote \( C = C_1 i + C_2 \), with \( C_1 = \beta(1 - \gamma)^3 \) and \( C_2 = (1 - \gamma)\gamma(1 - \beta)^2 \), and the last line is a definition. Functions \( F \) and \( G \) can be simplified to

\[ F(\theta) = -\frac{(e^\theta - 1)\beta(1 - \beta)[(1 - \beta)\gamma - e^\theta(\gamma - \beta)]}{AB} \]  

(20)

\[ G(\theta) = -\frac{(e^\theta - 1)\gamma(1 - \beta)(1 - \beta \gamma)[(1 - \beta - e^\theta(\gamma - \beta)]}{(1 - \gamma)AB}. \]  

(21)

Since \( \phi_i(0) = 1 \), we have \( \psi(0) = 0 \). We consider the case \( \mu \in (\lambda, \infty) \), that is, \( \gamma \in (0, 1) \). Then both \( A \) and \( B \) are strictly positive for all \( t \in [0, \infty) \), provided that \( e^\theta < \mu/\lambda \). Moreover, \( F \) and \( G \) are continuous on \( [0, \mu/\lambda) \), smooth on \( (0, \mu/\lambda) \) and \( F(0) = G(0) = 0 \).

**B Proofs**

To prove Theorem 2 (and Theorem 1 from which it follows), that is, to obtain the desired upper bound, (6), on

\[ \mathbb{P}^{\Pi} \left[ F_k(\bar{X}_{\beta T^k}) \neq \bar{X}_\rho^k \right] = \sum_{\bar{x} \in S} \mathbb{P}^{x} \left[ F_k(\bar{X}_{\beta T^k}) \neq \bar{x} \right] \Pi(\bar{x}), \]  

(22)
we first observe that from the construction of \( F_k \) in Section 2.3, if the estimator is wrong, then either the estimated length is wrong or the length is correct but the sequence is wrong. Hence we have

\[
\mathbb{P}^{\bar{x}} \left[ F_k(\bar{X}_{\partial T^k}) \neq \bar{x} \right] \leq \mathbb{P}_{|\bar{x}|} \left[ M^{k,*} \neq |\bar{x}| \right] + \mathbb{P}^{\bar{x}} \left[ F_k(|\bar{x}|)(\bar{X}_{\partial T^k}) \neq \bar{x} \right],
\]

for all \( \bar{x} \in S \setminus \{\, \bullet \, \} \), where \( \mathbb{P}^{\bar{x}} \) denotes the probability law when the root state is \( \bar{x} \). The proof involves bounding the first and second terms on the RHS of (23), formulated as Propositions 1 and 2 respectively in the next two subsections.

### B.1 Reconstructing the sequence length

In this subsection, we bound the first term on the RHS of (23), which is the probability of incorrect estimation of the root sequence length. Proposition 1 is a quantitative statement about how this error tends to zero exponentially fast in \( m := |\partial T^k(s)| \), as \( k \to \infty \) and \( s \to 0 \).

**Proposition 1** (Sequence length estimation error). There exist constants \( C_1, C_2 \in (0, \infty) \) which depend only on \( h^*, \mu \) and \( \lambda \) such that

\[
\mathbb{P}_0(M^{k,*} \neq 0) \leq 2 \exp \left( -C_1 |\partial T^k(s)| \right) + C_2 s \quad \text{and} \quad \mathbb{P}_M(M^{k,*} \neq M) \leq 2 \exp \left( -C_1 \frac{|\partial T^k(s)|}{M} \right) + C_2 (M + 1) s
\]

for all \( s \in (0, h^*/2] \), \( k \in \mathbb{N} \) and \( M \in \mathbb{N} \).

**Outline of the proof of Proposition 1**  Fix \( k \geq 1 \) and \( s > 0 \). For convenience, we let \( m := |\partial T^k(s)| \). Our sequence length estimator \( M^{k,*} \) is correct if the empirical average

\[
A^{k,*} = \frac{1}{m} \sum_{v \in \partial T^k,s} \mathbb{E}_{\bar{X}_v}[|I_{h^* - \ell_v}|]
\]

is close to its expectation. Indeed, all terms \( \mathbb{E}_{\bar{X}_v}[|I_{h^* - \ell_v}|] \), for \( v \in \partial T^k,s \), have mean \( \nu_M \), where by Markov property and formula (8)

\[
\nu_M := \mathbb{E}_M[|I_{h^*}|] = M \beta_{h^*} + \gamma \frac{(1 - \beta_{h^*})}{1 - \gamma}, \quad \text{where recall that} \quad \beta_t = e^{-(\mu - \lambda)t} \quad \text{and} \quad \gamma = \frac{\lambda}{\mu}.
\]

Formula (8) also tells us that the function \( M \mapsto \Phi_h^{(1)}(M) \) is linear with slope \( \beta_{h^*} \). So if \( |A^{k,*} - \nu_M| < \beta_{h^*}/2 \) then

\[
\left[ (\Phi_{h^*}^{(1)})^{-1}(A^{k,*}) \right] = \left[ (\Phi_{h^*}^{(1)})^{-1}(\nu_M) \right] = M.
\]

Hence, the error probability satisfies

\[
\mathbb{P}_M(M^{k,*} \neq M) \leq \mathbb{P}_M \left( \left| A^{k,*} - \nu_M \right| \geq \beta_{h^*}/2 \right),
\]

(25)
for all $M \geq 0$. To bound of the RHS of (25), we first note that the terms $E_{|\vec{X}_v|} [I_{h^* - \ell_v}]$, for $v \in \partial \tilde{T}^k,s$, are correlated. However, the construction of $\tilde{T}^k,s$ guarantees that this correlation is “small” as the paths to the root from any two leaves of the restriction overlap only “above level $s$.” To control the correlation, we condition on the leaf states of the truncation $\vec{X}_{\partial T(s)} = \{\vec{X}_v : v \in \partial T(s)\}$. By the Markov property

$$E_M \left[ A^{k,s} \bigg| \vec{X}_{\partial T(s)} \right] = \frac{1}{m} \sum_{u \in \partial T^k(s)} E_{|\vec{X}_u|} [I_{h^* - s}].$$

(26)

We first bound the probability that this conditional expectation is close to its expectation, which is also $\nu_M$. Then, conditioned on this event, we establish concentration of $A^{k,s}$ based on conditional independence. We detail the above argument in Steps A-C as follows. We use some properties of the length process derived in Section A.

(A) Decomposition from conditioning on level $s$ For $\epsilon > 0$, $\delta \in (0, \infty)$ and $s \in (0, h^*)$, we have

$$P_M \left( \left| A^{k,s} - \nu_M \right| \geq \epsilon \right) \leq P_M \left( \left| A^{k,s} - \nu_M \right| \geq \epsilon \cap E_{\delta,s} \right) + P_M (E_{\delta,s}),$$

(27)

where

$$E_{\delta,s} := \left\{ \left| E_M \left[ A^{k,s} \bigg| \vec{X}_{\partial T(s)} \right] - \nu_M \right| > \delta \right\}.$$

(28)

As we shall see, Proposition 1 is then be obtained by taking $\delta = \epsilon/2 = \beta_{h^*}/4$.

(B) Bounding $P_M (E_{\delta,s})$ The second term on the RHS of (27) is treated in Lemma 2 below. Because of the correlation above level $s$, we use Chebyshev’s inequality to control the deviation of the conditional expectation.

Lemma 2 (Conditional expectation given level $s$). For all $M \in \mathbb{Z}_+$, $\delta \in (0, \infty)$ and $s \in (0, h^*)$, we have

$$P_M (E_{\delta,s}) \leq \delta^{-2} C (M + 1) s,$$

where $C \in (0, \infty)$ is a constant which depends only on $h^*$, $\mu$ and $\lambda$.

Proof. By (26) and Chebyshev’s inequality,

$$P_M (E_{\delta,s}) = P_M \left[ \left| \sum_{u \in \partial T^k(s)} E_{|\vec{X}_u|} [I_{h^* - s}] - m\nu_M \right| > m\delta \right] \leq \frac{1}{m^2 \delta^2} E_M \left[ \left( \sum_{u \in \partial T^k(s)} E_{|\vec{X}_u|} [I_{h^* - s}] - \nu_M \right)^2 \right].$$

(29)
The numerator, by Cauchy-Schwarz, symmetry, (8) and (19), is bounded as follows

\[
\mathbb{E}_M \left[ \left( \sum_{u \in \partial T^k(s)} \mathbb{E}_{|\tilde{X}_u|} [ |I_{h^* - s}] - \nu_M \right)^2 \right] \\
= \sum_{u \in \partial T^k(s)} \sum_{\bar{u} \in \partial T^k(s)} \mathbb{E}_M \left[ \left( \mathbb{E}_{|\tilde{X}_u|} [ |I_{h^* - s}] - \nu_M \right) \left( \mathbb{E}_{|\tilde{X}_{\bar{u}}|} [ |I_{h^* - s}] - \nu_M \right) \right] \\
\leq \left[ \sum_{u \in \partial T^k(s)} \sqrt{\text{Var}_M \left( \mathbb{E}_{|\tilde{X}_u|} [ |I_{h^* - s}] \right)} \right]^2 \\
= m^2 \text{Var}_M \left( \mathbb{E}_{|\tilde{X}_u|} [ |I_{h^* - s}] \right) \\
= m^2 \beta_{h^*, s}^2 \text{Var}_M (|\tilde{X}_u|) \\
= m^2 \beta_{h^*, s}^2 \left( M \beta_s (1 - \beta_s)(1 + 3\gamma - 2\beta_s) \frac{1}{1 - \gamma} + \frac{\gamma(1 - \beta_s)(1 - \beta_s)}{(1 - \gamma)^2} \right) \\
\leq m^2 (1 - \beta_s) C (M + 1),
\]

where \( C \in (0, \infty) \) is a constant which depends only on \( h^* \), \( \mu \) and \( \lambda \), where we used that \( \gamma < 1 \) and \( \beta \) is decreasing. Putting the above inequality into (29), we obtain the desired inequality. \( \square \)

(C1) Deviation of \( A_{k, s} \) conditioned on \( \mathcal{E}_{\delta, s} \) The key step of the analysis is to control the first term on the RHS of (27) by taking advantage of the conditional independence of the leaves of the restriction given \( \tilde{X}_{\partial T^k(s)} \) (done in (30)). By the definition of \( A_{k, s} \), that term is equal to

\[
P_M \left( \left. \left\{ \sum_{i \in \partial T^k(s)} \mathbb{E}_{|\tilde{X}_u|} [ |I_{h^* - \ell_i}] \right\} \cap \mathcal{E}_{\delta, s}^c \right\} \right) \geq m \epsilon \}
\]

which, by the Markov property and conditional independence, is further equal to

\[
\sum_{\bar{u} \in Z_{\delta, s}^k} P \left( \left. \left\{ \sum_{i=1}^m |x^{(u_i)}|_{h^* - s} - m \nu_M \right\} \geq m \epsilon \right\} \right) P_M \left( |\tilde{X}_{\partial T^k(s)}| = \bar{u} \right),
\]

where the set \( Z_{\delta, s} \) is analogous to \( \mathcal{E}_{\delta, s} \) and defined as

\[
Z_{\delta, s} := \left\{ \bar{u} = (u_1, \cdots, u_m) \in \mathbb{Z}_+^m : \left| \sum_i \mathbb{E}_{x_i}[|I_{h^* - s}]] - m \nu_M \right| > m \delta \right\},
\]

and \( \{x^{(u_i)}\}_{i=1}^m \) are, under probability \( P \), independent copies of the birth-death process \( |I_t| \) starting from \( \{u_i\}_{i=1}^m \) respectively. By the triangle inequality, we have for all \( s \in (0, h^*) \),

\[
(31) \leq \max_{\bar{u} \in Z_{\delta, s}^k} P \left( \left. \left\{ \sum_{i=1}^m |x^{(u_i)}|_{h^* - s} - m \nu_M \right\} \geq m \epsilon \right\} \right) \\
\leq \max_{\bar{u} \in Z_{\delta, s}^k} P \left( \left. \left\{ \sum_{i=1}^m (|x^{(u_i)}|_{h^* - s} - \mathbb{E}_{x_i}[|I_{h^* - s}]] \right\} \geq m (\epsilon - \delta) \right\} \right).
\]

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Write \( t = h^* - s \) for convenience. A typical term in the sum of the last display is
\[
\xi_i = |x^{(u_i)}|_t - E_{u_i}(|I_t|),
\]
which are mean zero, unbounded random variables. To control the deviation, we bound the exponential moment generating function of \(|I_t|\) under \( P_{u_i} \). Although this type of argument is standard in large deviations theory (see, e.g., [Dur96]), a non-trivial requirement here is to obtain a bound that is \( \text{uniform in} \ (u_1, \cdots, u_m) \in Z_{c, \delta} \). Note that the condition \( \vec{u} \in Z_{c, \delta} \) is equivalent to
\[
|\vec{u}| \leq \beta t + \frac{\gamma (1 - \beta t)}{1 - \gamma} - \nu M \leq \delta.
\]
(33)

(C2) Uniform control of moment generating function  Let \( \delta = \epsilon/2 = \beta h^*/4 \) and fix \( \vec{u} \in Z_{\delta} \).
Write \( t = h^* - s \) for convenience. The moment generating function \( \varphi_M(\theta) := E_M[e^{\theta |I_t|}] \) of the length process \(|I_t|\) starting at \( M \in Z_+ \) is given in (17) in Section A. Markov’s inequality and the independence of \( \{\xi_i\} \) s yields, for all \( a \in (0, \infty) \) and \( \theta \in \mathbb{R} \),
\[
\mathbb{P} \left( \sum_{i=1}^{m} \xi_i \geq m a \right) = \mathbb{P} \left( \exp \left( \theta \sum_{i=1}^{m} \xi_i \right) \geq e^{\theta m a} \right)
\]
\[
\leq e^{-\theta m a} \prod_{i=1}^{m} E[e^{\theta \xi_i}] = e^{-\theta m a} \prod_{i=1}^{m} \exp (-\theta E_{u_i}([I_t])) \varphi_{u_i}(\theta) = \exp (-m \Phi(\theta)),
\]
where
\[
\Phi(\theta) := \theta a + \frac{\theta}{m} \sum_{i=1}^{m} \varphi'_{u_i}(0) - \frac{1}{m} \sum_{i=1}^{m} \log \varphi_{u_i}(\theta).
\]
(34)
Standard calculations easily give \( \Phi(\hat{\theta}) > 0 \) for some \( \hat{\theta} \in (0, \infty) \) small enough. However, we need to show that \( \hat{\theta} \in (0, \infty) \) can be chosen to be \text{independent of the vector} \( \vec{u} = (u_1, \cdots, u_m) \in Z_{\delta} \) and \( t \in (h^*/2, h^*) \).

Recall that definitions of the functions \( F \) and \( G \) in (20) and (21). It holds that \( \Phi(0) = 0, \Phi \) is continuous at 0 and differentiable on \((0, \infty)\) with derivative
\[
\Phi'(\theta) = a + \frac{1}{m} \sum_{i=1}^{m} \left( \varphi'_{u_i}(0) - \varphi'_{u_i}(\theta) \right) = a + G(\theta) + F(\theta) \sum_{i=1}^{m} u_i \\
\geq a + G(\theta) + F(\theta) \left( \nu_M - \frac{\gamma (1 - \beta t)}{1 - \gamma} + \delta \right),
\]
(36)
for \( \theta \in [0, \theta^*_1] \), where in the second last inequality we have used condition (33) and the fact that \( F(\theta) \leq 0 \) for all \( t \in (h^*/2, h^*) \) and \( \theta \in [0, \theta^*_1] \) for some \( \theta^*_1 > 0 \) which depends only on \( \mu, \lambda \) and \( h^* \).

Recall that \( t = h^* - s \) and take \( a = \epsilon - \delta = \beta h^*/4 \). From (24) and (36) and the fact that both \( F \) and \( G \) are continuously differentiable and tend to 0 as \( \theta \to 0 \), we have

\[
\Phi'(\theta) \geq \frac{\beta h^*}{4} + G(\theta) \frac{F(\theta)}{\beta_t} \left( M \beta h^* - \frac{\gamma (\beta_t - \beta h^*) + \beta h^*}{1 - \gamma} \right)
\geq \frac{\beta h^*}{4} + G(\theta) \frac{F(\theta)}{\beta_t} \left( M \beta h^* + \frac{\beta h^*}{4} \right)
\geq \frac{\beta h^*}{8} + F(\theta) (M + 1) e^{(\lambda - \mu)h^*/2},
\]

for \( \theta \in [0, \theta^*] \) and \( s \in [0, s_s] \), where \( s_s \in [0, h^*/2] \) and \( \theta^* > 0 \) are constants which depend only on \( \mu, \lambda \) and \( h^* \), but not on \( M \). Again, we also used that \( F(\theta) \) is non-positive for small \( \theta \). Note that, when \( t \in [h^*/2, h^*] \), we have \( F(\theta) \leq (1 - e^\theta) \) up to a constant depending on \( \mu, \lambda \) and \( h^* \). More precisely, there exists \( C_* \in (0, \infty) \) which depends only on \( \mu, \lambda, h^* \), but not on \( M \), \( s \in (0, h^*/2) \) or \( \bar{u} \in Z_{\delta}^{\xi} \), such that

\[
-\frac{e^{(\lambda - \mu)h^*/2}}{16} = -\frac{\beta h^*}{16 e^{(\lambda - \mu)h^*/2}} \leq (M + 1) F(\theta) \leq 0
\]

for all \( \theta \in [0, C_* / M] \), where \( C_* \) takes care of the factor \( F(\theta)/(1 - e^\theta) \) (which is between positive constant for \( t \in [h^*/2, h^*] \) and small \( \theta \)) and the LHS is chosen in view of the expression in (37). Therefore, from (37), we have

\[
\inf_{s \in (0, h^*/2)} \inf_{\theta \in [0, C_* / M]} \Phi'(\theta) \geq \frac{\beta h^*}{16}.
\]

From (34) and (38) we obtain

\[
P \left( \sum_{i=1}^{m} \xi_i \geq ma \right) \leq \exp \left( \frac{-m \beta h^* C_*}{16 M} \right).
\]

The same inequality can be obtained for \( P \left( \sum_{i=1}^{m} \xi_i \leq -ma \right) \) by replacing \( \xi_i \) by \(-\xi\) in the above arguments. Hence from (32) we finally obtain

\[
(30) \leq 2 \exp \left( \frac{-m \beta h^* C_*}{16 M} \right).
\]

**Proof of Proposition 1.** Take \( \delta = \epsilon / 2 = \beta h^*/4 \). Then apply (39) to the first term on the RHS of (27) and Lemma 2 to the second term on the RHS of (27). The proof of Proposition 1 is complete by collecting inequalities (25) and (27). \( \square \)
B.2 Reconstructing root sequence given sequence length

In this subsection, we bound the second term on the RHS of (23), which is the probability of incorrectly reconstructing the root sequence, given its length. Suppose we assume (or know) that the ancestral sequence length is \( M \geq 1 \), that is, the ancestral state is an element of \( \{A, T, C, G\}^M \). Let \( F_k^{(M)} \) denote the estimator in (5) when \( M^{k,s} = M \). Formally, we prove the following.

**Proposition 2** (Sequence reconstruction error). For all \( M \in \mathbb{Z}_+ \), \( \bar{x} \in \{A, T, C, G\}^M \) and \( s \in (0, h^*) \),

\[
P_{\bar{x}} \left[ F_k^{(M)} \left( \hat{X}_{\partial T^k} \right) \neq \bar{x} \right] \leq 8M \exp \left( -\frac{\left| \partial T_k^k(s) \right|}{8 \hat{C}} \right) + CM^4 \hat{C} s
\]

where \( \hat{C} := \|V^{-1}\Psi^{-1}\|_{\infty \to \infty} \in (0, \infty) \) is a constant which depends only on \( \mu, \lambda, h^* \) and \( \{t_j\}_{j=1}^M \), and \( C \in (0, \infty) \) is a constant which depends only on \( \nu, \mu \) and \( \lambda \).

**Outline of the proof of Proposition 2** Fix \( k \geq 1, s = s_k > 0, M \geq 1 \) and \( \{t_j\}_{j=1}^M \) in the construction of \( F_k^{(M)} \). By the construction of \( F_k^{(M)} \) in (5), our sequence estimator \( F_k^{(M)}(\hat{X}_{\partial T^k}) \in \{A, T, C, G\}^M \) is correct if it is close to the argmax over the columns of the matrix \( V^{-1}\Psi^{-1}U \). By the definitions of \( U, \Psi, V \), our analysis boils down to bounding the deviations of the empirical frequencies \( f_{k,s}^k(t_j) \) from their expectations \( p_{\bar{x}}^k(h^* + t_j) \). This is established using similar arguments to that of Proposition 1. Here is an outline.

(i) Reduction from deviation of matrices to deviation of frequencies Recall that \( \chi_{\bar{x}} \) is the \( M \times 4 \) matrix whose entries are \( 1_{\{x_j = \sigma\}} \). By (5), \( F_k^{(M)}(\hat{X}_{\partial T^k}) = \bar{x} \) is implied by \( \|V^{-1}\Psi^{-1}U - \chi_{\bar{x}}\|_{\max} < 1/2 \), where \( \|A\|_{\max} := \max_{i,j} |a_{ij}| \) is the maximum among the absolute values of all entries of \( A \). On the other hand,

\[
\|V^{-1}\Psi^{-1}U - \chi_{\bar{x}}\|_{\max} = \|V^{-1}\Psi^{-1}(U - \Psi V \chi_{\bar{x}})\|_{\max} \\
\leq \|V^{-1}\Psi^{-1}\|_{\infty \to \infty} \|U - \Psi V \chi_{\bar{x}}\|_{\max},
\]

where \( \|A\|_{\infty \to \infty} := \max_i \sum_j |a_{ij}| \) is the maximum absolute row sum of a matrix \( A = (a_{ij}) \). The above two facts give

\[
P_{\bar{x}} \left[ F_k^{(M)} \left( \hat{X}_{\partial T^k} \right) \neq \bar{x} \right] \leq P_{\bar{x}} \left[ \|V^{-1}\Psi^{-1}U - \chi_{\bar{x}}\|_{\max} \geq 1/2 \right] \leq P_{\bar{x}} \left[ \|U - \Psi V \chi_{\bar{x}}\|_{\max} \geq \frac{1}{2 \|V^{-1}\Psi^{-1}\|_{\infty \to \infty}} \right].
\]

By definitions of \( U, \Psi, V \), we have

\[
\|U - \Psi V \chi_{\bar{x}}\|_{\max} = \max_{\sigma \in \{A,T,C,G\}} \max_{1 \leq j \leq M} \left| f_{\sigma}^{k,s}(t_j) - p_{\bar{x}}^k(h^* + t_j) \right|
\]

Therefore we can bound the target probability by the probabilities of deviations of empirical frequencies \( f_{\sigma}^{k,s}(t_j) \) as follows

\[
P_{\bar{x}} \left[ F_k^{(M)} \left( \hat{X}_{\partial T^k} \right) \neq \bar{x} \right] \leq \sum_{\sigma \in \{A,T,C,G\}} \sum_{j=1}^M P_{\bar{x}} \left[ |f_{\sigma}^{k,s}(t_j) - p_{\bar{x}}^k(h^* + t_j)| \geq \frac{1}{2 \|V^{-1}\Psi^{-1}\|_{\infty \to \infty}} \right].
\]

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(ii) **Estimating deviation of frequencies** We then bound each term on the RHS of (41) using similar arguments to that of Proposition 1. As before we let $m := |\partial T^k(s)|$ for convenience. Recall from (3) that for $t \in [0, \infty)$

$$f^{k,s}_\sigma(t) = \frac{1}{m} \sum_{v \in \partial T^k,s} p^\sigma_{X_v}(t + h^* - \ell_v).$$

All the terms $p^\sigma_{X_v}(t + h^* - \ell_v)$, for $v \in \partial T^k,s$, have expectation $p^\sigma(h^* + t)$ under $\mathbb{P}^\tilde{X}$, by the Markov property. Therefore, for $\epsilon \in (0, \infty)$ and $t \in [0, \infty)$, we have

$$\mathbb{P}^{\tilde{X}} \left( |f^{k,s}_\sigma(t) - p^\sigma(h^* + t)| > \epsilon \right) = \mathbb{P}^{\tilde{X}} \left( \left| \frac{1}{m} \sum_{v \in \partial T^k,s} y_v \right| > \epsilon \right)$$

where

$$y_v := p^\sigma_{X_v}(t + h^* - \ell_v) - p^\sigma(h^* + t_j) \quad \text{for} \quad v \in \partial T^k,s,$$

are centered but correlated random variables under $\mathbb{P}^{\tilde{X}}$. To bound (42) we use the same method that we used to bound (25), namely by considering the conditional expectation of $f^{k,s}_\sigma(t)$ given the states $\tilde{X}_{\partial T(s)} = \{ \tilde{X}_v : v \in \partial T(s) \}$, which by the Markov property is equal to

$$\mathbb{E}^{\tilde{X}} \left[ f^{k,s}_\sigma(t) \bigg| \tilde{X}_{\partial T(s)} \right] = \frac{1}{m} \sum_{u \in \partial T^k(s)} p^\sigma_{X_u}(h^* + t - s).$$

As before we first bound the probability of the event that this conditional expectation is close to its expectation (which is also $p^\sigma(h^* + t)$), then conditioned on this event we establish a concentration inequality for $f^{k,s}_\sigma(t)$, based on conditional independence. Since all $\eta_v$ are bounded between 1 and -1, we apply Hoeffding’s inequality [Hoe63] for this purpose.

We detail the above argument in Steps A-C as follows.

(A) **Decomposition by conditioning on level $s$** Similarly to (27) we have

$$\mathbb{P}^{\tilde{X}} \left( |f^{k,s}_\sigma(t) - p^\sigma(h^* + t)| > \epsilon \right) \leq \mathbb{P}^{\tilde{X}} \left( \left| f^{k,s}_\sigma(t) - p^\sigma(h^* + t) \right| > \epsilon \right| (F^t_{\delta,s})^c + \mathbb{P}^{\tilde{X}}(F^t_{\delta,s}),$$

where

$$F^t_{\delta,s} := \left\{ \mathbb{E}_{\tilde{X}} \left[ f^{k,s}_\sigma(t) \bigg| \tilde{X}_{\partial T(s)} \right] - p^\sigma(h^* + t) \right\} > \delta \right\}.$$  

We then control the two terms on the RHS of (44). As we will see, the proof of Proposition 2 will be completed by taking

$$\epsilon = \frac{1}{2 \| V^{-1} \Psi^{-1} \|_{\infty} \to \infty}, \quad \delta := \epsilon/2 \quad \text{and} \quad t = t_j.$$  

in (44) and combining with (41).
Lemma 3. There exists a constant $C \in (0, \infty)$ which depends only on $\lambda, \nu$ and $\mu$ such that for all $\bar{x} \in \{A, T, C, G\}^M$, $\delta \in (0, \infty)$ and $s \in (0, h^*)$, we have

$$\sup_{t \in (0, \infty)} \mathbb{P}^\delta(\mathcal{F}_t^{\delta, s}) \leq \delta^{-2} CMs,$$

where event $\mathcal{F}_t^{\delta, s}$ is defined in (45).

Proof. Similarly to the proof of Lemma 2 we use Chebyshev’s inequality to control the deviation of $\sum_{u \in \partial T^k(s)} p_{X_u}^\sigma(h^* + t - s)$. By the Cauchy-Schwarz inequality, the variance can be bounded as follows

\[
\text{Var}_\bar{x} \left[ \sum_{u \in \partial T^k(s)} p_{X_u}^\sigma(h^* + t - s) \right] = \sum_{u \in \partial T^k(s)} \sum_{v \in \partial T^k(s)} \mathbb{E}^\bar{x} \left[ \left( p_{X_u}^\sigma(h^* + t - s) - p_{X_v}^\sigma(h^* + t) \right) \left( p_{X_v}^\sigma(h^* + t - s) - p_{X_v}^\sigma(h^* + t) \right) \right] \\
\leq \sum_{u \in \partial T^k(s)} \sum_{v \in \partial T^k(s)} \sqrt{\text{Var}_\bar{x} \left[ p_{X_u}^\sigma(h^* + t - s) \right] \text{Var}_\bar{x} \left[ p_{X_v}^\sigma(h^* + t - s) \right]} \\
= m^2 \text{Var}_\bar{x} \left[ p_{X_u}^\sigma(h^* + t - s) \right].
\]

(47)

Using the explicit formula (14) and the general inequality $\text{Var}(X + Y) \leq 2 (\text{Var}(X) + \text{Var}(Y))$ (which can be seen by applying Cauchy-Schwarz to the covariance and then the AM-GM inequality), we have

\[
\text{Var}_\bar{x} \left[ p_{X_u}^\sigma(h^* + t - s) \right] = \text{Var}_\bar{x} \left[ -\pi_\sigma \phi(h^* + t - s) A^{\bar{X}_u} + \psi(h^* + t - s) \sum_{i=1}^{\bar{X}_u} 1_{\{X_u, i = \sigma\}} A^{i-1} \right] \\
\leq 2 \pi_\sigma^2 \phi^2(h^* + t - s) \text{Var}_\bar{x} \left[ A^{\bar{X}_u} \right] + 2 \psi^2(h^* + t - s) \text{Var}_\bar{x} \left[ \sum_{i=1}^{\bar{X}_u} 1_{\{X_u, i = \sigma\}} A^{i-1} \right],
\]

(48)

where $A := \eta(h^* + t - s)$. (Note that the $A$ here is distinct from that in Section A.)

The term $\text{Var}_\bar{x} \left[ A^{\bar{X}_u} \right]$ can be bounded as follows. Fix $u \in \partial T^k(s)$ and let $E_u$ be the event that the sequence never left state $\bar{x}$ along the unique path from the root to $u$. Then

$$\mathbb{P}^\bar{x}(E_u) = e^{-q_M s} \quad \text{where} \quad q_M := M \nu + (M + 1) \lambda + M \mu,$$

and

$$\mathbb{E}^\bar{x} \left[ A^{\bar{X}_u} \right] = A^M \mathbb{P}^\bar{x}(E_u) + \mathbb{E}^\bar{x} \left[ A^{\bar{X}_u} ; E_u^c \right].$$
Since $A \in [0, 1]$, we have
\[ 0 \leq \mathbb{E}^\mathcal{F} \left[ A^{|X_u|} \right] - A^M e^{-qM s} \leq 1 - e^{-qM s}. \]

Similarly,
\[ 0 \leq \mathbb{E}^\mathcal{F} \left[ A^2|X_u| \right] - A^{2M} e^{-qM s} \leq 1 - e^{-qM s}. \]

The last two displays give
\[
\begin{align*}
\text{Var}_\mathcal{F} \left[ A^{|X_u|} \right] &= \mathbb{E}^\mathcal{F} \left[ A^2|X_u| \right] - \left( \mathbb{E}^\mathcal{F} \left[ A^{|X_u|} \right] \right)^2 \\
&\leq \left( A^{2M} e^{-qM s} + 1 - e^{-qM s} \right) - (A^M e^{-qM s})^2 \\
&= A^{2M} e^{-qM s} (1 - e^{-qM s}) + 1 - e^{-qM s} \\
&\leq 2(1 - e^{-qM s}),
\end{align*}
\]
where we used that $A \in [0, 1]$ on the last line.

For the second variance term in (48), a similar argument gives
\[
\begin{align*}
\mathbb{E}^\mathcal{F} \left[ \sum_{i=1}^{|X_u|} 1\{X_u,i=\sigma\} A^{i-1} \right] &= \left( \sum_{i=1}^M 1\{x_i=\sigma\} A^{i-1} \right) \mathbb{P}(E_u) + \mathbb{E}^\mathcal{F} \left[ \sum_{i=1}^{|X_u|} 1\{X_u,i=\sigma\} A^{i-1}; E_u \cap \{|X_u| \geq 1\} \right]. \\
\end{align*}
\]
Observe that almost surely
\[ 0 \leq \sum_{i=1}^{|X_u|} 1\{X_u,i=\sigma\} A^{i-1} \leq \frac{1}{1-A}, \]
because $A \in (0, 1)$ when $h^* + t - s > 0$. Hence we obtain
\[ 0 \leq \mathbb{E}^\mathcal{F} \left[ \sum_{i=1}^{|X_u|} 1\{X_u,i=\sigma\} A^{i-1} \right] - \left( \sum_{i=1}^M 1\{x_i=\sigma\} A^{i-1} \right) e^{-qM s} \leq \frac{1 - e^{-qM s}}{1-A}. \]

Similarly we have
\[ 0 \leq \mathbb{E}^\mathcal{F} \left[ \left( \sum_{i=1}^{|X_u|} 1\{X_u,i=\sigma\} A^{i-1} \right)^2 \right] - \left( \sum_{i=1}^M 1\{x_i=\sigma\} A^{i-1} \right)^2 e^{-qM s} \leq \frac{1 - e^{-qM s}}{(1-A)^2}. \]

From the above two displays and (50), we obtain, as in (49), the following estimate
\[ \text{Var}_\mathcal{F} \left[ \sum_{i=1}^{|X_u|} 1\{X_u,i=\sigma\} A^{i-1} \right] \leq \frac{2(1 - e^{-qM s})}{(1-A)^2}. \]
From (48)-(51) we have

$$\text{Var}_X \left[ p_{X_u}^\sigma (h^* + t - s) \right]$$

$$\leq 4 \pi^2 \phi^2(h^* + t - s) \left( 1 - e^{-qM^s} ) + 4 \psi^2(h^* + t - s) \frac{1 - e^{-qM^s}}{(1 - \lambda)^2}$$

$$= 4 (1 - e^{-qM^s}) \left[ \pi^2 \phi^2(h^* + t - s) + \frac{\psi^2(h^* + t - s)}{(1 - \eta(h^* + t - s))^2} \right]$$

$$\leq 4 (1 - e^{-qM^s}) \left[ \|\phi\|_\infty^2 \pi^2 + \frac{\gamma^2}{(1 - \gamma)^2} \right]$$

$$\leq C_1 M s$$

for all \( s \in (0, h^*) \) and \( t \in (0, \infty) \), where \( C_1 \in (0, \infty) \) is a constant which depends only on \( \lambda, \nu \) and \( \mu \). In the second to last inequality, we used the following facts that follow directly from the definitions: (i) \( \eta \) is a strictly increasing function with \( \eta(0) = 0 \) and \( \lim_{t \to \infty} \eta(t) = 1/\gamma \), (ii) the supremum norm \( \|\phi\|_\infty < \infty \) and (iii) \( \psi(t) \) is a decreasing function bounded above by 1.

The result follows by (47) and Chebyshev’s inequality. \( \square \)

(C) Deviation of \( f^{k,s}_\sigma(t) \) conditioned on \( F^t_{\delta,s} \) By the Markov property and conditional independence as in (32), the first term on the RHS of (44) is equal to

$$\mathbb{P}_X \left( | f^{k,s}_\sigma(t) - p_{X_u}^\sigma(h^* + t) | > \epsilon \bigg| (F^t_{\delta,s})^c \right)$$

$$= \mathbb{P}_X \left( \left| \sum_{v \in \partial T^{k,s}} p_{X_v}^\sigma(t + h^* - t_v) - m p_{X_u}^\sigma(h^* + t) \right| > m \epsilon \bigg| (F^t_{\delta,s})^c \right)$$

$$\leq \max_{(\tilde{u}_i)_{i=1}^m \in Z_{\delta,s}^c} \mathbb{P}_X \left( \left| \sum_{i=1}^m p_{X_{\tilde{u}_i}(h^* - t)}^\sigma(t) - m p_{X_u}^\sigma(h^* + t) \right| \leq m \delta \right).$$

(53)

where

$$Z_{\delta,s}^c := \left\{ (\tilde{u}_i)_{i=1}^m \in S^m : \left| \sum_{i=1}^m p_{\tilde{u}_i}^\sigma(h^* + t - s) - m p_{X_u}^\sigma(h^* + t) \right| \leq m \delta \right\}$$

and \( \{ \tilde{X}_{\tilde{u}_i}(h^* - s) \}_{i=1}^m \) are independent copies of the TKF91 process starting from \( \{ \tilde{u}_i \}_{i=1}^m \) respectively, evaluated at time \( h^* - s \). By the triangle inequality and then Hoeffding’s inequality [Hoe63], we have

$$\left| \sum_{i=1}^m \left( p_{X_{u_i}(h^* - t)}^\sigma(t) - p_{\tilde{u}_i}^\sigma(h^* + t - s) \right) \right| \geq m (\epsilon - \delta)$$

$$\leq 2 \exp \left( -2m \left( \epsilon - \delta \right)^2 \right).$$

(54)

Proof of Proposition 2. As pointed out in (46), we will take

$$\epsilon = \frac{1}{2 \| V^{-1} \psi^{-1} \|_{\infty \to \infty}}, \quad \delta := \epsilon/2 \quad \text{and} \quad t = t_j.$$
From (54) we have
\[ (53) \leq 2 \exp \left( \frac{-m}{8 \| V^{-1} \Psi^{-1} \|_{\infty \to \infty}^2} \right). \]

Taking \( t \in \{ t_j \} \) in (44), we see that a typical term on the RHS of (41) is
\[
P\bar{x} \left[ \left| f^{k,s}_\sigma (t_j) - p^{\sigma}_{\bar{x}} (h^* + t_j) \right| \geq \frac{1}{2 \| V^{-1} \Psi^{-1} \|_{\infty \to \infty}} \right]
\leq 2 \exp \left( \frac{-m}{8 \| V^{-1} \Psi^{-1} \|_{\infty \to \infty}^2} \right) + P\bar{x} \left[ F_{t_j}^{s,s} \right]. \tag{55} \]

The proof of Proposition 2 is completed upon applying Lemma 3 and plugging into (41).

\[ \square \]

### B.3 Proof of Theorem 2

Applying Propositions 1 and 2 to the first and the second terms on the RHS of (23) respectively, we obtain constants \( C_1, C_2, C_3 \in (0, \infty) \) which depend only on \( h^*, \mu \) and \( \lambda \) such that
\[
P\bar{x} \left[ F_k (\bar{X}_{\partial T^k}) \neq \bar{x} \right] \leq 2 \exp \left( \frac{-C_1 \| \partial T^k (s) \|}{M} \right) + C_2 M s
+ 8M \exp \left( \frac{-\| \partial T^k (s) \|}{8 \hat{C}} \right) + C_3 M^4 \hat{C} s \tag{56} \]
for all \( s \in (0, h^*/2] \) and \( k \in \mathbb{N} \), where \( M = |\bar{x}| \) and \( \hat{C} := \| V^{-1} \Psi^{-1} \|_{\infty \to \infty} \in (0, \infty) \) is a constant which depends only on \( \mu, \lambda, h^* \) and \( \{ t_j \}_{j=1}^M \).

For any \( \epsilon \in (0, \infty) \), there exists \( M_\epsilon \) such that \( \sum_{\{ x : |x| > M_\epsilon \}} \Pi(x) < \epsilon/2 \). Hence
\[
P\Pi \left[ F_k (\bar{X}_{\partial T^k}) \neq \bar{x} \right] < \sum_{\{ x : |x| \leq M_\epsilon \}} P\bar{x} \left[ F_k (\bar{X}_{\partial T^k}) \neq \bar{x} \right] \Pi(x) + \frac{\epsilon}{2}
\leq \max_{\{ x : |x| \leq M_\epsilon \}} P\bar{x} \left[ F_k (\bar{X}_{\partial T^k}) \neq \bar{x} \right] + \frac{\epsilon}{2}. \]

From (56), there exist constants \( C_4, C_5 \in (0, \infty) \) which depend only on \( \mu, \lambda, h^*, M_\epsilon \) and \( \{ t_j \}_{j=1}^M \) such that
\[
\max_{\{ x : |x| \leq M_\epsilon \}} P\bar{x} \left[ F_k (\bar{X}_{\partial T^k}) \neq \bar{x} \right] \leq 16 M_\epsilon \exp \left( \frac{-\| \partial T^k (s) \|}{C_4} \right) + C_5 s
\]
for all \( s \in (0, h^*/2] \) and \( k \in \mathbb{N} \). Inequality (6) follows from this. The proof of Theorem 2 is complete.

### B.4 Proof of Theorem 1

Theorem 1 follows from Theorem 2 upon taking sequences \( \epsilon_m \downarrow 0 \) and \( s_m \downarrow 0 \) and then a subsequence \( k_m \to +\infty \) such that the error in (6) goes to 0. This is possible thanks to the big bang condition, which guarantees \( |\partial T^k (s_m) | \to +\infty \) as \( k \to \infty \).
Our estimator runs in time polynomial in the size of the input data. Indeed the length estimator is linear in the length of the longest input sequence and the matrix manipulations in the sequence estimator are polynomial in that quantity.