Near-Optimal Clustering in Mixture of Markov Chains

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Abstract

We study the problem of clustering T trajectories of length H, each generated by one of K unknown ergodic Markov chains over a finite state space of size S. The goal is to accurately group trajectories according to their underlying generative model. We begin by deriving an instance-dependent, high-probability lower bound on the clustering error rate, governed by the weighted KL divergence between the transition kernels of the chains. We then present a novel two-stage clustering algorithm. In Stage I, we apply spectral clustering using a new injective Euclidean embedding for ergodic Markov chains—a contribution of independent interest that enables sharp concentration results. Stage II refines the initial clusters via a single step of likelihood-based reassignment. Our method achieves a near-optimal clustering error with high probability, under the conditions $H = \widetilde{\Omega}(\gamma_{\rm ps}^{-1}(S^2 \vee \pi_{\rm min}^{-1}))$ and $TH = \widetilde{\Omega}(\gamma_{\rm ps}^{-1}S^2)$, where $\pi_{\rm min}$ is the minimum stationary probability of a state across the \widetilde{K} chains and γ_{ps} is the minimum pseudo-spectral gap. These requirements provide significant improvements, if not at least comparable, to the state-of-the-art guarantee (Kausik et al., 2023), and moreover, our algorithm offers a key practical advantage: unlike existing approach, it requires no prior knowledge of model-specific quantities (e.g., separation between kernels or visitation probabilities). We conclude by discussing the inherent gap between our upper and lower bounds, providing insights into the unique structure of this clustering problem.

1 Introduction

Clustering, or community detection for graphs, is a fundamental statistical problem with applications across diverse scientific disciplines, including social science, biology, and statistical physics (Ezugwu et al., 2022; Fortunato, 2010; Kiselev et al., 2019; McLachlan et al., 2019). The precise statistical characterization of clustering has been rigorously investigated under various probabilistic frameworks, such as stochastic block models (SBMs; Abbe (2018)), Gaussian mixture models (GMMs; Chen and Zhang (2024); Löffler et al. (2021); Lu and Zhou (2016)), and block Markov chains (BMCs; Jedra et al. (2023); Sanders et al. (2020)).

However, the aforementioned models primarily focus on clustering static data points or nodes, where individual elements often lack inherent informative structure in isolation: the clustering signal typically emerges only when considering the entire data. In contrast, many real-world applications involving multiple underlying processes, such as astronomy (Yang et al., 2020), mobile social networks (Tang et al., 2021), and human conversation traces (Park et al., 2024), deal with *trajectories*

with a mixture of temporal information. The task is to cluster the trajectories based on their generating process or model. The longer each trajectory (e.g., a user's interaction sequence or a time series) is, the more information it potentially reveals about its generating model, facilitating clustering.

The **Mixture of Markov Chains (MCC)** provides a fundamental yet powerful probabilistic framework for the mentioned problem of trajectory clustering in the most basic scenario with no controllable actions. In this model, we are given T trajectories, each of length H, where each trajectory is generated by one of K unknown Markov chains defined over a finite state space of size S. This model has been studied in a variety of context, originally by Blumen et al. (1955) for modeling heterogeneous labor mobility patterns, and later frequently utilized for learning underlying usage patterns from user trails of app usages, music playlists, web browsing, and more (Cadez et al., 2003; Girolami and Kabán, 2003; Gupta et al., 2016; Maystre et al., 2022; Poulsen, 1990; Spaeh and Tsourakakis, 2023). A more recent motivating example arises in personalized reinforcement learning from human feedback (RLHF) in large language models (LLMs) interacting with diverse users possessing heterogeneous preferences (Park et al., 2024). To provide the best personalized experiences for users of the same preference, LLMs must effectively identify and group feedback data, where the feedback is given on users' conversation traces, according to these underlying preferences, and then perform RLHF.

In MCC, two primary and closely intertwined objectives emerge: *learning* the underlying K Markov chain models (Gupta et al., 2016; Kausik et al., 2023; Spaeh and Tsourakakis, 2023) and *clustering* the observed trajectories according to their generative source (Kausik et al., 2023). Successful clustering can significantly simplify the learning task by allowing for information aggregation within each identified group of trajectories. Conversely, while learning each model accurately can indeed facilitate clustering, it is expected to necessitate stringent requirements on the trajectory length H, because each trajectory is solely responsible for its own amount of information helpful for clustering. Thus, beyond its intrinsic value as an exploratory data analysis technique, accurate clustering can lead to statistically more efficient inference than analyzing each trajectory independently.

As done in prior clustering literature, one can ask two critical questions regarding clustering in MCC:

- 1. What is the fundamental limit on the misclassification rate?
- 2. Given sufficiently long (but not excessively so) trajectories, is there a *computationally tractable, parameter-free*¹ algorithm whose performance (clustering error rate) matches the lower bound? What is the requirement on T and H?

Several studies have algorithmically addressed the second question (Gupta et al., 2016; Kausik et al., 2023; Spaeh and Tsourakakis, 2023, 2024; Spaeh et al., 2024), often without rigorous statistical guarantees. One notable exception is Kausik et al. (2023), where the authors proposed a clustering algorithm that provably performs exact clustering (i.e., zero misclassification error) in MCC when $T = \widetilde{\Omega}(K^2S)$ and $H = \widetilde{\Omega}(K^{3/2}t_{\rm mix})$. However, they do not provide the clustering error rate across various regimes of T and H (and appropriate separation parameters); for instance, they do not address the asymptotic regime where $T \to \infty$, commonly studied in prior clustering literature (Lu and Zhou, 2016; Yun and Proutière, 2016). Moreover, Kausik et al. (2023) lacks a corresponding lower bound and related discussions, making it difficult to assess the optimality of their sample complexity on T and H. Furthermore, their algorithm relies on explicit knowledge of problem-specific quantities, often unavailable in practice. We will elaborate on this comparison in Section 5. Consequently, despite their importance, both of the aforementioned questions have remained elusive in the literature.

Contributions. In short, we answer both questions fully. Specifically:

- (a) We prove an instance-specific high-probability lower bound on the clustering error rate for MCC. This reveals the problem-difficulty quantity \mathcal{D} : the minimum weighted KL divergence between the transition kernels (Section 3).
- (b) We propose a two-stage clustering algorithm that achieves near-optimal clustering error. Notably, it does not require any *a priori* knowledge of the underlying model, yet fully adapts to the given problem difficulty (Section 4). Especially for Stage I, we introduce a new injective Euclidean embedding specifically designed for ergodic Markov chains. This embedding, a contribution of independent interest, facilitates sharp concentration results for spectral clustering analysis (Section 4.1).

¹An algorithm that does not require *a-priori* knowledge of problem-dependent parameters.

(c) Our upper and lower bounds reveal gaps in misclassification errors and the required trajectory length H. Building on recent advances in concentration inequalities (Fan et al., 2021; Paulin, 2015) and estimation techniques (Wolfer and Kontorovich, 2021) for Markov chains, we elucidate the inherent complexities of clustering in MMC that currently render these gaps unavoidable (Appendix D).

Notation. For a positive integer $n \geq 1$, let $[n] := \{1, 2, \cdots, n\}$. For a set X, let $\Delta(X)$ be the set of probability distributions over X. Let $a \vee b := \max\{a, b\}$ and $a \wedge b := \min\{a, b\}$. We will utilize the asymptotic notations $\mathcal{O}, o, \Omega, \omega, \Theta$ freely throughout. For aesthetic purpose, we will also use $f \gtrsim g, f \lesssim g, f \asymp g$, defined as $f = \Omega(g), f = \mathcal{O}(g), f = \Theta(g)$, respectively.

2 Problem Setting

Mixture of Markov chains (MMCs). There are K unknown Markov chains. The k-th Markov chain is denoted as $\mathcal{M}^{(k)}=(\mathcal{S},H,\mu^{(k)},p^{(k)})$. \mathcal{S} is a finite state space of cardinality $S,H\geq 2$ is the horizon or (episode length), $\mu^{(k)}$ is a initial state distribution, and $p^{(k)}(\cdot|\cdot)$ and $P^{(k)}$ are the transition kernel and matrix. We make the following assumption: denoting $\min_{k,s}:=\min_{k\in[K]}\min_{s\in\mathcal{S}}$,

Assumption 1. Each $\mathcal{M}^{(k)}$ is ergodic, with pseudo-spectral gap³ at least $\gamma_{ps} > 0$ and stationary distribution $\pi^{(k)}$. We also have $\pi_{\min} := \min_{k,s} \pi^{(k)}(s), v_{\min} := \min_{k,s} \pi^{(k)}(s)(1 - \pi^{(k)}(s)) > 0$.

For ergodic chains, it is known that γ_{ps} and the mixing time t_{mix} are of same order, up to $\log \frac{1}{\pi_{min}}$:

Proposition 2.1 (Proposition 3.4 of Paulin (2015)).
$$\frac{1}{2} \leq \gamma_{\rm ps} t_{\rm mix} \leq 1 + 2\log 2 + \log \frac{1}{\pi_{\rm min}}$$
, where $t_{\rm mix} := \max_{k \in [K]} t_{\rm mix}^{(k)}$ and $t_{\rm mix}^{(k)} := \min\{t \in \mathbb{N} : \max_{s \in \mathcal{S}} \mathsf{TV}((P^{(k)})^t(s, \cdot), \pi^{(k)}) \leq \frac{1}{4}\}.$

Clustering Problem and Learner's Objective. The learner observes T trajectories generated as follows: for each $t \in [T]$, a trajectory of length H is sampled from $\mathcal{M}^{(f(t))}$. Specifically, trajectory $\mathcal{T}_t = (s_{t,1}, \ldots, s_{t,H})$ is generated as $s_{t,1} \sim \mu^{(f(t))}$ and $s_{t,h+1} \sim p^{(f(t))}(\cdot|s_{t,h})$, which we denote as $\mathcal{T}_t \sim \mathcal{M}^{(f(t))}$. Here, $f:[T] \to [K]$ is the (unknown) ground-truth decoding function that maps each trajectory to its generating Markov chain. The learner's objective is to recover f—that is, to cluster the T trajectories according to their generating models. Let $\hat{f}:[T] \to [K]$ denote the learner's estimated decoding function. The number of misclassified trajectories is measured as:

$$E_T(\widehat{f}, f) := \min_{\sigma \in \text{Sym}(K)} \sum_{t=1}^{T} \mathbb{1}[\widehat{f}(t) \neq \sigma(f(t))],$$

where $\mathrm{Sym}(K)$ is the symmetric group over [K]. The goal is to design an algorithm such that, for any confidence level $\delta \in (0,1)$ and misclassification rate $\varepsilon \in (0,1)$, the following guarantee holds: $\mathbb{P}(E_T(\widehat{f},f) \leq \varepsilon T) \geq 1-\delta$, where the probability \mathbb{P} is over the randomness of both the trajectory generation and the clustering algorithm, and \mathcal{E} is an upper bound on the number of misclassified trajectories with *optimal* dependence on T,H,S,K, and δ . We will assume that the only information available of the learner is γ_{ps} (or some viable lower bound). In particular, the learner does *not* know K a priori, which adds to the complexity of the algorithm design.

Remark 1 (About the knowledge of γ_{ps} or t_{mix}). There has been some recent advancements on estimating γ_{ps} (Hsu et al., 2019; Wolfer and Kontorovich, 2024) and t_{mix} (Wolfer, 2020, 2023; Wolfer and Kontorovich, 2019). Later, we can see that under our requirements on H, both quantities can be estimated accurately.

3 Instance-Specific High Probability Lower Bound

In this section, we present the first instance-specific high-probability lower bound on the number of misclassified trajectories in the MMC problem. We define an instance of the MMC as a tuple

 $^{^2}$ We assume uniform ergodicity: there exist $\rho \in (0,1), M>0$ such that $\max_{s\in\mathcal{S}} \mathsf{TV}\left(P^H(s,\cdot),\pi\right) \leq M\rho^H$ for all $H\in\mathbb{N}$, which is implied by aperiodicity and irreducibility (Levin and Peres, 2017, Theorem 4.9). 3 For ergodic Markov chain with transition matrix P, its pseudo-spectral gap is defined as $\gamma_{\mathrm{ps}} := \max_{k\geq 1} \frac{1}{k} \gamma\left((P^*)^k P^k\right)$, where $\gamma(\cdot)$ is the spectral gap of the self-adjoint operator (Paulin, 2015, Section 3).

 $\Phi_T := ((\mathcal{M}^{(k)})_{k \in [K]}, f, T)$, where $(\mathcal{M}^{(k)})_{k \in [K]}$ is a collection of K ergodic Markov chains, f is the decoding function, and $T \in \mathbb{N}$ is the total number of trajectories to be clustered. Note that each instance of **clustering in MMC** is fully described by Φ_T .

To derive instance-specific lower bounds, we must consider algorithms that for a given instance, genuinely adapt to perturbations of the decoding function. Indeed, an algorithm that would return $\widehat{f} = f$, would have no misclassified trajectories, but would fail for other decoding functions. Hence, we now introduce a class of "good" algorithms that are robust to small instance perturbations with a given confidence level: denoting $\alpha(f) := (\alpha_k(f))_{k \in [K]} \in \Delta([K])$ with $\alpha_k(f) := |f^{-1}(k)|/T$,

Definition 3.1 (Stable Clustering Algorithms). Let $(\varepsilon, \beta, \delta) \in [0, 1] \times \mathbb{R}_{\geq 0} \times (0, 1/2]$. A clustering algorithm \mathcal{A} is $(\varepsilon, \beta, \delta)$ -locally stable at $\Phi_T := ((\mathcal{M}^{(k)})_{k \in [K]}, f, T)$ if the following holds: for all $\Phi_T' = ((\mathcal{M}^{(k)})_{k \in [K]}, f', T)$ such that $\|\alpha(f') - \alpha(f)\|_2 \leq \beta$,

$$\mathbb{P}_{\Phi_T', \mathcal{A}}\left(E_T(\widehat{f}_{\mathcal{A}}, f') > \varepsilon T\right) \le \delta,\tag{1}$$

where $\widehat{f}_{\mathcal{A}}$ is the outputted clustering function from our algorithm \mathcal{A} that takes as input the T trajectories whose ground-truth clustering is given by f'. Furthermore, we say that \mathcal{A} is (ε, β) -asymptotically locally stable at $\Phi := ((\mathcal{M}^{(k)})_{k \in [K]}, f)$ if there exists a sequence $(\delta_T)_{T \in \mathbb{N}}$ with $\lim_{T \to \infty} \delta_T = 0$ such that \mathcal{A} is $(\varepsilon, \beta, \delta_T)$ -locally stable at Φ_T for all $T \in \mathbb{N}$.

Intuitively, the perturbation is the (slight) change in the relative cluster sizes $\alpha(f)$, inspired by the prior definitions of locally stable algorithms for clustering in SBMs (Yun and Proutière, 2019, Definition 1) and block Markov chains (Jedra et al., 2023; Sanders et al., 2020).

We now present our lower bound, whose full proof is deferred to Appendix A:

Theorem 3.1 (Instance-Specific High-Probability Lower Bound). Let $(\varepsilon, \delta) \in [0, 1] \times (0, 1/2]$. Then, a necessary condition for the existence of a $(\varepsilon, \beta, \delta)$ -locally stable algorithm at $\Phi_T := ((\mathcal{M}^{(k)})_{k \in [K]}, f, T)$ with $\beta \geq 2\sqrt{2}\varepsilon$ is as follows: denoting $\alpha_{\min} = \min_{k \in [K]} \alpha_k(f)$,

$$\delta \ge \frac{1}{2} \left(\frac{\alpha_{\min}}{16e\varepsilon} \right)^{\varepsilon T} \exp\left(-4\varepsilon T(H-1)\mathcal{D} \right) \Longleftrightarrow 4(H-1)\mathcal{D} \ge \frac{1}{\varepsilon T} \log \frac{1}{2\delta} + \log \frac{\alpha_{\min}}{16e\varepsilon}.$$
 (2)

For (ε, β) -asymptotically locally stable algorithm with the same β as above and $\varepsilon = o(1)$, we have the following necessary condition:

$$\liminf_{T \to \infty} \frac{2(H-1)\mathcal{D}}{\log \frac{\alpha_{\min}}{16c_c}} \ge 1.$$
(3)

The information-theoretic divergence is defined as $\mathcal{D} := \min_{k \neq k' \in [K]} \mathcal{D}^{(k,k')}$, where

$$\mathcal{D}^{(k,k')} := \frac{1}{H-1} \, \mathsf{KL}\left(\mu^{(k)}, \mu^{(k')}\right) + \sum_{s \in \mathcal{S}} \mathbb{P}_{H}^{(k)}(s) \, \mathsf{KL}\left(p^{(k)}(\cdot|s), p^{(k')}(\cdot|s)\right), \tag{4}$$

where
$$\mathbb{P}_{H}^{(k)}(s) := \frac{1}{H-1} \sum_{h=1}^{H-1} \mathbb{P}^{(k)}(s_h = s)$$
.

Proof sketch. The proof proceeds by first constructing a large number of hypotheses, each corresponding to different cluster allocations of the observations using combinatorial arguments of Yun and Proutière (2019). These hypotheses are slight perturbations of the given instance of clustering in MMC. We then utilize the change-of-measure argument (Lai and Robbins, 1985) and data-processing inequality (Garivier et al., 2019, Lemma 1) to relate the error of any "good" clustering algorithm to the KL divergences between the true and alternate models. Lastly, we "optimize" the resulting lower bound over our construction of different allocations. The proof is largely inspired by Yun and Proutière (2019, Theorem 1) and Jedra and Proutière (2023, Theorem 2), where high-probability lower bounds are proved for the clustering in SBMs and linear system identification, respectively. □

Remark 2 (Chernoff Information). *Dreveton et al.* (2024) recently highlighted Chernoff information as a universal measure of clustering difficulty for sub-exponential mixtures, extending earlier results in SBM clustering (Abbe and Sandon, 2015a,b; Dreveton et al., 2023). While our analysis uses KL divergence, the two quantities are closely related (van Erven and Harremos, 2014) and become equivalent as $T \to \infty$ in many settings, including labeled SBMs (Yun and Proutière, 2016, Claim 4).

Remark 3 (Comparison to Wang and Choi (2023)). One notable related result is Wang and Choi (2023, Theorem 4.1), which establishes an asymptotic equipartition property (Cover and Thomas, 2006, Theorem 11.8.1) of binary hypothesis testing between two Markov chains from $\{(X_{h,1}, X_{h,2})\}_{h \in [H]}$, where $X_{h,1} \stackrel{i.i.d.}{\sim} \nu$ and $X_{h,2} \sim P(\cdot|X_{h,1})$. Our asymptotic lower bound is a generalization of theirs, as we consider the full Markov chain instead of a collection of single hops.

Asymptotically Exact Recovery. The necessary condition for asymptotically exact recovery, i.e., when $\varepsilon = \mathcal{O}(1/T)$ is $H\mathcal{D} = \Omega(\log T)$. This mirrors the minimax lower bound for GMM clustering (Lu and Zhou, 2016, Theorem 3.3), where strong consistency demands that $\Delta^2/\sigma^2 = \Omega(\log n)$ —with Δ denoting the minimum mean separation (referred to as the signal-to-noise ratio, or SNR), σ the isotropic variance of the GMM, and n the number of data points. Analogously, in our setting, the SNR is given by \mathcal{D} , the minimum KL divergence between Markov chains, and H plays a role similar to $1/\sigma^2$: longer trajectories reduce variance, much like smaller σ^2 does in the GMM.

Interpretation of \mathcal{D} . Note that in \mathcal{D} , as $H \to \infty$ the first term vanishes, given that the initial distributions share the same support. Thus, the difficulty of clustering in MMC is determined by $\sum_{s \in \mathcal{S}} \mathbb{P}^{(k)}(s) \operatorname{KL}(p^{(k)}(\cdot|s), p^{(k')}(\cdot|s))$, which quantifies the distinguishing⁴ power from different emission probabilities from each state, *weighted* by its average visitation probability. In other words, even though state s has been visited sufficiently often, if s can't distinguish between the two chains (i.e., $p^{(k)}(\cdot|s) \approx p^{(k')}(\cdot|s)$), its contribution diminishes. Vice versa, even though state s has sufficient distinguishing power, its contribution diminishes if it is not visited sufficiently often.

4 Near-Optimal Clustering Algorithm for MMC

Motivated by prior clustering literature (Gao et al., 2017; Lu and Zhou, 2016; Yun and Proutière, 2016), our algorithm consists of two stages. The full pseudocodes are provided in Algorithm 1 and 2.

4.1 Stage I. Initial Spectral Clustering, Without Knowing K

Algorithm Design. We utilize a variant of spectral clustering (von Luxburg, 2007) that does not require the knowledge of K (Kannan and Vempala, 2009; Yun and Proutière, 2016). The key novelty here is the data matrix on which we perform the spectral decomposition, which we describe here.

For an ergodic Markov chain \mathcal{M} with transition probability matrix \mathbf{P} and stationary distribution π , we introduce the following S^2 -dimensional Euclidean embedding and its empirical version:

$$L: \mathcal{M} \mapsto \operatorname{vec}\left(\operatorname{diag}(\pi)^{1/2} \mathbf{P}\right), \quad \widehat{L}: \mathcal{T} = (s_1, s_2, \cdots, s_H) \mapsto \left(\widehat{N}(s, s') / \sqrt{H\widehat{N}(s)}\right)_{(s, s') \in \mathcal{S}^2},$$

where
$$\mathcal{T} \sim \mathcal{M}, \, \widehat{N}(s) := \sum_{h=1}^{H} \mathbb{1}[s_h = s], \, \text{and} \, \, \widehat{N}(s,s') := \sum_{h=1}^{H-1} \mathbb{1}[s_h = s, s_{h+1} = s'].$$

Remark 4. To the best of our knowledge, such Euclidean embedding of ergodic Markov chain has not been reported in the literature yet. Without the square root, this is precisely the doublet frequency (Vidyasagar, 2014; Wolfer and Kontorovich, 2021), which is known to encode all information about the ergodic Markov chain. This vaguely resembles the diffusion map (Coifman and Lafon, 2006) or weighted Laplacian (Chung, 1997), but we could not establish a clear connection.

We show below that our L also encodes all information about the chain:

Proposition 4.1. Over the space of ergodic Markov chains with a common initial state distribution, L is an injective mapping, i.e., $L(\mathcal{M}) = L(\mathcal{M}') \iff \mathcal{M} = \mathcal{M}'$.

⁴The precise interpretation of KL is the "measure of the inefficiency of assuming that the Markov chain is k-th, when it is actually k'-th. This is clear when one considers the proof of our lower bound, where we swap the trajectories from two distinct clusters.

```
Algorithm 1: Initial Spectral Clustering (without knowing K)
```

```
Input: t_{\text{mix}}, \{\mathcal{T}_t = (s_{t,1}, s_{t,2}, \cdots, s_{t,H})\}_{t \in [T]}
        /* Adaptive Spectral Decomposition
                                                                                                                                                                                                                                                                 */
  \mathbf{1} \ \widehat{\boldsymbol{U}} \widehat{\boldsymbol{\Sigma}} \widehat{\boldsymbol{V}}^{\top} \leftarrow \text{SVD of } \widehat{\boldsymbol{W}} \in [0,1]^{T \times S^2} \text{ (see Eqn. (5)), with } \widehat{\boldsymbol{\Sigma}} := \operatorname{diag}(\{\widehat{\sigma}_i\}_{i \in [\min(T,S^2)]});
  \mathbf{2} \ \widehat{R} \leftarrow \sum_{i=1}^{\min(T,S^2)} \mathbb{1} \left[ \widehat{\sigma}_i \geq \widehat{\sigma}_{\text{thres}} \triangleq 8\sqrt{\frac{TS}{H\gamma_{\text{ps}}} \log \frac{TH}{\delta}} \right];
  3 \widehat{m{X}} \leftarrow \widehat{m{U}}_{1:\widehat{R}} \widehat{m{\Sigma}}_{1:\widehat{R}} ; 
 /* Adaptive Clustering
                                                                                                                      // Spectral representation for each t \in [T]
   \textbf{4 Define } \mathcal{Q}_t \leftarrow \left\{t' \in [T]: \left\|\widehat{\boldsymbol{X}}_{t',:} - \widehat{\boldsymbol{X}}_{t,:}\right\|_2^2 \leq (\widehat{\sigma}_{\mathrm{thres}})^2 \right\} \text{ for each } t \in [T]; 
  5 Initialize S_0 \leftarrow \emptyset, k \leftarrow 1, and \rho \leftarrow T;
  6 while \rho \geq \frac{32\widehat{R}T}{\log \frac{TH}{\varepsilon}} do
 7  \begin{vmatrix} t_k^{\star} \leftarrow \arg\max_{t \in [T]} \left| \mathcal{Q}_t \setminus \bigcup_{\ell=0}^{t-1} \mathcal{S}_{\ell} \right|; \\ \mathbf{8} & \mathcal{S}_k \leftarrow \mathcal{Q}_{t_k^{\star}} \setminus \bigcup_{\ell=0}^{k-1} \mathcal{S}_{\ell}; \\ \mathbf{9} & \left| \mathcal{S}_k \right|, k \leftarrow k+1; 
 10 \hat{K} := k - 1:
                                                                                                                                          //\ \widehat{K}\colon Estimated number of clusters
 11 \widehat{f}_0(t) := k for t \in \mathcal{S}_k and k \in [\widehat{K}];
12 for t \in [T] \setminus \bigcup_{k=1}^{\widehat{K}} \mathcal{S}_k do
13 \widehat{f}_0(t) := \arg\min_{k \in |\widehat{K}|} \|\widehat{X}_{t_k^{\star},:} - \widehat{X}_{t,:}\|_{\mathcal{L}}
        Return: \widehat{K}, \ \widehat{f}_0: [T] \to [\widehat{K}]
```

Proof. By definition, we must have that for all $s, s' \in \mathcal{S}$, $\sqrt{\pi(s)}p(s'|s) = \sqrt{\pi'(s)}p'(s'|s)$. Summing over $s' \in \mathcal{S}$, we have that $\pi(s) = \pi'(s) > 0$ for all $s \in \mathcal{S}$, where the ergodicity of the chains implies the strict positivity. This then implies that p = p', i.e., $\mathcal{M} = \mathcal{M}'$.

We now define our ground-truth and empirical data matrices as follows:

$$\boldsymbol{W} = \left[L(\mathcal{M}^{(f(t))}) \right]_{t \in [T],:} \in [0, 1]^{T \times S^2}, \quad \widehat{\boldsymbol{W}} = \left[\widehat{L}(\mathcal{T}_t) \right]_{t \in [T],:} \in [0, 1]^{T \times S^2},$$
 (5)

i.e., by row-concatenating the embeddings. Then, the minimum (row-wise) ℓ_2 -separation of W is

$$\Delta_{\mathbf{W}}^2 := \min_{k \neq k'} \left\| L(\mathcal{M}^{(k)}) - L(\mathcal{M}^{(k')}) \right\|_2^2 = \min_{k \neq k'} \sum_{s \in \mathcal{S}} \left\| \sqrt{\pi^{(k)}(s)} p^{(k)}(\cdot | s) - \sqrt{\pi^{(k')}(s)} p^{(k')}(\cdot | s) \right\|_2^2.$$

By Proposition 4.1, $\Delta_{W}=0$ iff at least two of the K Markov models are exactly the same. This also provides an intuitive motivation for our choice of L. Informally, Δ_{W}^{2} can be viewed as roughly corresponding to $\min_{k\neq k'}\sum_{s\in\mathcal{S}}\pi^{(k)}(s)\|p^{(k)}(\cdot|s)-p^{(k')}(\cdot|s)\|_{2}^{2}$, which, up to a constant, is upper bounded by $\mathcal{D}=\min_{k\neq k'}\sum_{s\in\mathcal{S}}\pi^{(k)}(s)$ KL $(p^{(k)}(\cdot|s),p^{(k')}(\cdot|s))$ (see Lemma D.1). Hence, our L facilitates a more "direct" comparison between the ℓ_{2} -based separation Δ_{W}^{2} and the KL-based separation \mathcal{D} . We discuss in more detail on the relations between different gaps in Section 5(3).

Theoretical Analysis. We now present the performance guarantee of Stage I, whose full proof is deferred to Appendix B:

Theorem 4.1 (Performance Guarantee of Stage I). Let $\delta \in (0,1)$, and suppose that $H \gtrsim \frac{1}{v_{\min}\gamma_{\mathrm{ps}}}\log\frac{1}{\pi_{\min}\delta} \vee \frac{S}{\Delta_{\boldsymbol{W}}^2\gamma_{\mathrm{ps}}}\log\frac{H}{\delta}\log\frac{TH}{\delta}$. Then, we have the following: with $R = \mathrm{rank}(\boldsymbol{W})$,

$$\mathbb{P}\left(E_T(\widehat{f}_0, f) \lesssim \frac{TRS}{H\gamma_{\text{ps}}\Delta_{\boldsymbol{W}}^2} \log \frac{TH}{\delta}\right) \ge 1 - \delta. \tag{6}$$

Algorithm 2: Likelihood Improvement

Input: $\widehat{f}_0:[T] \to [K]$ from Algorithm 1, $\{\mathcal{T}_t = (s_{t,1},s_{t,2},\cdots,s_{t,H})\}_{t\in[T]}$

1 Estimate $p^{(k)}(\cdot|\cdot)$ for each $k \in [K]$ as follows: for all $s, s' \in \mathcal{S}$,

$$\widehat{p}_{0}^{(k)}(s'|s) \leftarrow \frac{\sum_{t \in (\widehat{f}_{0})^{-1}(k)} \sum_{h \in [H-1]} \mathbb{1}[s_{t,h} = s, s_{t,h+1} = s']}{\sum_{t \in (\widehat{f}_{0})^{-1}(k)} \sum_{h \in [H-1]} \mathbb{1}[s_{t,h} = s]}.$$
(7)

2 Refine the cluster estimates via trajectory-wise maximum likelihood estimator: for each $t \in [T]$,

$$\widehat{f}(t) \leftarrow \underset{k \in [K]}{\operatorname{arg max}} \left\{ \mathcal{L}(k;t) \triangleq \sum_{h=1}^{H-1} \log \widehat{p}_0^{(k)}(s_{t,h+1}|s_{t,h}) \right\}$$
(8)

Return: $\widehat{f}:[T] \to [K]$

Proof sketch. We first prove $\left\| \boldsymbol{W} - \widehat{\boldsymbol{W}} \right\|_{2 \to \infty} \lesssim \sqrt{\frac{S}{H\gamma_{\mathrm{ps}}}} \log \frac{TH}{\delta}$ (Lemma B.1), our key technical novelty. From here, the proof largely follows that of Yun and Proutière (2016, Algorithm 2). Note that the decay rate is *independent* of π_{\min}^{-1} , which is crucial in obtaining a tight requirement on H when combined with Stage II. Such rate is possible as the weighting by $\sqrt{\pi(s)}$ in our embedding L cancels out with both $\widetilde{\mathcal{O}}\left(1/\sqrt{H\pi(s)}\right)$ for ℓ_2 -estimation of $p(\cdot|s)$ and $\widetilde{\mathcal{O}}\left(1/\sqrt{H\pi(s)\gamma_{\mathrm{ps}}}\right)$ for the estimation of $\sqrt{\pi(s)}$, which come up when decomposition the error via the triangle inequality. \square

4.2 Stage II. One-Shot Trajectory Likelihood Improvement

Algorithm Design. By the Neyman-Pearson lemma (Neyman and Pearson, 1933) and from our information-theoretic lower bound (Theorem 3.1), we must perform trajectory-wise likelihood testing to achieve the optimal performance. But, we do not know the transition kernels p beforehand. Hence, we first utilize the "good enough" $\hat{f}_0: [T] \to [K]$ from Stage I to estimate the transition kernels \hat{p}_0 (line 1). Then, we perform likelihood-based reassignment of the cluster labels based on \hat{p}_0 (line 2).

Theoretical Analysis. Here, we consider the following additional regularity assumption:

Assumption 2 (η -regularity *across* the chains). $\exists \eta_{\mu}, \eta_{\pi}, \eta_{p} > 1$ *s.t.*

$$\max_{s \in \mathcal{S}} \max_{k,k' \in [K]} \frac{\mu^{(k)}(s)}{\mu^{(k')}(s)} \le \eta_{\mu}, \ \max_{s \in \mathcal{S}} \max_{k,k' \in [K]} \frac{\pi^{(k)}(s)}{\pi^{(k')}(s)} \le \eta_{\pi}, \ \max_{s,s' \in \mathcal{S}} \max_{k,k' \in [K]} \frac{p^{(k)}(s'|s)}{p^{(k')}(s'|s)} \le \eta_{p}. \quad (9)$$

Remark 5. The assumption above does not require the chains to be uniform. For example, it does not impose $\pi^{(k)}(s) = \Theta(1)$, as done in SBMs (Yun and Proutière, 2014a) or block Markov chains (Jedra et al., 2023; Sanders et al., 2020) where all edge/transition probabilities are roughly 1/S (S is the number of states). Instead, our assumption only requires that if one chain exhibits non-uniformity in certain states, then the other chains must exhibit similar non-uniformity in those same states.

Recall from our lower bound (Theorem 3.1) that in the asymptotic regime $T \to \infty$, a necessary condition for asymptotically accurate (or exact) recovery is $H\mathcal{D} = \Omega(\log T)$, implying $H \to \infty$ as well. Given this and under Assumptions 1 (ergodicity) and 2 (η -regularity), we observe that $\mathsf{KL}(\mu^{(k)}, \mu^{(k')}) \le \log \eta_{\mu} < \infty$ and hence:

$$\begin{split} \mathcal{D}^{(k,k')} &= \frac{1}{H-1} \operatorname{KL}\left(\mu^{(k)}, \mu^{(k')}\right) + \sum_{s \in \mathcal{S}} \mathbb{P}_H^{(k)}(s) \operatorname{KL}\left(p^{(k)}(\cdot|s), p^{(k')}(\cdot|s)\right) \\ &\stackrel{H \to \infty}{\longrightarrow} \sum_{s \in \mathcal{S}} \pi^{(k)}(s) \operatorname{KL}\left(p^{(k)}(\cdot|s), p^{(k')}(\cdot|s)\right) =: \mathcal{D}_{\pi}^{(k,k')}. \end{split}$$

We define the **stationary version of** \mathcal{D} as $\mathcal{D}_{\pi} := \min_{k \neq k'} \mathcal{D}_{\pi}^{(k,k')}$. As $H \to \infty$, the contribution from the divergence between initial state distributions, $\mathsf{KL}(\mu^{(k)}, \mu^{(k')})$, becomes negligible compared

to the cumulative signal from transitions. This is reflected in Algorithm 2, which performs likelihood tests based solely on transition dynamics.

We now present the final error guarantee of Algorithm 2; the proof is deferred to Appendix C:

Theorem 4.2 (Performance Guarantee of Stage I+II). Suppose Assumptions 1 and 2 hold, and that the following requirements on H and T hold:

$$TH \gtrsim \frac{(S\log T)^2}{\alpha_{\min}\mathcal{D}_{\pi}^2\gamma_{\mathrm{ps}}} \text{ and } H \gtrsim \frac{1}{\gamma_{\mathrm{ps}}} \left(S^2\log T \vee \frac{\log\frac{TH}{\pi_{\min}}}{v_{\min}} \vee \frac{\eta_p\eta_{\pi}RS\log(TH)}{\alpha_{\min}\mathcal{D}_{\pi}\Delta_{\pmb{W}}^2}\right).$$

Then, for some $C_{\eta} \asymp \frac{1}{\eta_p^2}$, we have that w.h.p.^a,

$$E_T(\widehat{f}, f) \lesssim T \exp\left(-C_\eta \gamma_{\rm ps} H \mathcal{D}_\pi\right).$$
 (10)

^awith probability tending to 1 as $T \to \infty$.

One can immediately see that the obtained upper bound on the clustering error rate nearly matches the lower bound (Theorem 3.1), up to some constants and a factor of $\gamma_{\rm ps}$ in the exponential, which we elaborate in the subsequent section.

5 Discussions

(1) Gaps Between Upper and Lower Bounds. By comparing our performance upper bound (Theorem 4.2) and lower bound (Theorem 3.1), we identify two key gaps.

The first concerns the clustering error rates: the lower bound scales as $T\exp(-2H\mathcal{D})$, while the upper bound scales as $T\exp(-C_\eta\gamma_{\rm ps}H\mathcal{D}_\pi)$, where C_η is a constant depending on the regularity parameters η_p and η_π . The upper bound thus contains an additional multiplicative factor of $\gamma_{\rm ps}$ in the exponential term. The second gap pertains to the requirement on the horizon length H. Specifically, the lower bound holds for any $H \geq 2$ and $T \geq 1$, while the upper bound requires $H = \widetilde{\Omega}(\gamma_{\rm ps}^{-1}(S^2 \vee \pi_{\rm min}^{-1}))$ and $TH = \widetilde{\Omega}(\gamma_{\rm ps}^{-1}S^2)$, omitting logarithmic and other secondary factors.

We believe these gaps indicate that the current lower bound may be loose. Both stem from the fact that the transition kernels p are not known a priori and must be estimated by the learner, whereas the lower bound analysis assumes full knowledge of the p's.

The first gap arises from employing the Markovian Bernstein concentration inequality of Paulin (2015), which relies on decomposing the trajectories of the Markov chain into nearly independent blocks of length proportional to $\gamma_{\rm ps}H$ (Janson, 2004; Lezaud, 1998; Yu, 1994). Recent results confirm that this dependence on $\gamma_{\rm ps}$ in the exponent is indeed unavoidable for (reversible) Markov chains: there exist chains for which the concentration rate matches this dependency (Fan et al., 2021; Jiang et al., 2018; Rabinovich et al., 2020). The second gap stems from the concentration of \widehat{W} around W, which in turn requires accurate estimation of the transition kernels. Wolfer and Kontorovich (2021, Theorem 3.2) show the following requirement on H: if $H = o\left(\frac{1}{\varepsilon^2\pi_{\min}} + \frac{S}{\gamma_{\rm ps}}\right)$, then no estimator can achieve ε -accuracy in $\|\cdot\|_{2\to\infty}$.

We leave to future work the development of a more comprehensive lower bound that explicitly accounts for the learner's uncertainty about the transition kernels p. Broadly, this challenge can be framed as a nonparametric statistical question (Tsybakov, 2009): to what extent does uncertainty in the underlying probability measures degrade the power of hypothesis testing?

(2) Comparison with Kausik et al. (2023). We first recall their result on exact cluster recovery: Assumption 3 (Assumption 2 of Kausik et al. (2023)). There are $\alpha, \Delta > 0$ such that: $\forall k \neq k' \in [K]$,

$$\exists s = s(k, k') \text{ s.t. } \pi^{(k)}(s), \pi^{(k')}(s) \ge \alpha \text{ and } \left\| p^{(k)}(\cdot|s) - p^{(k')}(\cdot|s) \right\|_2 \ge \Delta. \tag{11}$$

 $^{^5}$ Their theorem is stated for $\|\cdot\|_{1\to\infty}$, but the same argument applies to $\|\cdot\|_{2\to\infty}$ with minimal modification.

Theorem 5.1 (Theorem 3 of Kausik et al. (2023)). Suppose that Assumptions 1 and 3 hold. Set the algorithm hyperparameters, occurrence and histogram clustering thresholds, as $\beta = \frac{\alpha}{3}$ and $\tau = \frac{3\Delta^2}{4}$, respectively. Then, with $H \gtrsim K^{3/2} t_{\text{mix}} \frac{\left(\log(T/(\alpha\delta))\right)^4}{\alpha^3 \Delta^6}$ and $T \gtrsim K^2 S \frac{\log(1/\delta)}{\alpha^3 \Delta^8}$, their Algorithm 2 attains exact clustering (i.e., no misclassifications) with probability at least $1 - \delta$.

Kausik et al. (2023) treat α and Δ as constants, independent of the number of states S and the trajectory length H. This assumption allows their condition on H to avoid any polynomial dependence on S, and ensures that the requirement on T scales only linearly with S. In effect, they implicitly assume that for every pair $k \neq k'$, there exists a highly visited state s(k,k') with constant separation and from which clusters can be identified. However, this assumption does not hold in general. For example, in uniform-like Markov chains where $\pi(s) = \Theta(1/S)$, they require $H \gtrsim t_{\rm mix} S^3 (\log T)^4$ and $T \gtrsim S^4 \log T$ (with $\delta = 1/T$), which are impractically large. In the same regime, our algorithm requires only $H \gtrsim t_{\rm mix}(S^2 \vee \pi_{\rm min}^{-1}) \log T$ and $TH \gtrsim t_{\rm mix}S^2$, a significant improvement.

Moreover, a major limitation of their algorithm is that it requires prior knowledge of α and Δ for Theorem 5.1 to apply. In contrast, our algorithm is completely parameter-free (see Remark 1 for relaxing the knowledge of $\gamma_{\rm ps}$). Also, our requirements of H and T, albeit worse by a factor of $\pi_{\rm min}^{-1}$ in the ideal scenario mentioned above, are generally much better, and are believed to be minimax optimal as discussed in (1). An interesting future direction is whether an instance-wise optimal algorithm is possible, i.e., when the condition on H for cluster recovery is $H\gtrsim t_{\rm mix}$ under Assumption 3 with $\alpha=\Omega(1)$, and $H\gtrsim \gamma_{\rm ps}^{-1}(S^2\vee\pi_{\rm min}^{-1})$, or better, in the worst-case.

(3) **Different gaps:** \mathcal{D}_{π} , Δ_{W} , Δ and α . Throughout this paper, we have introduced different notions of separability: the KL gap \mathcal{D}_{π} , the "aggregated" ℓ_{2} gap Δ_{W} , and the separability quantities Δ , α from Kausik et al. (2023). The following proposition, proved in Appendix D.1, shows the three-way relationship between these gaps:

Proposition 5.1. Define $p_{\max} := \max_{k \in [K]} \max_{s,s' \in S} p^{(k)}(s'|s)$. We then have the following:

(a)
$$p_{\text{max}} \mathcal{D}_{\pi} \gtrsim \alpha \Delta^2$$
; (b) $p_{\text{max}} \mathcal{D}_{\pi} + \sqrt{\mathcal{D}_{\pi}/\pi_{\text{min}}} \gtrsim \Delta_{\boldsymbol{W}}^2$;

(c) under Assumption 2,
$$\Delta_{\mathbf{W}}^2 \gtrsim \alpha \Delta^2 - \mathcal{O}((\sqrt{\eta_{\pi}} - 1)^2)$$
.

The inequality (b) holds up to uniform ergodicity contraction constants, see Appendix D.1 for details. Note that due to our choice of W (Eqn. (5)), Δ_W^2 and the other gaps become comparable. Indeed, for η -regular ergodic Markov chains with $\alpha\Delta^2\gtrsim (\sqrt{\eta_\pi}-1)^2$, we roughly have $\alpha\Delta^2\lesssim \Delta_W^2\lesssim p_{\max}\mathcal{D}_\pi$.

Although our optimal clustering error rates depend only on \mathcal{D}_{π} , ensuring the success of ℓ_2 -based spectral clustering in Stage I requires that $H\gtrsim \frac{1}{\mathcal{D}_{\pi}\Delta_{W}^{2}}$. Note that Kausik et al. (2023)'s algorithm also relies on a similar notion of ℓ_2 -separation, as reflected in their requirement $H\gtrsim \frac{1}{(\alpha\Delta^2)^3}$. While our dependence on the separation gap is already clearly better, we make this comparison explicit by proving that the ratio between $\alpha\Delta^2$ and Δ_{W}^2 can be as large as S (see Appendix D.2 for details).

Proposition 5.2. There exists an instance of clustering in MMC such that $\Delta_W^2 \simeq S\alpha\Delta^2 \lesssim \frac{\mathcal{D}_\pi}{S}$.

Intuitively, Kausik et al. (2023)'s $\alpha\Delta^2$ accounts for separation from a single "good" state, whereas our Δ_W aggregates separation information across all states. Also, for uniform-like Markov chains where $p_{\max} \approx \frac{1}{S}$, an additional gap of S pops up due to Proposition 5.1(b).

It remains an interesting question whether the dependence of H on Δ_W is unavoidable or merely an artifact of our current algorithm design, which relies on ℓ_2 -based spectral clustering. We believe that because the "natural" gap \mathcal{D}_{π} requires knowledge of the transition kernels—which we do not assume—the use of Δ_W or a similarly weaker proxy is unavoidable. Since spectral initialization is a standard Stage I for two-stage procedures (Gao et al., 2017; Lu and Zhou, 2016; Yun and Proutière, 2016), we believe our dependency on Δ_W is optimal among ℓ_2 -based methods.

6 Conclusion and Future Work

This paper investigates clustering in a mixture of ergodic Markov chains. We derived an instancespecific lower bound on clustering error, which is, to our knowledge, the first of its kind in this literature. We also proposed a computationally efficient, two-stage algorithm that delivers near-optimal error rates without requiring model-specific knowledge. Among various technical novelties, our primary contribution is the design of Stage I, which introduces a new injective Euclidean embedding for ergodic Markov chains. This novel embedding is crucial for achieving sharp concentration results and accurately clustering trajectories via spectral methods, reinforcing the growing body of literature on the efficacy of spectral algorithms in structured reinforcement learning environments (Azizzadenesheli et al., 2016, 2017; Jedra et al., 2023; Kausik et al., 2023).

We present several future directions for this work. First, our algorithm requires $\mathcal{O}(TS^2)$ space complexity, which is quite intensive. Making the algorithm more space-efficient by considering streaming settings (Yun et al., 2014) and/or using tools from randomized linear algebra (Woodruff, 2014) is important for large-scale applications. It would also be interesting to explore the relationship between the distances considered here for Markov chains (KL divergence and our L-based ℓ_2 distance) and other information divergences beyond KL (Wang and Choi, 2023), as well as the recently studied bisimulation metric (Calo et al., 2024, 2025). Extending our algorithm to controlled Markov chains (Banerjee et al., 2025; Kausik et al., 2023) is another important direction, as having actions often presents unique challenges (Jedra et al., 2023) and naturally connects to latent MDPs (Kwon et al., 2021, 2024a,b) with real-world applications like personalized RLHF (Park et al., 2024).

Acknowledgments and Disclosure of Funding

J. Lee and S.-Y. Yun were supported by the Institute of Information & Communications Technology Planning & Evaluation (IITP) grant funded by the Korean government(MSIT) (No. RS-2022-II220311, Development of Goal-Oriented Reinforcement Learning Techniques for Contact-Rich Robotic Manipulation of Everyday Objects, No. RS-2024-00457882, AI Research Hub Project, and No. RS-2019-II190075, Artificial Intelligence Graduate School Program (KAIST)). Y. Jedra was supported by the Knut and Alice Wallenberg Foundation Postdoctoral Scholarship Program under grant KAW 2022.0366.

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A Proof of Theorem 3.1 – Fundamental Lower Bound

Let $(\varepsilon, \delta) \in [0, 1] \times (0, 1/2]$, $\alpha \in \Delta([K])$, and $T \in \mathbb{N}$ be fixed. Let $c = \varepsilon T$ be the "target" number of misclassifications. Let $f^{(0)} \triangleq f : [T] \to [K]$ be the ground-truth clustering satisfying $\alpha^{(0)} := \alpha(f^{(0)}) = \alpha$, and let us denote $\mathcal{C}_k^{(0)} := (f^{(0)})^{-1}(k) = \{t \in [T] : f^{(0)}(t) = k\}$ be the set of trajectories in the k-th cluster.

We recall the following notion of distance between two clustering functions $f, g : [T] \to [K]$:

$$E_T(f,g) := \min_{\sigma \in \text{Sym}(K)} \sum_{t \in [T]} \mathbb{1}[f(t) \neq \sigma(g(t))]. \tag{12}$$

This is a proper metric on a suitable space of allocations, as shown in the following proposition (its proof deferred to the end of this section):

Proposition A.1. Let $\mathcal{F}(T,K) := [K]^T = \{f \mid f : [T] \to [K]\}$ and $\widetilde{\mathcal{F}}(T,K) := \mathcal{F}(T,K) / \sim$, where $f \sim g$ iff $\exists \sigma \in \operatorname{Sym}(K)$ s.t. $f = \sigma \circ g$. Then, $E_T(\cdot, \cdot)$ is a proper metric on $\widetilde{\mathcal{F}}(T,K)$.

Let us arbitrarily fix $a \neq b \in [K]$ that we will optimize later. We construct M_T alternate hypotheses $\{f^{(m)}: [T] \to [K]\}_{m \in [M_n]}$ by re-allocating some trajectories from cluster b to a. We denote the probability measure and expectation w.r.t. each m-th allocation as \mathbb{P}_m and \mathbb{E}_m , respectively.

The construction will satisfy the following conditions for all $m \in [M_T]$: denoting $C_k^{(m)} := (f^{(m)})^{-1}(k)$ for $k \in [K]$,

(C1)
$$\mathcal{C}_a^{(0)} \subset \bigcap_{m \in [M_T]} \mathcal{C}_a^{(m)}, |\mathcal{C}_a^{(m)}| = \alpha_a n + 2c$$
, and $|\mathcal{C}_b^{(m)}| = \alpha_b n - 2c$,

(C2)
$$E_T(f^{(m)}, f^{(\ell)}) > 2c, \quad \forall m, \ell \in \{0\} \cup [M_T],$$

(C3)
$$C_k^{(m)} = C_k^{(0)}, \quad \forall k \in [K] \setminus \{a, b\}.$$

The following lemma quantifies the minimum number of such hypotheses:

Lemma A.1.
$$M_T \geq 2 \left(\frac{\alpha_b T}{16ec}\right)^c$$
.

Proof. The combinatorial argument here is due to Yun and Proutière (2019, Appendix B), which we reproduce here for completeness.

First, note that there are total of $\binom{\alpha_b T}{2c}$ partitions satisfying (C1) and (C3) by moving 2c trajectories from $\mathcal{C}_b^{(0)}$ to $\mathcal{C}_a^{(m)}$. For each such partition, there are at most $\sum_{\ell=0}^c \binom{2c}{\ell} \binom{\alpha_b T - 2c}{\ell}$ partitions that still satisfy (C1) and (C3) but violate (C2), as such partitions must be created via swapping ℓ elements from $\mathcal{C}_b^{(m)}$ and ℓ elements from $\mathcal{C}_a^{(m)} \setminus \mathcal{C}_a^{(0)}$ with $\ell \leq c$. Thus, we have that

$$M_T \ge \frac{\binom{\alpha_b T}{2c}}{\sum_{\ell=0}^{c} \binom{2c}{\ell} \binom{\alpha_b T - 2c}{\ell}} \stackrel{(*)}{\ge} \frac{\left(\frac{\alpha_b T}{2c}\right)^{2c}}{2^{2c-1} \left(\frac{e\alpha_b T}{c}\right)^c} = 2\left(\frac{\alpha_b T}{16ec}\right)^c,$$

where at (*), we use the elementary inequalities $\left(\frac{n}{m}\right)^m \leq {n \choose m} \leq \left(\frac{en}{m}\right)^m$ for $n \geq m \geq 1$.

Then, for a clustering algorithm A that outputs a $\widehat{f}_A : [T] \to [K]$, consider the following hypothesis testing procedure:

$$R_{a}(\mathcal{A}) = \underset{m \in \{0\} \cup [M_{T}]}{\min} \min_{\sigma \in \operatorname{Sym}(K)} \left| \mathcal{C}_{a}^{(m)} \triangle \widehat{f}_{\mathcal{A}}^{-1}(\sigma(a)) \right|, \tag{13}$$

where for two sets $A, B, A \triangle B := (A \setminus B) \cup (B \setminus A)$ is their symmetric difference.

Intuitively, R_a outputs the most likely hypothesis out of $\{0\} \cup [M_T]$, given some estimated cluster for a. Let $\mathcal{E}^{(m)} := \{R_a(\mathcal{A}) = m\}$ be disjoint events across $m \in \{0\} \cup [M_T]$. Note that for each hypothesis $m \in [M_T]$, the corresponding $\boldsymbol{\alpha}^{(m)} := \boldsymbol{\alpha}(f^{(m)})$ satisfies $\|\boldsymbol{\alpha} - \boldsymbol{\alpha}^{(m)}\|_2 = \frac{2\sqrt{2}c}{T} = 2\sqrt{2}\varepsilon \leq \beta$. As

 \mathcal{A} is $(\varepsilon, \beta, \delta)$ -locally stable and any Type I/II error w.r.t. each model $\Psi_n^{(m)}$ results in at least s+1 misclassifications (see condition (C2)), we must have that

$$\min \left\{ \mathbb{P}_0 \left(\mathcal{E}^{(0)} \right), \, \min_{m \in [M_T]} \mathbb{P}_m \left(\mathcal{E}^{(m)} \right) \right\} \ge 1 - \delta. \tag{14}$$

Furthermore, we note that

$$\mathbb{P}_0\left(\bigcup_{m\in[M_T]}\mathcal{E}^{(m)}\right) \le \delta,\tag{15}$$

as if $\mathcal{E}^{(m)}$ is true for some $m \in [M_T]$, then

$$2c < E_T(f, f^{(m)}) \le E_T(\widehat{f}_{\mathcal{A}}, f) + E_T(\widehat{f}_{\mathcal{A}}, f^{(m)}) \le E_T(\widehat{f}_{\mathcal{A}}, f) + c \Longrightarrow E_T(\widehat{f}_{\mathcal{A}}, f) > c$$
, which holds with probability at most δ due to \mathcal{A} being $(\varepsilon, \beta, \delta)$ -stable. Note that due to the disjointness of $\mathcal{E}^{(m)}$'s, we additionally have that

$$\frac{1}{M_T} \sum_{m \in [M_T]} \mathbb{P}_0\left(\mathcal{E}^{(m)}\right) \le \delta \Longrightarrow \min_{m \in [M_T]} \mathbb{P}_0\left(\mathcal{E}^{(m)}\right) \le \frac{\delta}{M_T}.$$
 (16)

We now define the log-likelihood ratio of the given trajectories $\{\mathcal{T}_t = (s_{t,1}, \cdots, s_{t,H})\}_{t \in [T]}$ under the true model (m=0) and the m-th alternate model:

$$Q_T^{(m)} := \log \frac{\mathbb{P}_m(\{\mathcal{T}_t\}_{t \in [T]})}{\mathbb{P}_0(\{\mathcal{T}_t\}_{t \in [T]})} = \sum_{t \in \mathcal{C}_a^{(m)} \setminus \mathcal{C}_a^{(0)}} \log \frac{\mathbb{P}^{(a)}(s_{t,1}, \dots, s_{t,H})}{\mathbb{P}^{(b)}(s_{t,1}, \dots, s_{t,H})}.$$
 (17)

Taking the expectation w.r.t. the m-th alternate model, we have

$$\mathbb{E}_{m}\left[\mathcal{Q}_{T}^{(m)}\right] = \sum_{t \in \mathcal{C}_{a}^{(m)} \backslash \mathcal{C}_{a}^{(0)}} \mathbb{E}_{m}\left[\log \frac{\mathbb{P}^{(a)}\left(s_{t,1}, \cdots, s_{t,H}\right)}{\mathbb{P}^{(b)}\left(s_{t,1}, \cdots, s_{t,H}\right)}\right]$$

$$= \sum_{t \in \mathcal{C}_{a}^{(m)} \backslash \mathcal{C}_{a}^{(0)}} \mathbb{E}_{m}\left[\log \frac{\mu^{(a)}(s_{t,1})}{\mu^{(b)}(s_{t,1})} + \sum_{h=1}^{H-1} \log \frac{p^{(a)}\left(s_{t,h+1} | s_{t,h}\right)}{p^{(b)}\left(s_{t,h+1} | s_{t,h}\right)}\right]$$

$$= 2c\left[\mathsf{KL}\left(\mu^{(a)}, \mu^{(b)}\right) + \sum_{h=1}^{H-1} \sum_{s \in \mathcal{S}} \mathbb{P}^{(a)}\left(s_{t,h} = s\right) \mathsf{KL}\left(p^{(a)}(\cdot | s), p^{(b)}(\cdot | s)\right)\right]$$
(Law of total expectation w.r.t. $s_{t,h}$)
$$= 2(H-1)c\left[\frac{1}{H-1} \mathsf{KL}\left(\mu^{(a)}, \mu^{(b)}\right) + \sum_{s \in \mathcal{S}} \mathbb{P}^{(a)}_{H}(s) \mathsf{KL}\left(p^{(a)}(\cdot | s), p^{(b)}(\cdot | s)\right)\right].$$

$$= 2\mathcal{D}^{(a,b)}$$

$$(\mathbb{P}^{(a)}_{H}(s) := \frac{1}{H-1} \sum_{h=1}^{H-1} \mathbb{P}^{(a)}\left(s_{t,h} = s\right)$$

There are two paths from here, one inspired by the arguments of Jedra and Proutière (2023) that utilizes data processing inequality, and another inspired by Yun and Proutière (2019) that utilizes Markov's inequality. The former leads to the non-asymptotic guarantee, while the latter leads to the asymptotic guarantee.

Non-asymptotic guarantee. We recall the likelihood version of the data processing inequality⁶: **Lemma A.2** (Data Processing Inequality; Lemma 1 of Garivier et al. (2019)). *Consider a measurable space* (Γ, \mathcal{G}) *equipped with two probability measure* \mathbb{P}_1 *and* \mathbb{P}_2 . *Then, we have that*

$$\mathsf{KL}(\mathbb{P}_1, \mathbb{P}_2) \ge \sup_{Z} \mathsf{kl}(\mathbb{E}_1[Z], \mathbb{E}_2[Z]),\tag{18}$$

where \sup_Z is over all possible \mathcal{G} -measurable random variable $Z:\Omega\to[0,1]$ and kl is the Bernoulli KL divergence, i.e., $\mathsf{kl}(p,q):=p\log\frac{p}{q}+(1-p)\log\frac{1-p}{1-q}$ for $p,q\in(0,1)$.

⁶This has been referred to as the "Fundamental Inequality" in Garivier et al. (2019), as using this allows for a strikingly simple proof of distribution-dependent bandit regret lower bounds.

In the above lemma, let (Γ, \mathcal{G}) be our observation space of T trajectories, $\mathbb{P}_1 = \mathbb{P}_m$, $\mathbb{P}_2 = \mathbb{P}_0$, and $Z = \mathbb{1}\{\mathcal{E}^{(m)}\}$.

Then, we have that

$$\begin{split} 2(H-1)c\mathcal{D}^{(a,b)} &= \frac{1}{M_T} \sum_{m \in [M_T]} \mathsf{KL}\left(\mathbb{P}_m, \mathbb{P}_0\right) \\ &\geq \frac{1}{M_T} \sum_{m \in [M_T]} \mathsf{kl}\left(\mathbb{P}_m(\mathcal{E}^{(m)}), \mathbb{P}_0(\mathcal{E}^{(m)})\right) \qquad \qquad \text{(Lemma A.2)} \\ &\geq \mathsf{kl}\left(\frac{1}{M_T} \sum_{m \in [M_T]} \mathbb{P}_m(\mathcal{E}^{(m)}), \frac{1}{M_T} \sum_{m \in [M_T]} \mathbb{P}_0\left(\mathcal{E}^{(m)}\right)\right) \\ &= \mathsf{kl}\left(\frac{1}{M_T} \sum_{m \in [M_T]} \mathbb{P}_m(\mathcal{E}^{(m)}), \frac{1}{M_T} \mathbb{P}_0\left(\bigcup_{m \in [M_T]} \mathcal{E}^{(m)}\right)\right) \quad (\mathcal{E}^{(m)}\text{'s are disjoint)} \\ &\stackrel{(*)}{\geq} \mathsf{kl}\left(1-\delta, \frac{\delta}{M_T}\right) \\ &\stackrel{(**)}{\geq} (1-\delta)\log\frac{M_T}{\delta} - \log 2 \\ &\geq \frac{1}{2}\log\frac{1}{\delta} + \frac{c}{2}\log\frac{\alpha_{\mathrm{b}}T}{16ec} - \frac{1}{2}\log 2 \quad \qquad \text{(Lemma A.1, } \delta \in (0, 1/2]) \\ &\geq \frac{1}{2}\log\frac{1}{2\delta} + \frac{c}{2}\log\frac{\alpha_{\mathrm{min}}T}{16ec}. \end{split}$$

(*) follows from $\mathbb{P}_m(\mathcal{E}^{(m)}) \ge 1 - \delta$ (as the algorithm is $(\varepsilon, \beta, \delta)$ -stable), Eqn. (15), and the following well-known properties of kl:

• $q \mapsto \mathsf{kl}(p,q)$ is increasing in [p,1], as

$$\partial_q \mathrm{kl}(p,q) = -\frac{p}{q} + \frac{1-p}{1-q} = \frac{q-p}{q(1-q)} \geq 0,$$

• $p\mapsto \mathsf{kl}(p,q)$ is increasing on $p\in [1/2,1]$ when q<1/2, as

$$\partial_p \mathsf{kl}(p,q) = \log \frac{p}{q} - \log \frac{1-p}{1-q} = \log \frac{p}{1-p} + \frac{1-q}{q} \ge 0.$$

(**) follows from $kl(p,q) \ge p \log \frac{1}{q} - \log 2$ (Eqn. (11) of Garivier et al. (2019)).

We conclude by rearranging the resulting inequality in terms of δ and optimizing over $a \neq b \in [K]$.

 \Box (for non-asymptotic)

Asymptotic guarantee. Let $m^* = \arg\min_{m \in [M_T]} \mathbb{P}_0[\mathcal{E}^{(m)}]$. Then,

$$\begin{split} \mathbb{P}_{m^*}[\mathcal{Q}_T^{(m^*)} &\leq \log M_T] = \mathbb{P}_{m^*} \left[\mathcal{Q}_T^{(m^*)} \leq \log M_T, \mathcal{E}^{(m^*)} \right] + \mathbb{P}_{m^*} \left[\mathcal{Q}_T^{(m^*)} \leq \log M_T, (\mathcal{E}^{(m^*)})^{\complement} \right] \\ &\leq \exp(\log M_T) \mathbb{P}_0 \left[\mathcal{Q}_T^{(m^*)} \leq \log M_T, \mathcal{E}^{(m^*)} \right] + \mathbb{P}_{m^*} \left[(\mathcal{E}^{(m^*)})^{\complement} \right] \\ & \text{(change of measure from the alternate model } m^* \text{ to the true model)} \\ &\leq M_T \mathbb{P}_0 [\mathcal{E}^{(m^*)}] + \delta_T \\ &\leq 2\delta_T, \end{split} \tag{Eqn. (16)}$$

where $(\delta_T)_{T\in\mathbb{N}}$ is such that $\delta_T\to 0$ as $T\to \infty$.

Thus, by Markov's inequality,

$$1 - 2\delta_T \le \mathbb{P}_{m^*} \left[\mathcal{Q}_T^{(m^*)} > \log M_T \right]$$

$$\leq \frac{2(H-1)c\mathcal{D}^{(a,b)}}{\log M_T}$$

$$\leq \frac{2(H-1)c\mathcal{D}^{(a,b)}}{c\log\frac{\alpha_b T}{16ec} + \log 2}.$$
(Lemma A.1)
$$\leq \frac{2(H-1)c\mathcal{D}^{(a,b)}}{c\log\frac{\alpha_{\min} T}{16ec} + \log 2}.$$

Taking the min over $a \neq b \in [K]$ and the limit $n \to \infty$, we have that

$$\liminf_{T \to \infty} \frac{2(H-1)\mathcal{D}}{\log \frac{\alpha_{\min}}{16e\varepsilon}} \ge 1.$$
(19)

 \Box (for asymptotic)

Proof of Proposition A.1. Positivity and symmetricity are trivial. Thus, it remains to show the triangle inequality. Let $f, g, h \in \mathcal{F}(T, K)$. Then,

$$\begin{split} E_T(f,h) &= \min_{\sigma \in \operatorname{Sym}(K)} \sum_{t \in [T]} \mathbbm{1}[f(t) \neq \sigma(h(t))] \\ &\leq \min_{\nu \in \operatorname{Sym}(K)} \min_{\sigma \in \operatorname{Sym}(K)} \sum_{t \in [T]} \mathbbm{1}[f(t) \neq \nu(g(t)) \vee \nu(g(t)) \neq \sigma(h(t))] \\ &\leq \min_{\nu \in \operatorname{Sym}(K)} \min_{\sigma \in \operatorname{Sym}(K)} \sum_{t \in [T]} \left(\mathbbm{1}[f(t) \neq \nu(g(t))] + \mathbbm{1}[\nu(g(t)) \neq \sigma(h(t))] \right) \\ &\leq \min_{\nu \in \operatorname{Sym}(K)} \sum_{t \in [T]} \mathbbm{1}[f(t) \neq \nu(g(t))] + \min_{\nu \in \operatorname{Sym}(K)} \min_{\sigma \in \operatorname{Sym}(K)} \sum_{t \in [T]} \mathbbm{1}[\nu(g(t)) \neq \sigma(h(t))] \\ &= E_T(f,g) + \min_{\nu' \in \operatorname{Sym}(K)} \mathbbm{1}[g(t) \neq \nu'(h(t))] \qquad (\nu' = \nu^{-1} \circ \sigma) \\ &= E_T(f,g) + E_T(g,h). \end{split}$$

B Proof of Theorem 4.1 – Initial Spectral Clustering

We remark in advance that the proofs of all supporting lemmas and propositions are deferred to the end of this section.

We begin by establishing the following concentration result for $\widehat{\boldsymbol{W}}$:

Lemma B.1 (Concentration of $\widehat{\boldsymbol{W}}$ to \boldsymbol{W}). Let $\delta \in (0,1)$. For each $s \in \mathcal{S}$ and $t \in [T]$, the following holds with probability at least $1-\delta$, given that $H \geq \left(\frac{25}{1-\pi(s)} \vee 52\right) \frac{2}{\pi(s)\gamma_{\mathrm{ps}}} \log \frac{8}{\pi_{\min}\delta^2}$:

If we <u>additionally</u> assume that $H \ge \frac{9\pi(s)}{\pi_{\min}}$, the following holds with probability at least $1 - \delta$:

$$\left| (\boldsymbol{W})_{t,:} - (\widehat{\boldsymbol{W}})_{t,:} \right| \leq \widehat{r} \triangleq 8\sqrt{\frac{S}{H\gamma_{\text{ps}}} \log \frac{H}{\delta}} \Longrightarrow \left\| \boldsymbol{W} - \widehat{\boldsymbol{W}} \right\|_{2 \to \infty} \leq 8\sqrt{\frac{S}{H\gamma_{\text{ps}}} \log \frac{TH}{\delta}}. \quad (21)$$

First, as $\left\| \boldsymbol{W} - \widehat{\boldsymbol{W}} \right\|_2 \leq \sqrt{T} \left\| \boldsymbol{W} - \widehat{\boldsymbol{W}} \right\|_{2 \to \infty}$ (Cape et al., 2019, Proposition 6.3), with our choice of $\widehat{\sigma}_{\mathrm{thres}} := 8 \sqrt{\frac{TS}{H\gamma_{\mathrm{ps}}}} \log \frac{TH}{\delta}$ (line 3), we have from Lemma B.1 and Weyl's inequality for singular values (Horn and Johnson, 2012, Problem 7.3.P16) that $\mathbb{P}\left(\widehat{R} \leq R = \mathrm{rank}(\boldsymbol{W})\right) \geq 1 - \delta$. We will condition on this event throughout the remainder of the proof.

Then, we have that

$$\begin{split} \left\| \widehat{\boldsymbol{X}} \widehat{\boldsymbol{V}}_{1:R}^{\top} - \boldsymbol{W} \right\|_F^2 &\leq 2R \left\| \widehat{\boldsymbol{X}} \widehat{\boldsymbol{V}}_{1:R}^{\top} - \boldsymbol{W} \right\|_2^2 \\ &\leq 4R \left(\left\| \widehat{\boldsymbol{X}} \widehat{\boldsymbol{V}}_{1:R}^{\top} - \widehat{\boldsymbol{W}} \right\|_2^2 + \left\| \widehat{\boldsymbol{W}} - \boldsymbol{W} \right\|_2^2 \right) \\ &\leq 8R (\widehat{\sigma}_{\text{thres}})^2, \qquad \text{(with probability at least } 1 - \delta) \\ &= 2^9 R \frac{TS}{H\gamma_{\text{DS}}} \log \frac{TH}{\delta}. \end{split}$$

Let us denote $\widehat{Y} := \widehat{X}\widehat{V}_{1:R}$. We now have the following lemma:

Lemma B.2. If $t \in [T]$ is misclassified from Algorithm 1, then $\|\widehat{\mathbf{Y}}_{t,:} - \mathbf{W}_{t,:}\|_2 \geq \frac{\Delta_{\mathbf{W}}}{4}$.

Then, we have that with probability at least $1 - \delta$,

$$E_T(\widehat{f_0}, f) \le \frac{\left\|\widehat{\boldsymbol{Y}} - \boldsymbol{W}\right\|_F^2}{\frac{\Delta_{\boldsymbol{W}}^2}{2^4}} \le \frac{2^{13}TRS}{H\gamma_{\mathrm{ps}}\Delta_{\boldsymbol{W}}^2} \log \frac{TH}{\delta}.$$

B.1 Proof of Lemma B.1

Note that

 $\left\| \sqrt{\pi^{(f(t))}(s)} p^{(f(t))}(\cdot|s) - \frac{1}{\sqrt{H\widehat{N}_{t}(s)}} \widehat{N}_{t}(s,\cdot) \right\|_{2}$ $\leq \sqrt{\pi^{(f(t))}(s)} \underbrace{\left\| p^{(f(t))}(\cdot|s) - \frac{\widehat{N}_{t}(s,\cdot)}{\widehat{N}_{t}(s)} \right\|_{2}}_{(i)} + \underbrace{\left\| \sqrt{\pi^{(f(t))}(s)} - \sqrt{\frac{\widehat{N}_{t}(s)}{H}} \right\| \frac{\widehat{N}_{t}(s,\cdot)}{\widehat{N}_{t}(s)} \right\|_{2}}_{(ii)}$

Let us bound (i) and (ii) separately. For simplicity, we omit the dependency on $t \in [T]$.

Bounding (i). Here, we follow the proof strategy of Wolfer and Kontorovich (2021, Theorem 3.1), with two crucial modifications: the quantity being bounded is the ℓ_2 -norm (not ℓ_1 -norm) error, and we only need to bound the error stemming from a single state s.

Let $n_s \in \mathbb{N}$ to be determined later, and let \mathbb{P}_{π} be the probability measure induced when the Markov chain starts from its stationary distribution. Then,

$$\begin{split} & \mathbb{P}_{\pi} \left(\left\| p(\cdot|s) - \frac{\widehat{N}(s, \cdot)}{\widehat{N}(s)} \right\|_{2} > \varepsilon \right) \\ & \leq \sum_{n=n_{s}}^{3n_{s}} \mathbb{P}_{\pi} \left(\left\| p(\cdot|s) - \frac{\widehat{N}(s, \cdot)}{\widehat{N}(s)} \right\|_{2} > \varepsilon, \ \widehat{N}(s) = n_{s} \right) + \mathbb{P}_{\pi} \left(\widehat{N}(s) \notin \llbracket n_{s}, 3n_{s} \rrbracket \right). \end{split}$$

For the first term, we utilize the scheme of reducing learning the Markovian transition kernel to learning a discrete distribution, as described in the proof of Billingsley (1961, Theorem 3.1). Then, denoting $\widehat{p}_n(\cdot|s)$ to be the estimate of $p(\cdot|s)$ from n i.i.d. samples of $p(\cdot|s)$, we have that

$$\sum_{n=n_s}^{3n_s} \mathbb{P}_{\pi} \left(\left\| p(\cdot|s) - \frac{\widehat{N}(s,\cdot)}{\widehat{N}(s)} \right\|_2 > \varepsilon, \ \widehat{N}(s) = n \right) \le \sum_{n=n_s}^{3n_s} \mathbb{P}_{\pi} \left(\left\| p(\cdot|s) - \widehat{p}_n(\cdot|s) \right\|_2 > \varepsilon \right)$$

$$\stackrel{(*)}{\le} \sum_{n=n_s}^{3n_s} \exp\left(-\frac{\varepsilon^2 n}{2} \right)$$

$$\le (2n_s + 1) \exp\left(-\frac{\varepsilon^2 n_s}{2} \right),$$

where (*) follows from the following ℓ_2 -concentration of learning discrete distribution:

Lemma B.3 (Theorem 9 of Canonne (2020)). Let S be a finite state space, $p \in \mathcal{P}(S)$, and $\delta \in (0,1)$. We are given $\{s_i\}_{i \in [N]}$ with $s_i \overset{i.i.d.}{\sim} p$. Let $\hat{p}_N \in \mathcal{P}(S)$ be defined as $\hat{p}_N(s) := \frac{1}{N} \sum_{i \in [N]} \mathbb{1}[s_i = s]$ for each $s \in S$. Then, we have the following:

$$\mathbb{P}\left(\|p - \hat{p}_N\|_2 \ge \varepsilon\right) \le \exp\left(-\frac{\varepsilon^2 N}{2}\right),\tag{22}$$

We now choose $n_s = \frac{H\pi(s)}{2}$ and utilize the Markovian Bernstein concentration, which we recall here: **Lemma B.4** (Theorem 3.4 of Paulin (2015)). Suppose of $(X_h)_{h\geq 1}$ is an ergodic Markov chain over S with transition probability p, initial distribution μ , and pseudo spectral gap γ_{ps} . Let $\phi \in L^2(\pi)$ with $\sup_{s\in S} |\phi(s) - \mathbb{E}_{\pi}[\phi]| \leq C$ for some C>0, and $V_{\phi}:= \mathrm{Var}_{\pi}[\phi]$. Then, we have the following: for any $u\geq 0$,

$$\mathbb{P}\left(\sum_{h=1}^{H} (\phi(X_h) - \mathbb{E}_{\pi}[\phi(X_h)]) \ge u\right) \le \exp\left(-\frac{u^2 \gamma_{\text{ps}}}{8\left(H + \frac{1}{\gamma_{\text{ps}}}\right) V_{\phi} + 20Cu}\right). \tag{23}$$

For two integers $a \ge b$, denote $[a, b] := \{a, a+1, \dots, b\}$. We then have that

$$\mathbb{P}_{\pi}\left(\widehat{N}(s) \notin \left[\left[\frac{H\pi(s)}{2}, \frac{3H\pi(s)}{2}\right]\right]\right) = \mathbb{P}_{\pi}\left(\widehat{N}(s) - H\pi(s) \notin \left[\left[-\frac{H\pi(s)}{2}, \frac{H\pi(s)}{2}\right]\right]\right) \\
\leq \mathbb{P}_{\pi}\left(\left|\widehat{N}(s) - H\pi(s)\right| > \frac{H\pi(s)}{2}\right) \\
\leq 2\exp\left(-\frac{(H\pi(s)/2)^{2}\gamma_{\mathrm{ps}}}{8\left(H + \frac{1}{\gamma_{\mathrm{ps}}}\right)\pi(s)(1 - \pi(s)) + 20(H\pi(s)/2)}\right)$$

$$\leq 2 \exp\left(-\frac{H\pi(s)\gamma_{\mathrm{ps}}}{104}\right). \tag{Assume that } H > \tfrac{1}{\gamma_{\mathrm{ps}}})$$

Combining everything, we have that

$$\mathbb{P}_{\pi}\left(\left\|p(\cdot|s) - \frac{\widehat{N}(s,\cdot)}{\widehat{N}(s)}\right\|_{2} > \varepsilon\right) \leq (H\pi(s) + 1) \exp\left(-\frac{\varepsilon^{2}H\pi(s)}{2}\right) + 2\exp\left(-\frac{H\pi(s)\gamma_{\mathrm{ps}}}{104}\right),$$

and thus, with $H \geq \frac{1}{\gamma_{\rm ps}} \vee \frac{104}{\pi(s)\gamma_{\rm ps}}\log\frac{2}{\delta},$ we have that

$$\mathbb{P}_{\pi} \left(\left\| p(\cdot|s) - \frac{\widehat{N}(s,\cdot)}{\widehat{N}(s)} \right\|_{2} > \sqrt{\frac{2}{H\pi(s)} \log \frac{2(H\pi(s)+1)}{\delta}} \right) \leq \delta. \tag{24}$$

Here, we recall the following result that quantifies the price of non-stationarity due to the initial distribution μ not necessarily being the stationary distribution π :

Lemma B.5 (Proposition 3.10 of Paulin (2015)). Let (X_1, \dots, X_H) be a (time-homogeneous) Markov chain with stationary distribution π . For any measurable $g: \mathcal{S}^H \to \mathbb{R}$ and initial distribution $\mu \in \Delta(\mathcal{S})$, we have that for any $u \geq 0$,

$$\mathbb{P}_{\mu}\left(g(X_1,\cdots,X_H)\geq u\right)\leq \sqrt{\left[\sum_{s\in\mathcal{S}}\frac{\mu(s)^2}{\pi(s)}\right]}\,\mathbb{P}_{\pi}\left(g(X_1,\cdots,X_H)\geq u\right). \tag{25}$$

Especially as $|S| < \infty$, we can bound $\sum_{s \in S} \frac{\mu(s)^2}{\pi(s)} \le \frac{1}{\pi_{\min}}$.

Thus,

$$\mathbb{P}\left(\left\|p(\cdot|s) - \frac{\widehat{N}(s,\cdot)}{\widehat{N}(s)}\right\|_2 > \sqrt{\frac{2}{H\pi(s)}\log\frac{2(H\pi(s)+1)}{\delta}}\right) \leq \sqrt{\frac{\delta}{\pi_{\min}}}.$$

Reparametrizing finally gives

$$\mathbb{P}\left(\left\|p(\cdot|s) - \frac{\widehat{N}(s,\cdot)}{\widehat{N}(s)}\right\|_{2} > \sqrt{\frac{2}{H\pi(s)}\log\frac{8(H\pi(s)+1)}{\pi_{\min}\delta^{2}}}\right) \le \frac{\delta}{2},\tag{26}$$

given that $H \geq \frac{1}{\gamma_{\rm ps}} \vee \frac{104}{\pi(s)\gamma_{\rm ps}} \log \frac{8}{\pi_{\min}\delta^2}$

Bounding (ii). Note that

$$\left| \sqrt{\pi(s)} - \sqrt{\frac{\widehat{N}(s)}{H}} \right| = \frac{\left| \pi(s) - \frac{\widehat{N}(s)}{H} \right|}{\sqrt{\pi(s)} + \sqrt{\frac{\widehat{N}(s)}{H}}} \le \frac{1}{\sqrt{\pi(s)}} \left| \pi(s) - \frac{\widehat{N}(s)}{H} \right|.$$

Again, we invoke Lemma B.4:

$$\mathbb{P}_{\pi} \left(\left| \pi(s) - \frac{\widehat{N}(s)}{H} \right| > \sqrt{\frac{32\pi(s)(1 - \pi(s))}{H\gamma_{ps}} \log \frac{8}{\pi_{\min} \delta^{2}}} \right) \\
\leq 2 \exp \left(-\frac{32\pi(s)(1 - \pi(s))H \log \frac{8}{\pi_{\min} \delta^{2}}}{8\left(H + \frac{1}{\gamma_{ps}}\right)\pi(s)(1 - \pi(s)) + 20\sqrt{\frac{32\pi(s)(1 - \pi(s))H}{\gamma_{ps}} \log \frac{8}{\pi_{\min} \gamma_{ps}}}} \right) \\
\leq 2 \exp \left(-\frac{2\sqrt{H\pi(s)(1 - \pi(s))} \log \frac{8}{\pi_{\min} \delta^{2}}}{\sqrt{H\pi(s)(1 - \pi(s))} + 5\sqrt{\frac{2}{\gamma_{ps}} \log \frac{8}{\pi_{\min} \delta^{2}}}} \right) \qquad (H \geq \frac{1}{\gamma_{ps}})$$

$$\leq 2 \exp\left(-\frac{2\sqrt{H\pi(s)(1-\pi(s))}\log\frac{8}{\pi_{\min}\delta^2}}{2\sqrt{H\pi(s)(1-\pi(s))}}\right) \qquad (H \geq \frac{50}{\pi(s)(1-\pi(s))\gamma_{\text{ps}}}\log\frac{8}{\pi_{\min}\delta^2})$$
$$= \frac{\pi_{\min}\delta^2}{4}.$$

Using Lemma B.5, we then have

$$\mathbb{P}\left(\left|\pi(s) - \frac{\widehat{N}(s)}{H}\right| > \sqrt{\frac{32\pi(s)(1-\pi(s))}{H\gamma_{\text{ps}}}\log\frac{8}{\pi_{\min}\delta^2}}\right) \le \frac{\delta}{2}.$$
 (27)

Combining everything. By union bound, we have that with probability at least $1 - \delta$,

$$\left\| \sqrt{\pi^{(f(t))}(s)} p^{(f(t))}(\cdot|s) - \frac{1}{\sqrt{H\hat{N}_{t}(s)}} \hat{N}_{t}(s,\cdot) \right\|_{2}$$

$$\leq \sqrt{\frac{2}{H} \log \frac{8(H\pi(s)+1)}{\pi_{\min}\delta^{2}}} + \sqrt{\frac{32(1-\pi(s))}{H\gamma_{ps}} \log \frac{8}{\pi_{\min}\delta^{2}}}$$

$$\leq 4\sqrt{\frac{2}{H\gamma_{ps}} \log \frac{8(H\pi(s)+1)}{\pi_{\min}\delta^{2}}}.$$
(28)

B.2 Proof of Lemma B.2

Here, we are largely inspired by the proof strategies of Yun and Proutière (2014a, Appendix C) and Yun and Proutière (2016, Appendix C.2).

We start by defining the following sets:

$$\mathcal{I}_{k} := \left\{ t \in f^{-1}(k) : \left\| \widehat{\mathbf{Y}}_{t,:} - \mathbf{W}_{t,:} \right\|_{2}^{2} \le \frac{1}{4} (\widehat{r})^{2} \log \frac{TH}{\delta} \right\}, \quad k \in [K]$$
 (29)

$$\mathcal{O} := \left\{ t \in [T] : \min_{t' \in [T]} \left\| \widehat{\boldsymbol{Y}}_{t,:} - \boldsymbol{W}_{t',:} \right\|_{2}^{2} \ge 4(\widehat{r})^{2} \log \frac{TH}{\delta} \right\}.$$
 (30)

Intuitively, \mathcal{I}_k is the subset of trajectories of $f^{-1}(k)$ that will be classified accurately (with high probability), and \mathcal{O} is the set of trajectories that are clustered at the end (i.e., lines 12-13).

Then the following properties hold:

$$\begin{split} \text{(i)} \quad & \underline{\left(\bigcup_{k=1}^K \mathcal{I}_k\right) \cap \mathcal{Q}_t = \emptyset \text{ for any } t \in \mathcal{O}. \text{ This is because for any } t' \in \mathcal{I}_k,} \\ & \underline{\left\|\widehat{\boldsymbol{Y}}_{t,:} - (\widehat{\boldsymbol{Y}})_{t',:}\right\|_2^2 \geq \frac{1}{2} \left\|\widehat{\boldsymbol{Y}}_{t,:} - \boldsymbol{W}_{t,:}\right\|_2^2 - \left\|(\widehat{\boldsymbol{Y}})_{t',:} - \boldsymbol{W}_{t,:}\right\|_2^2} \quad ((a+b)^2 \leq 2(a^2+b^2)) \\ & \geq 2(\widehat{r})^2 \log \frac{TH}{\delta} - \frac{1}{4}(\widehat{r})^2 \log \frac{TH}{\delta} \qquad \text{(Definition of } \mathcal{O} \text{ and } \mathcal{I}_k)} \\ & = \frac{7}{4}(\widehat{r})^2 \log \frac{TH}{\delta} \geq (\widehat{r})^2 \log \frac{TH}{\delta}, \end{split}$$

i.e.,
$$t' \in \mathcal{Q}_t \Rightarrow t' \not\in \bigcup_{k=1}^{K_s} \mathcal{I}_k$$
.

(ii) $\left| [T] \setminus \bigcup_{k=1}^{K} \mathcal{I}_k \right| \leq \frac{RT}{\log \frac{TH}{\delta}}$. This is because

$$\left| [T] \setminus \bigcup_{k=1}^K \mathcal{I}_k \right| \leq \frac{\left\| \widehat{\boldsymbol{Y}} - \boldsymbol{W} \right\|_F^2}{\min_{t \in [T] \setminus \bigcup_{k=1}^K \mathcal{I}_k} \left\| \widehat{\boldsymbol{Y}}_{t,:} - \boldsymbol{W}_{t,:} \right\|_2^2} \leq \frac{8RT(\widehat{r})^2}{\frac{1}{4}(\widehat{r})^2 \log \frac{TH}{\delta}} = \frac{32RT}{\log \frac{TH}{\delta}}$$

(iii) $\mathcal{I}_k \subseteq \mathcal{Q}_t$ for any $t \in \mathcal{I}_k$. This is because for any $t, t' \in \mathcal{I}_k$,

$$\left\|\widehat{Y}_{t',:} - \widehat{Y}_{t,:}\right\|_{2}^{2} \le 2 \left\|\widehat{Y}_{t',:} - W_{t',:}\right\|_{2}^{2} + 2 \left\|\widehat{Y}_{t,:} - W_{t,:}\right\|_{2}^{2} \le (\widehat{r})^{2} \log \frac{TH}{\delta}$$

(iv) If $\mathcal{Q}_t \cap \mathcal{I}_k \neq \emptyset$, then $\mathcal{Q}_t \cap \bigcup_{k' \neq k} \mathcal{I}_k = \emptyset$. We show this via *reductio ad absurdum*. Suppose there exists $k \neq k'$ such that $\mathcal{Q}_t \cap \mathcal{I}_k \neq \emptyset$ and $\mathcal{Q}_t \cap \mathcal{I}_{k'} \neq \emptyset$. Let $t_k \in \mathcal{Q}_t \cap \mathcal{I}_k$ and $t_{k'} \in \mathcal{Q}_t \cap \mathcal{I}_{k'}$. Then, by definition of \mathcal{Q}_t ,

$$\begin{split} \widehat{r}\sqrt{\log\frac{TH}{\delta}} &\geq \left\|\widehat{\boldsymbol{Y}}_{t_{k},:} - \widehat{\boldsymbol{Y}}_{t_{k'},:}\right\|_{2} \\ &\geq \left\|\boldsymbol{W}_{t_{k},:} - \boldsymbol{W}_{t_{k'},:}\right\|_{2} - \left\|\widehat{\boldsymbol{Y}}_{t_{k},:} - \boldsymbol{W}_{t_{k},:}\right\|_{2} - \left\|\widehat{\boldsymbol{Y}}_{t_{k'},:} - \boldsymbol{W}_{t_{k'},:}\right\|_{2} \\ &\geq \Delta_{\boldsymbol{W}} - \widehat{r}\sqrt{\log\frac{TH}{\delta}}. \end{split}$$

Recalling the definition of \hat{r} , one can easily check that if $H \geq 2^8 \frac{S}{\Delta_W^2 \gamma_{\rm ps}} \log \frac{H}{\delta} \log \frac{TH}{\delta}$, above cannot be true, a contradiction.

Claim B.1. $\widehat{K} = K$.

Proof. WLOG, assume that $|\mathcal{I}_1| \geq |\mathcal{I}_2| \geq \cdots |\mathcal{I}_K|$.

We first show that for each $1 \le k \le K$,

$$\exists t_k^\star \in \bigcup_{k' \in [K]} \mathcal{I}_{k'} \setminus \bigcup_{\ell=1}^{k-1} \mathcal{S}_{\ell} \quad \text{s.t.} \quad \left| \mathcal{Q}_{t_k^\star} \setminus \bigcup_{\ell=0}^{k-1} \mathcal{S}_{\ell} \right| \geq |\mathcal{I}_k|.$$

Due to the properties (iii) and (iv), and the greedy nature of lines 7-10, the above is indeed true.

Let $\{t_1^{\star}, \dots, t_K^{\star}\}$ be the selected "centers" with $\mathcal{I}_k \subseteq \mathcal{Q}_{t_k^{\star}}$.

Now, we show that after k has reached K+1 in line 10, the **while** loop terminates. By property (ii), the number of remaining trajectories is

$$\left| [T] \setminus \bigcup_{k \in [K]} \mathcal{Q}_{t_k^{\star}} \right| \le \left| [T] \setminus \bigcup_{k \in [K]} \mathcal{I}_k \right| \stackrel{(ii)}{\le} \frac{32RT}{\log \frac{TH}{\delta}},$$

which is precisely the termination criterion at line 7.

Thus, if a trajectory t is misclassified in the sense that it gets assigned to $t_{k'}^{\star}$ instead of t_{k}^{\star} , then it must be that $\left\|\widehat{\boldsymbol{Y}}_{t,:}-\widehat{\boldsymbol{Y}}_{t_{k}^{\star}}^{\star}\right\|_{2}>\left\|\widehat{\boldsymbol{Y}}_{t,:}-\widehat{\boldsymbol{Y}}_{t_{k'}^{\star}}^{\star}\right\|_{2}$. By the triangle inequality, this then implies that

$$\begin{split} & \left\| \widehat{Y}_{t,:} - W_{t,:} \right\|_{2} + \left\| \widehat{Y}_{t_{k}^{\star},:} - W_{t_{k}^{\star},:} \right\|_{2} + \left\| W_{t_{k}^{\star},:} W_{t_{k}^{\star},:} \right\|_{2}^{0} \\ & \geq \left\| \widehat{Y}_{t,:} - \widehat{Y}_{t_{k}^{\star},:} \right\|_{2} \\ & > \left\| \widehat{Y}_{t,:} - \widehat{Y}_{t_{k'}^{\star},:} \right\|_{2} \\ & > \left\| W_{t,:} - W_{t_{k'}^{\star},:} \right\|_{2} - \left\| \widehat{Y}_{t,:} - W_{t,:} \right\|_{2} - \left\| \widehat{Y}_{t_{k'}^{\star},:} - W_{t_{k'}^{\star},:} \right\|_{2} \end{split}$$

i.e.,

$$\begin{split} \left\|\widehat{\boldsymbol{Y}}_{t,:} - \boldsymbol{W}_{t}\right\|_{2} &> \frac{1}{2} \left(\left\|\boldsymbol{W}_{t,:} - \boldsymbol{W}_{t_{k'}^{\star},:}\right\|_{2} - \left\|\widehat{\boldsymbol{Y}}_{t_{k'}^{\star},:} - \boldsymbol{W}_{t_{k}^{\star},:}\right\|_{2} - \left\|\widehat{\boldsymbol{Y}}_{t_{k}^{\star},:} - \boldsymbol{W}_{t_{k'}^{\star},:}\right\|_{2} \right) \\ &\geq \frac{1}{2} \left(\Delta_{\boldsymbol{W}} - \frac{1}{2}\Delta_{\boldsymbol{W}}\right) \qquad (t_{k}^{\star}, t_{k'}^{\star} \in \bigcup_{k=1}^{K} \mathcal{I}_{k}, \text{ see the proof of property (iv))} \\ &= \frac{1}{4} \Delta_{\boldsymbol{W}}. \end{split}$$

B.3 Proof of Lemma B.3

As the exact constants for the ℓ_2 -distance concentration have been left to exercise in Canonne (2020), we provide the complete proof here.

First, we have that

$$\mathbb{E}\left[\|\hat{p}_{N} - p\|_{2}^{2}\right] = \sum_{s \in \mathcal{S}} \mathbb{E}\left[(\hat{p}_{N}(s) - p(s))^{2}\right]$$

$$= \frac{1}{N^{2}} \sum_{s \in \mathcal{S}} \operatorname{Var}[\operatorname{Bin}(N, p(s))] \qquad (N\hat{p}_{N}(s) \sim \operatorname{Bin}(N, p(s)))$$

$$= \frac{1}{N} \sum_{s \in \mathcal{S}} p(s)(1 - p(s))$$

$$= \frac{1}{N} \left(1 - \sum_{s \in \mathcal{S}} p(s)^{2}\right)$$

$$\leq \frac{1}{N} \left(1 - \frac{1}{S}\right), \qquad (Cauchy-Schwartz inequality)$$

i.e., with $N \geq \frac{4}{\varepsilon^2} \left(1 - \frac{1}{S}\right)$,

$$\mathbb{E}\left[\left\|\hat{p}_{N}-p\right\|_{2}\right]\overset{(*)}{\leq}\sqrt{\mathbb{E}\left[\left\|\hat{p}_{N}-p\right\|_{2}^{2}\right]}\leq\frac{\varepsilon}{2},$$

where (*) follows from Jensen's inequality.

We now utilize the McDiarmid's inequality (McDiarmid, 1989) to turn this into a *tight* high-probability guarantee. For $s_N = (s_1, \dots, s_N)$, let us define

$$f(s_N) := \|\hat{p}_N - p\|_2 = \sqrt{\sum_{i=1}^N (\hat{p}_N(s_i) - p(s_i))^2}.$$

Now, let $s^{\neg i}=(s_1,\ldots,s_{i-1},s_i',s_{i+1},\ldots,s_N)$ for $s_i'\in\{0,1\}$ and $\hat{p}_N^{\neg i}$ be the empirical distribution using $x^{\neg i}$. Observe that

$$\begin{split} |f(s) - f(s^{\neg i})| &= \left| \|\hat{p}_N - p\|_2 - \|\hat{p}_N^{\neg i} - p\|_2 \right| \\ &\leq \|\hat{p}_N - \hat{p}_N^{\neg i}\|_2 \\ &= \frac{1}{N} |s_i - s_i'| \leq \frac{1}{N}. \end{split} \tag{Triangle inequality}$$

Thus, f satisfies the bounded difference property with $c_i = 1/N$.

Combining everything, we have that

$$\mathbb{P}\left(\|\hat{p}_{N} - p\|_{2} \ge \varepsilon\right) \le \mathbb{P}\left(\|\hat{p}_{N} - p\|_{2} - \mathbb{E}[\|\hat{p}_{N} - p\|_{2}] \ge \frac{\varepsilon}{2}\right) \qquad \text{(with } N \ge \frac{4}{\varepsilon^{2}} \left(1 - \frac{1}{S}\right)\text{)}$$

$$\le \exp\left(-\frac{2\left(\frac{\varepsilon}{2}\right)^{2}}{N\left(\frac{1}{N}\right)^{2}}\right)$$

$$= \exp\left(-\frac{\varepsilon^{2}N}{2}\right).$$

C Proof of Theorem 4.2 – Likelihood Improvement

The proof largely follows the recipe of likelihood improvement for SBM clustering (Yun and Proutière, 2014a,b), which dates back to the seminal works of Abbe (2018); Amini et al. (2013) and recently extended to other variants such as labeled SBM (Yun and Proutière, 2016) and block Markov chains (Jedra et al., 2023; Sanders et al., 2020).

Let $\mathcal{H} \subseteq [T]$ be the maximum subset satisfying the following: whenever $t \in f^{-1}(k) \cap \mathcal{H}$,

$$\sum_{s,s' \in S} \widehat{N}_t(s,s') \log \frac{p^{(k)}(s'|s)}{p^{(k')}(s'|s)} \ge C(H-1)\mathcal{D}_{\pi}, \quad \forall k' \ne k.$$
 (31)

The first proposition bounds $|\mathcal{H}^{\complement}|$ in-expectation, which then leads to a *w.h.p.* guarantee via Markov's inequality:

Proposition C.1. Suppose that $H \gtrsim \frac{\eta_p^2}{\gamma_{\rm ps}D_{\pi}}\log\frac{1}{\pi_{\rm min}}$. With $C=\frac{1}{2}$, We have that

$$\mathbb{E}[|\mathcal{H}^{\complement}|] \le T(K-1) \exp\left(-\frac{\gamma_{\mathrm{ps}}(H-1)\mathcal{D}_{\pi}}{128(4\eta_p^2 + 5\log\eta_p)}\right). \tag{32}$$

Thus, by Markov's inequality, we have that

$$\mathbb{P}\left(|\mathcal{H}^{\complement}| \ge T \exp\left(-\frac{\gamma_{\mathrm{ps}}(H-1)\mathcal{D}_{\pi}}{256(4\eta_{p}^{2}+5\log\eta_{p})}\right)\right) \le K \exp\left(-\frac{\gamma_{\mathrm{ps}}(H-1)\mathcal{D}_{\pi}}{256(4\eta_{p}^{2}+5\log\eta_{p})}\right). \tag{33}$$

We next show that all trajectories in \mathcal{H} are correctly classified with high probability:

Proposition C.2. Suppose that the following requirements on H and T hold:

$$H \gtrsim \frac{1}{\gamma_{\rm ps}} \left(S^2 \log T \vee \frac{1}{v_{\rm min}} \log \frac{TH}{\pi_{\rm min}} \vee \frac{\eta_p \eta_\pi RS}{\alpha_{\rm min} H \Delta_{\boldsymbol{W}}^2 \mathcal{D}_\pi} \log(TH) \right), \ TH \gtrsim \frac{(S \log T)^2}{\gamma_{\rm ps} \alpha_{\rm min} \mathcal{D}_\pi^2}.$$
 (34)

Then, all trajectories in \mathcal{H} are correctly classified with probability at least $1 - \frac{1}{\sqrt{\pi_{\min}T}} - \frac{1}{TH}$.

Note that the probability in Eqn. (33) goes to 0 as $T \to \infty$. from our requirement that $H \gtrsim \log T$ (ignoring other factors). Then, the proof concludes by taking the worst-case, namely, that all the trajectories in $\mathcal{H}^{\complement}$ are misclassified, and applying a union bound.

C.1 Proof of Proposition C.1

First note that

$$\mathbb{E}[|\mathcal{H}^{\complement}|] = \sum_{t \in [T]} \mathbb{P}\left(\exists k' \neq f(t) \in [K] \text{ s.t. } \sum_{s,s' \in \mathcal{S}} \widehat{N}_t(s,s') \log \frac{p^{(f(t))}(s'|s)}{p^{(k')}(s'|s)} < C(H-1)\mathcal{D}_{\pi}\right)$$

$$\leq (K-1) \sum_{t \in [T]} \max_{k' \neq f(t) \in [K]} \mathbb{P}\left(\sum_{s,s' \in \mathcal{S}} \widehat{N}_t(s,s') \log \frac{p^{(f(t))}(s'|s)}{p^{(k')}(s'|s)} < C(H-1)\mathcal{D}_{\pi}\right)$$

$$\leq (K-1) \sum_{t \in [T]} \max_{k' \neq f(t) \in [K]} \mathbb{P}\left(\sum_{s,s' \in \mathcal{S}} \widehat{N}_t(s,s') \log \frac{p^{(f(t))}(s'|s)}{p^{(k')}(s'|s)} < C(H-1)\mathcal{D}_{\pi}(t;k')\right),$$

where we denote $\mathcal{D}_{\pi}(t;k') := \mathcal{D}_{\pi}^{(f(t),k')} = \sum_{s \in \mathcal{S}} \pi^{(f(t))}(s) \operatorname{KL}(p^{(f(t))}(\cdot|s), p^{(k')}(\cdot|s)).$

As done in Jedra et al. (2023); Sanders et al. (2020), define an "augmented" Markov chain, $X_{t,h} := (s_{t,h}, s_{t,h+1})$. For notational simplicity, let us denote $p := p^{(f(t))}$ and $\pi = \pi^{(f(t))}$.

This is a Markov chain on $\mathcal{S} \times \mathcal{S}$, with transition probability kernel $\tilde{p}(s_{t,h+1},s_{t,h+2}|s_{t,h},s_{t,h+1}) = p(s_{t,h+2}|s_{t,h+1})$ and stationary distribution $\tilde{\pi}(s,s') = \pi(s)p(s'|s)$. We have the following property that we provide the proof at the end:

Lemma C.1. The pseudo-spectral gap of $X_{t,h}$ is also γ .

Now define a function $\phi_{k'}: \mathcal{S} \times \mathcal{S} \to \mathbb{R}$ as

$$\phi_{k'}(X_{t,h}) := \sum_{s,s' \in \mathcal{S}} \mathbb{1}[s_{t,h} = s, s_{t,h+1} = s'] \log \frac{p(s'|s)}{p^{(k')}(s'|s)} = \log \frac{p(s_{t,h+1}|s_{t,h})}{p^{(k')}(s_{t,h+1}|s_{t,h})}. \tag{35}$$

To apply the above concentration, we compute the necessary quantities. First, by Assumption 2, we have that for any $(s, s') \in \mathcal{S} \times \mathcal{S}$,

$$|\phi(s,s') - \mathbb{E}_{\pi}[\phi]| = \left| \log \frac{p(s'|s)}{p^{(k')}(s'|s)} - \sum_{s,s' \in \mathcal{S}} \pi(s)p(s'|s) \log \frac{p(s'|s)}{p^{(k')}(s'|s)} \right| \le 2\log \eta_p.$$

Also, note that

$$\begin{aligned} \operatorname{Var}_{\pi}[\phi] &\leq \mathbb{E}_{\pi}[\phi^{2}] \\ &= \sum_{s,s'} \pi(s) p(s'|s) \left(\log \frac{p(s'|s)}{p^{(k')}(s'|s)} \right)^{2} \\ &\leq 2 \left(\max_{s' \in \mathcal{S}} \frac{p(s'|s) \vee p^{(k')}(s'|s)}{p(s'|s) \wedge p^{(k')}(s'|s)} \right)^{2} \sum_{s \in \mathcal{S}} \pi(s) \operatorname{KL} \left(p(\cdot|s), p^{(k')}(\cdot|s) \right) \\ & (\operatorname{Lemma 19 of SM6.3 of Sanders et al. (2020))} \\ &\leq 2 \eta_{p}^{2} \mathcal{D}_{\pi}(t; k'). \end{aligned} \tag{Assumption 2}$$

With this, we have that

$$\begin{split} & \mathbb{P}_{\pi} \left(\sum_{s,s' \in \mathcal{S}} \widehat{N}_{t}(s,s') \log \frac{p^{(k)}(s'|s)}{p^{(k')}(s'|s)} < C(H-1)\mathcal{D}_{\pi}(t;k') \right) \\ & = \mathbb{P}_{\pi} \left(\sum_{h=1}^{H-1} (\phi_{k'}(X_{t,h}) - \mathbb{E}[\phi_{k'}(X_{t,h})]) < -(1-C)(H-1)\mathcal{D}_{\pi}(t;k') \right) \\ & \leq \exp \left(-\frac{(1-C)^{2}(H-1)^{2}(\mathcal{D}_{\pi}(t;k'))^{2}\gamma_{\mathrm{ps}}}{32\eta_{p}^{2}(H-1)\mathcal{D}_{\pi}(t;k') + 40(\log\eta_{p})(H-1)\mathcal{D}_{\pi}(t;k')} \right) \\ & \qquad \qquad \qquad \text{(Lemma B.4, Lemma C.1, and } H > \frac{1}{\gamma_{\mathrm{ps}}}) \\ & \leq \exp \left(-\frac{(1-C)^{2}}{8(4\eta_{p}^{2} + 5\log\eta_{p})} \gamma_{\mathrm{ps}}(H-1)\mathcal{D}_{\pi}(t;k') \right) \\ & \leq \exp \left(-\frac{(1-C)^{2}}{8(4\eta_{p}^{2} + 5\log\eta_{p})} \gamma_{\mathrm{ps}}(H-1)\mathcal{D}_{\pi} \right). \end{split}$$

We choose $C = \frac{1}{2}$ and invoke Lemma B.5, which yields

$$\mathbb{P}\left(\sum_{s,s'\in\mathcal{S}} \widehat{N}_t(s,s') \log \frac{p^{(k)}(s'|s)}{p^{(k')}(s'|s)} < \frac{(H-1)\mathcal{D}_{\pi}(t;k')}{2}\right) \\
\leq \sqrt{\frac{1}{\pi_{\min}} \exp\left(-\frac{1}{32(4\eta_p^2 + 5\log\eta_p)} \gamma_{ps}(H-1)\mathcal{D}_{\pi}\right)} \\
= \sqrt{\exp\left(\log \frac{1}{\pi_{\min}} - \frac{1}{32(4\eta_p^2 + 5\log\eta_p)} \gamma_{ps}(H-1)\mathcal{D}_{\pi}\right)} \\
\leq \exp\left(-\frac{\gamma_{ps}(H-1)\mathcal{D}_{\pi}}{128(4\eta_p^2 + 5\log\eta_p)}\right),$$

where the last inequality is true when
$$H-1>\frac{64(4\eta_p^2+5\log\eta_p)}{\gamma_{\rm ps}\mathcal{D}_\pi}\log\frac{1}{\pi_{\min}}$$
.

Proof of Lemma C.1. For notational simplicity, we omit the dependency on t. Let P and \tilde{P} be the (bounded) linear operators corresponding to the original Markov chain s_h and the augmented Markov chain $X_h := (s_h, s_{h+1})$, respectively. Then, it is clear that $\tilde{P} = \bigoplus_{s \in \mathcal{S}} P$, where \bigoplus denotes the (matrix) direct sum.

We now denote P^* and \widetilde{P}^* be their adjoints on $L^2(\pi)$ and $L^2(\widetilde{\pi})$, respectively, i.e., their time reversals (Lezaud, 1998). By a well-known property of direct sum (Horn and Johnson, 2012), we have that $\widetilde{P}^* = \bigoplus_{s \in S} P^*$. This can also be seen via explicit computation:

$$\tilde{p}^*(y,y'|x,x') := \frac{\tilde{\pi}(y,y')\tilde{p}(x,x'|y,y')}{\tilde{\pi}(x,x')} = \frac{\pi(y)p(y'|y)p(x'|x)\mathbb{1}[y'=x]}{\pi(x)\tilde{p}(x'|x)} = \underbrace{\frac{\pi(y)p(x|y)}{\pi(x)}}_{=p^*(y|x)}\mathbb{1}[y'=x].$$

The off-diagonal zero blocks correspond to where $\mathbb{1}[y'=x]=0$.

Thus, we have that for every $k \in \mathbb{N}$, $(\widetilde{\boldsymbol{P}}^*)^k \widetilde{\boldsymbol{P}}^k = \bigoplus_{s \in \mathcal{S}} (\boldsymbol{P}^*)^k \boldsymbol{P}^k$, i.e., the spectrum of $(\widetilde{\boldsymbol{P}}^*)^k \widetilde{\boldsymbol{P}}^k$ is precisely S copies of that of $(\boldsymbol{P}^*)^k \boldsymbol{P}^k$. This immediately implies that $\gamma_{\mathrm{ps}}(\widetilde{\boldsymbol{P}}) = \gamma_{\mathrm{ps}}(\boldsymbol{P})$.

C.2 Proof of Proposition C.2

Recall that

$$\mathcal{L}(k;t) := \sum_{h=1}^{H-1} \log \widehat{p}_0^{(k)}(s_{t,h+1}|s_{t,h}) = \sum_{s,s' \in \mathcal{S}} \widehat{N}_t(s,s') \log \widehat{p}_0^{(k)}(s'|s)$$
(36)

where

$$\widehat{p}_0^{(k)}(s'|s) := \frac{\sum_{t \in (\widehat{f}_0)^{-1}(k)} \sum_{h \in [H-1]} \mathbb{1}[s_{t,h} = s, s_{t,h+1} = s']}{\sum_{t \in (\widehat{f}_0)^{-1}(k)} \sum_{h \in [H-1]} \mathbb{1}[s_{t,h} = s]}.$$
(37)

Then, Algorithm 2 ensures that t is misclassified if and only if

$$E_t \triangleq \mathcal{L}(\widehat{f}(t);t) - \mathcal{L}(f(t);t) > 0. \tag{38}$$

We decompose E_t as

$$E_{t} = \underbrace{\sum_{s,s' \in \mathcal{S}} \widehat{N}_{t}(s,s') \log \frac{p^{(\widehat{f}_{0}(t))}(s'|s)}{p^{(f(t))}(s'|s)}}_{\triangleq E_{1,t}} + \underbrace{\sum_{s,s' \in \mathcal{S}} \widehat{N}_{t}(s,s') \log \frac{\widehat{p}_{0}^{(\widehat{f}_{0}(t))}(s'|s)}{p^{(\widehat{f}_{0}(t))}(s'|s)}}_{\triangleq E_{2,t}} + \underbrace{\sum_{s,s' \in \mathcal{S}} \widehat{N}_{t}(s,s') \log \frac{p^{(f(t))}(s'|s)}{\widehat{p}_{0}^{(f(t))}(s'|s)}}_{\triangleq E_{3,t}}$$

We now upper bound $E_{2,t}$ and $E_{3,t}$.

To do so, we start with the following concentration for $\widehat{N}_t(s,s')$, which can be derived via Lemma B.4 (similar to Eqn. (27)): for each $k \in [K]$ and $t \in f^{-1}(k)$

$$\mathbb{P}\left(\left|\widehat{N}_t(s,s') - (H-1)\pi^{(k)}(s)p^{(k)}(s'|s)\right| \gtrsim \sqrt{\frac{H\pi^{(k)}(s)p^{(k)}(s'|s)}{\gamma_{\mathrm{ps}}}\log\frac{1}{\pi_{\min}\delta^2}}\right) \le \delta, \quad (39)$$

i.e.,
$$\widehat{N}_t(s,s') \lesssim H\pi^{(k)}(s)p^{(k)}(s'|s) + \sqrt{\frac{H\pi^{(k)}(s)p^{(k)}(s'|s)}{\gamma_{\mathrm{ps}}}\log T}$$
 with probability at least $1 - \frac{1}{\sqrt{\pi_{\min}T^2}}$

We then bound the intermediate estimation error of the transition probabilities:

Lemma C.2. Let $\delta \in (0,1)$, and suppose that $H \gtrsim \frac{1}{\gamma_{\text{ps}}\pi_{\min}}$. Then, for each $k \in [K]$ and $s, s' \in \mathcal{S}$, the following holds with probability at least $1 - \delta$:

$$\left| \log \frac{\widehat{p}_0^{(k)}(s'|s)}{p^{(k)}(s'|s)} \right| \lesssim \sqrt{\frac{1}{\gamma_{\text{ps}}\alpha_k T H \pi^{(k)}(s) p^{(k)}(s'|s)} \log \frac{\alpha_k T}{\sqrt{\pi_{\min}\delta}} \log \frac{1}{\sqrt{\pi_{\min}\delta}} + \frac{\eta_p \eta_\pi e^{(0)}}{\alpha_k T}. \tag{40}$$

For simplicity, let $t \in f^{-1}(k)$. By union bound, we have that with probability at least $1 - \frac{1}{\sqrt{\pi_{\min}T^2}}$,

$$\begin{split} E_{2,t} &\lesssim \sum_{s,s' \in \mathcal{S}} H\pi^{(k)} p^{(k)}(s'|s) \left(\sqrt{\frac{1}{\gamma_{\mathrm{ps}} \alpha_k T H\pi^{(k)}(s) p^{(k)}(s'|s)}} \log T + \frac{\eta_p \eta_\pi e^{(0)}}{\alpha_k T} \right) \\ &+ \sum_{s,s' \in \mathcal{S}} \sqrt{\frac{H\pi^{(k)}(s) p^{(k)}(s'|s)}{\gamma_{\mathrm{ps}}}} \log T \left(\sqrt{\frac{1}{\gamma_{\mathrm{ps}} \alpha_k T H\pi^{(k)}(s) p^{(k)}(s'|s)}} \log T + \frac{\eta_p \eta_\pi e^{(0)}}{\alpha_k T} \right) \\ &= \sum_{s,s' \in \mathcal{S}} \left(\sqrt{\frac{H\pi^{(k)}(s) p^{(k)}(s'|s)}{\gamma_{\mathrm{ps}} \alpha_k T}} \log T \right) + \frac{H\eta_p \eta_\pi e^{(0)}}{\alpha_k T} \\ &+ \sum_{s,s' \in \mathcal{S}} \left(\sqrt{\frac{1}{\alpha_k T}} \frac{(\log T)^{3/2}}{\gamma_{\mathrm{ps}}} + \sqrt{\frac{H\pi^{(k)}(s) p^{(k)}(s'|s)}{\gamma_{\mathrm{ps}}}} \log T \frac{\eta_p \eta_\pi e^{(0)}}{\alpha_k T} \right) \\ &\leq S \sqrt{\frac{H}{\gamma_{\mathrm{ps}} \alpha_k T}} \log T + \frac{H\eta_p \eta_\pi e^{(0)}}{\alpha_k T} + \frac{S^2 (\log T)^{3/2}}{\gamma_{\mathrm{ps}} \sqrt{\alpha_k T}} + S \sqrt{\frac{H}{\gamma_{\mathrm{ps}}}} \log T \frac{\eta_p \eta_\pi e^{(0)}}{\alpha_k T} \\ &\lesssim S \sqrt{\frac{H}{\gamma_{\mathrm{ps}} \alpha_k T}}} \log T + \frac{H\eta_p \eta_\pi e^{(0)}}{\alpha_k T} \end{aligned} \tag{when } H \gtrsim \frac{S^2 \log T}{\gamma_{\mathrm{ps}}}) \end{split}$$

and the same for $E_{3,t}$.

Now invoking Theorem 4.1 and the union bound, we have that with probability at least $1 - \frac{1}{\sqrt{\pi_{\min}T^2}} - \frac{1}{T^2H}$,

$$E_{2,t}, E_{3,t} \lesssim S \sqrt{\frac{H}{\gamma_{\rm ps}\alpha_{\min}T}} \log T + \frac{H\eta_p\eta_\pi}{\alpha_{\min}T} \frac{TRS}{\gamma_{\rm ps}H\Delta_{\boldsymbol{W}}^2} \log(TH).$$
 (41)

With this, we deduce that $t \in \mathcal{H}$ is misclassified *only if*

$$H\mathcal{D}_{\pi} \lesssim -E_{1,t} < E_{2,t} + E_{3,t} \lesssim S\sqrt{\frac{H}{\gamma_{\mathrm{ps}}\alpha_{\mathrm{min}}T}}\log T + \frac{\eta_{p}\eta_{\pi}}{\alpha_{\mathrm{min}}}\frac{RS}{\gamma_{\mathrm{ps}}\Delta_{\boldsymbol{W}}^{2}}\log(TH),$$

where the first inequality follows from the definition of \mathcal{H} . By taking the contrapositive, we can deduce that if both

$$H\mathcal{D}_{\pi} \gtrsim S\sqrt{rac{H}{\gamma_{
m ps}lpha_{
m min}T}}\log T ext{ and } H\mathcal{D}_{\pi} \gtrsim rac{\eta_p\eta_{\pi}}{lpha_{
m min}}rac{RS}{\gamma_{
m ps}\Delta_{m{W}}^2}\log(TH)$$

hold, then $t \in \mathcal{H}$ must be classified correctly after one-shot likelihood improvement. Combining the other requirement of $H \gtrsim \frac{S^2 \log T}{\gamma_{\mathrm{ps}}}$ and by applying union bound over $t \in \mathcal{H}$, we are done.

C.3 Proof of Lemma C.2

We denote $N_t(s) := (H-1)\pi^{(f(t))}(s)$ and $N_t(s,s') := (H-1)\pi^{(f(t))}(s)p^{(f(t))}(s'|s)$ as the expected number of visitations/transitions under the respective chain's stationary distribution.

As
$$\frac{x}{1+x} \le \log(1+x) \le x$$
 for $x > -1$, we have that

$$\left|\log \frac{\widehat{p}_0^{(k)}(s'|s)}{p^{(k)}(s'|s)}\right|$$

$$\leq \left| \frac{\widehat{p}_{0}^{(k)}(s'|s)}{p^{(k)}(s'|s)} - 1 \right|$$

$$= \left| \frac{\sum_{t \in (\widehat{f}_{0})^{-1}(k)} \widehat{N}_{t}(s, s')}{\sum_{t \in (\widehat{f}_{0})^{-1}(k)} \widehat{N}_{t}(s)} \frac{1}{p^{(k)}(s'|s)} - 1 \right|$$

$$= \left| \underbrace{\frac{\sum_{t \in (\widehat{f}_{0})^{-1}(k)} \widehat{N}_{t}(s, s')}{\sum_{t \in (\widehat{f}_{0})^{-1}(k)} \widehat{N}_{t}(s)}}_{\underline{\sum_{t \in (\widehat{f}_{0})^{-1}(k)} \widehat{N}_{t}(s)}} \underbrace{\frac{\sum_{t \in (\widehat{f}_{0})^{-1}(k)} N_{t}(s, s')}{\sum_{t \in (\widehat{f}_{0})^{-1}(k)} \widehat{N}_{t}(s)}}_{\underline{\sum_{t \in (\widehat{f}_{0})^{-1}(k)} N_{t}(s, s')}} \underbrace{\frac{\sum_{t \in (\widehat{f}_{0})^{-1}(k)} N_{t}(s, s')}{\sum_{t \in (\widehat{f}_{0})^{-1}(k)} \widehat{N}_{t}(s)}}_{\underline{\triangleq_{E_{cluster}}}} - 1 \right|.$$

Throughout the proof, let $\mathcal{E}_0^{(k)} := \widehat{f}_0^{-1}(k) \setminus f^{-1}(k)$ and $\mathcal{C}_0^{(k)} := f^{-1}(k) \cap \widehat{f}_0^{-1}(k)$, which satisfies $\widehat{f}_0^{-1}(k) = \mathcal{E}_0^{(k)} \dot{\cup} \mathcal{C}_0^{(k)}$.

We first bound E_{est} :

$$\left| \frac{\sum_{t \in \widehat{f}_{0}^{-1}(k)} \widehat{N}_{t}(s, s')}{\sum_{t \in \widehat{f}_{0}^{-1}(k)} N_{t}(s, s')} - 1 \right| = \frac{\left| \sum_{t \in \widehat{f}_{0}^{-1}(k)} \left(\widehat{N}_{t}(s, s') - N_{t}(s, s') \right) \right|}{\sum_{t \in \mathcal{C}_{0}^{(k)}} N_{t}(s, s') + \sum_{t \in \mathcal{C}_{0}^{(k)}} N_{t}(s, s')} \\
\leq \frac{\left| \sum_{t \in \widehat{f}_{0}^{-1}(k)} \left(\widehat{N}_{t}(s, s') - N_{t}(s, s') \right) \right|}{\sum_{t \in \mathcal{C}_{0}^{(k)}} N_{t}(s, s')} \\
\leq \frac{\left| \sum_{t \in \widehat{f}_{0}^{-1}(k)} \left(\widehat{N}_{t}(s, s') - N_{t}(s, s') \right) \right|}{(\alpha_{k}T - |\mathcal{E}_{0}^{(k)}|)(H - 1)\pi^{(k)}(s)p^{(k)}(s'|s)} \quad (|\mathcal{C}_{0}^{(k)}| \geq \alpha_{k}T - |\mathcal{E}_{0}^{(k)}|) \\
\leq \frac{2\left| \sum_{t \in \widehat{f}_{0}^{-1}(k)} \left(\widehat{N}_{t}(s, s') - N_{t}(s, s') \right) \right|}{\alpha_{k}T(H - 1)\pi^{(k)}(s)p^{(k)}(s'|s)} \\
\leq \frac{2\left| \sum_{t \in \widehat{f}_{0}^{-1}(k)} \left(\widehat{N}_{t}(s, s') - N_{t}(s, s') \right) \right|}{(|\mathcal{E}_{0}^{(k)}| \leq e^{(0)} \leq \frac{\alpha_{\min}T}{\alpha}} \leq \frac{\alpha_{k}T}{\alpha} \right\}$$

Defining $X_t := \widehat{N}_t(s,s') - N_t(s,s')$, note that X_t 's are independent across t and satisfy $\mathbb{E}_{\pi}[X_t] = 0$. Let us define an event $\mathcal{M} := \left\{ |X_t| \leq M, \ \forall t \in \widehat{f}_0^{-1}(k) \right\}$, where M>0 is chosen later. By Hoeffding's inequality (Hoeffding, 1963) conditioned on \mathcal{M} , we have that for any $z \geq 0$,

$$\mathbb{P}_{\pi} \left(\left| \sum_{t \in \widehat{f}_0^{-1}(k)} \left(\widehat{N}_t(s, s') - N_t(s, s') \right) \right| \ge z \middle| \mathcal{M} \right) \le \exp\left(-\frac{z^2}{2M^2 |\widehat{f}_0^{-1}(k)|} \right).$$

By Lemma B.5 and the fact that $|\widehat{f}_0^{-1}(k)| \leq \frac{3\alpha_k T}{2}$, we have

$$\mathbb{P}\left(\left|\sum_{t\in\widehat{f}_0^{-1}(k)} \left(\widehat{N}_t(s,s') - N_t(s,s')\right)\right| \ge z \middle| \mathcal{M}\right) \le \frac{1}{\sqrt{\pi_{\min}}} \exp\left(-\frac{z^2}{6M^2\alpha_k T}\right).$$

We choose $M \asymp \sqrt{\frac{H\pi(s)p(s'|s)}{\gamma_{\mathrm{ps}}}\log\frac{\alpha_k T}{\sqrt{\pi_{\min}\delta}}}$. Then, by Eqn. (39), we have that $\mathbb{P}(\mathcal{M}^{\complement}) \leq \frac{\delta}{2}$. By reparametrizing $z \asymp M\sqrt{\alpha_k T\log\frac{1}{\sqrt{\pi_{\min}\delta}}}$ and union bound, we have that

$$\mathbb{P}\left(\left|\sum_{t\in\widehat{f}_0^{-1}(k)} \left(\widehat{N}_t(s,s') - N_t(s,s')\right)\right| \ge \sqrt{\frac{\alpha_k T H \pi(s) p(s'|s)}{\gamma_{\mathrm{ps}}} \log \frac{\alpha_k T}{\sqrt{\pi_{\min}\delta}} \log \frac{1}{\sqrt{\pi_{\min}\delta}}}\right) \le \delta.$$

Then, combining everything, the following holds with probability at least $1 - \delta$:

$$\left| \frac{\sum_{t \in \widehat{f}_0^{-1}(k)} \widehat{N}_t(s, s')}{\sum_{t \in \widehat{f}_0^{-1}(k)} N_t(s, s')} - 1 \right| \lesssim \sqrt{\frac{1}{\gamma_{\text{ps}} \alpha_k T H \pi(s) p(s'|s)} \log \frac{\alpha_k T}{\sqrt{\pi_{\min} \delta}} \log \frac{1}{\sqrt{\pi_{\min} \delta}}.$$
 (42)

Under the requirement of $H \gtrsim \frac{1}{\gamma_{\rm ps}\pi_{\rm min}}$, we similarly have that with probability at least $1 - \delta$:

$$\left| \frac{\sum_{t \in \widehat{f}_0^{-1}(k)} \widehat{N}_t(s)}{\sum_{t \in \widehat{f}_0^{-1}(k)} N_t(s)} - 1 \right| \lesssim \sqrt{\frac{1}{\gamma_{\text{ps}} \alpha_k T H \pi(s)} \log \frac{\alpha_k T}{\sqrt{\pi_{\min}} \delta} \log \frac{1}{\sqrt{\pi_{\min}} \delta}}, \tag{43}$$

We now bound $E_{cluster}$:

$$\begin{split} \frac{\sum_{t \in (\widehat{f_0})^{-1}(k)} N_t(s,s')}{\sum_{t \in (\widehat{f_0})^{-1}(k)} N_t(s)} & \frac{1}{p^{(k)}(s'|s)} = \frac{\sum_{t \in \mathcal{C}_0^{(k)}} p^{(k)}(s'|s) N_t(s) + \sum_{t \in \mathcal{E}_0^{(k)}} p^{(\widehat{f_0}(t))}(s'|s) N_t(s)}{\left(\sum_{t \in \mathcal{C}_0^{(k)}} N_t(s) + \sum_{t \in \mathcal{E}_0^{(k)}} N_t(s)\right) p^{(k)}(s'|s)} \\ & \leq \frac{\sum_{t \in \mathcal{C}_0^{(k)}} N_t(s) + \eta_p \sum_{t \in \mathcal{E}_0^{(k)}} N_t(s)}{\sum_{t \in \mathcal{C}_0^{(k)}} N_t(s) + \sum_{t \in \mathcal{E}_0^{(k)}} N_t(s)} & \text{(Assumption 2)} \\ & \leq \frac{\sum_{t \in \mathcal{C}_0^{(k)}} N_t(s) + \eta_p \sum_{t \in \mathcal{E}_0^{(k)}} N_t(s)}{\sum_{t \in \mathcal{C}_0^{(k)}} N_t(s)} & \\ & = 1 + \frac{\eta_p \sum_{t \in \mathcal{E}_0^{(k)}} N_t(s)}{\sum_{t \in \mathcal{C}_0^{(k)}} N_t(s)}. \end{split}$$

Recalling that $\pi^{(k)}(s)$'s satisfy η -regularity (Assumption 2), we then have that

$$\begin{split} \frac{\sum_{t \in (\widehat{f_0})^{-1}(k)} N_t(s,s')}{\sum_{t \in (\widehat{f_0})^{-1}(k)} N_t(s)} \frac{1}{p^{(k)}(s'|s)} - 1 &\leq \frac{\eta_p \sum_{t \in \mathcal{E}_0^{(k)}} (H-1) \pi^{(\widehat{f_0}(t))}(s)}{(\alpha_k T - |\mathcal{E}_0^{(k)}|)(H-1) \pi^{(k)}(s)} \\ & \qquad \qquad (|\mathcal{C}_0^{(k)}| \geq \alpha_k T - |\mathcal{E}_0^{(k)}|) \\ & \leq \frac{2\eta_p \eta_\pi |\mathcal{E}_0^{(k)}|}{\alpha_k T} \\ & \qquad \qquad (\text{Assumption 2, } |\mathcal{E}_0^{(k)}| \leq e^{(0)} \leq \frac{\alpha_{\min} T}{2} \leq \frac{\alpha_k T}{2}) \end{split}$$

We also have that

$$\begin{split} \frac{\sum_{t \in (\widehat{f_0})^{-1}(k)} N_t(s,s')}{\sum_{t \in (\widehat{f_0})^{-1}(k)} N_t(s)} \frac{1}{p^{(k)}(s'|s)} &= \frac{\sum_{t \in \mathcal{C}_0^{(k)}} p^{(k)}(s'|s) N_t(s) + \sum_{t \in \mathcal{E}_0^{(k)}} p^{(\widehat{f_0}(t))}(s'|s) N_t(s)}{\left(\sum_{t \in \mathcal{C}_0^{(k)}} N_t(s) + \sum_{t \in \mathcal{E}_0^{(k)}} N_t(s)\right) p^{(k)}(s'|s)} \\ &\geq \frac{\sum_{t \in \mathcal{C}_0^{(k)}} N_t(s) + \eta_p^{-1} \sum_{t \in \mathcal{E}_0^{(k)}} N_t(s)}{\sum_{t \in \mathcal{C}_0^{(k)}} N_t(s) + \sum_{t \in \mathcal{E}_0^{(k)}} N_t(s)} & \text{(Assumption 2)} \\ &= 1 + \frac{(\eta_p^{-1} - 1) \sum_{t \in \mathcal{E}_0^{(k)}} N_t(s)}{\sum_{t \in \mathcal{C}_0^{(k)}} N_t(s) + \sum_{t \in \mathcal{E}_0^{(k)}} N_t(s)} > 0, \end{split}$$

i.e., we can bound $E_{cluster}$ as

$$|E_{cluster} - 1| \le \frac{2\eta_p \eta_\pi e^{(0)}}{\alpha_\nu T}.\tag{44}$$

Combining everything, we are done.

D Deferred Proofs from Section 5

D.1 Proof of Proposition 5.1 – Relationship between different gaps

D.1.1 (a) Relationship between \mathcal{D}_{π} and Kausik et al. (2023)'s α, Δ

We first recall the following lemma connecting the KL divergence and the L_2 -distance between two probability measures on a finite state space S:

Lemma D.1. For two probability mass functions p, q over a finite state space S, we have

$$\frac{\log \frac{e}{2}}{q_{\max} \vee p_{\max}} L_2(p, q) \le \mathsf{KL}(p, q) \le \frac{1}{\min_{s \in \mathcal{S}} q(s)} L_2(p, q), \tag{45}$$

where $p_{\max} := \max_{s \in \mathcal{S}} p(s)$, $q_{\max} := \max_{s \in \mathcal{S}} q(s)$, and $L_2(p,q) := \sum_{s \in \mathcal{S}} (p(s) - q(s))^2$

Then, note that for each $k \neq k'$,

$$\mathcal{D}^{(k,k')} \geq \pi^{(k)}(s(k,k')) \operatorname{KL}\left(p^{(k)}(\cdot|s(k,k')), p^{(k')}(\cdot|s(k,k'))\right) \geq \left(\log \frac{e}{2}\right) \frac{\alpha \Delta^2}{p_{\max}},$$

where we recall that $p_{\max} := \max_{k \in [K]} \max_{s,s' \in \mathcal{S}} p^{(k)}(s'|s)$.

Remark 6. Note that the first inequality is tight if such s(k,k') is unique because s(k,k') is the only state from which k and k' can be meaningfully distinguished. Also, if there are W(k,k') number of such s(k,k')'s, then the lower bound can be improved to $\left(\log\frac{e}{2}\right)W(k,k')\frac{\alpha\Delta^2}{n_{\max}}$.

Proof of Lemma D.1. The second inequality is due to Csiszar and Talata (2006, Lemma 6.1). The first inequality is due to a Stackoverflow post and user Ze-Nan Li's answer, whose proof we reproduce here for completeness.

Let us define $\eta(s) := \frac{q(s) - p(s)}{p(s)}$ and partition ${\mathcal S}$ as follows:

$$S = \underbrace{\left\{s \in S : \eta(s) > 1\right\}}_{\triangleq S} \dot{\cup} \underbrace{\left\{s \in S : \eta(s) \le 1\right\}}_{\triangleq S}.$$
 (46)

Then it is easy to see that

(i) For
$$s \in S_+$$
, $1 + \eta(s) \le 2^{\eta(s)} = e^{\eta(s) \log 2}$, and

(ii) For
$$s \in \mathcal{S}_-$$
, $1 + \eta(s) \le e^{\eta(s) - c\eta(s)^2}$, where $c := \log \frac{e}{2}$.

Then,

$$\begin{split} \mathsf{KL}(p,q) &:= \sum_{s \in \mathcal{S}} p(s) \log \frac{p(s)}{q(s)} \\ &= -\sum_{s \in \mathcal{S}_+} p(s) \log(1+\eta(s)) - \sum_{s \in \mathcal{S}_-} p(s) \log(1+\eta(s)) \\ &\geq -\log 2 \sum_{s \in \mathcal{S}_+} p(s) \eta(s) - \sum_{s \in \mathcal{S}_-} p(s) (\eta(s) - c \eta(s)^2) \\ &= c \sum_{s \in \mathcal{S}_+} p(s) \eta(s) - \sum_{s \in \mathcal{S}_-} p(s) \eta(s) + c \sum_{s \in \mathcal{S}_-} p(s) \eta(s)^2 \\ &= c \sum_{s \in \mathcal{S}_+} (q(s) - p(s)) + c \sum_{s \in \mathcal{S}_-} \frac{(q(s) - p(s))^2}{p(s)} \\ &\geq c \sum_{s \in \mathcal{S}_+} q(s) \frac{q(s) - p(s)}{q(s)} + \frac{c}{p_{\max}} \sum_{s \in \mathcal{S}_-} (q(s) - p(s))^2. \end{split}$$

Now, for $s \in \mathcal{S}_+$, we have that $0 < \frac{q(s) - p(s)}{q(s)} \le 1$, and thus,

$$\begin{aligned} \mathsf{KL}(p,q) &\geq c \sum_{s \in \mathcal{S}_+} q(s) \frac{q(s) - p(s)}{q(s)} + \frac{c}{p_{\max}} \sum_{s \in \mathcal{S}_-} (q(s) - p(s))^2 \\ &\geq c \sum_{s \in \mathcal{S}_+} q(s) \left(\frac{q(s) - p(s)}{q(s)} \right)^2 + \frac{c}{p_{\max}} \sum_{s \in \mathcal{S}_-} (q(s) - p(s))^2 \\ &\geq \frac{c}{q_{\max} \vee p_{\max}} \underbrace{\sum_{s \in \mathcal{S}} (q(s) - p(s))^2}_{=L_2(p,q)}. \end{aligned}$$

D.1.2 (b) Relationship between \mathcal{D}_{π} and $\Delta_{\mathbf{W}}$

Here, we provide the full statement of (b) and prove it:

Proposition D.1. We have

$$\Delta_{\mathbf{W}}^{2} \leq \min_{k \neq k'} \left\{ \frac{2p_{\max}}{\log \frac{e}{2}} \mathcal{D}_{\pi}^{(k,k')} + 4H^{2} \left(\pi^{(k)}, \pi^{(k')} \right) \right\},\tag{47}$$

where $H^2(\cdot,\cdot)$ is the Hellinger distance: $H^2(p,q):=\frac{1}{2}\left(\sum_{s\in\mathcal{S}}(\sqrt{p(s)}-\sqrt{q(s)})^2\right)^{\frac{1}{2}}$. Furthermore, we also have the following slightly more relaxed bound:

$$\Delta_{\mathbf{W}}^{2} \le 7 \left(p_{\max} \mathcal{D}_{\pi} + \left(\lceil \log_{\rho} M^{-1} \rceil + \frac{1}{1 - \rho} \right) \sqrt{\frac{1}{2\pi_{\min}} \mathcal{D}_{\pi}} \right), \tag{48}$$

where ρ and M are the contraction constants from the definition of uniformly ergodic Markov chains⁷.

Proof. For each $s \in \mathcal{S}$,

$$\begin{split} & \left\| \sqrt{\pi^{(k)}(s)} p^{(k)}(\cdot|s) - \sqrt{\pi^{(k')}(s)} p^{(k')}(\cdot|s) \right\|_2^2 \\ & = \left\| \sqrt{\pi^{(k)}(s)} \left(p^{(k)}(\cdot|s) - p^{(k')}(\cdot|s) \right) + \left(\sqrt{\pi^{(k)}(s)} - \sqrt{\pi^{(k')}(s)} \right) p^{(k')}(\cdot|s) \right\|_2^2 \\ & \leq 2\pi^{(k)}(s) \left\| p^{(k)}(\cdot|s) - p^{(k')}(\cdot|s) \right\|_2^2 + 2 \left(\sqrt{\pi^{(k)}(s)} - \sqrt{\pi^{(k')}(s)} \right)^2 \left\| p^{(k')}(\cdot|s) \right\|_2^2 \\ & \leq 2\pi^{(k)}(s) \left\| p^{(k)}(\cdot|s) - p^{(k')}(\cdot|s) \right\|_2^2 + 2 \left(\sqrt{\pi^{(k)}(s)} - \sqrt{\pi^{(k')}(s)} \right)^2 \\ & \leq \frac{2p_{\max}}{\log \frac{e}{2}} \pi^{(k)}(s) \operatorname{KL} \left(p^{(k)}(\cdot|s), p^{(k')}(\cdot|s) \right) + 2 \left(\sqrt{\pi^{(k)}(s)} - \sqrt{\pi^{(k')}(s)} \right)^2 \end{split} \tag{Lemma D.1}$$

We conclude the first part by summing over $s \in \mathcal{S}$ and taking a minimum over $k \neq k'$.

For the second part, we start by recalling Le Cam's inequality (Tsybakov, 2009, Lemma 2.3):

$$H^2\left(\pi^{(k)}, \pi^{(k')}\right) \le \mathsf{TV}\left(\pi^{(k)}, \pi^{(k')}\right).$$

We utilize the perturbation bound for Markov chains (Mitrophanov, 2005, Corollary 3.1) to obtain

$$\mathsf{TV}\left(\pi^{(k)}, \pi^{(k')}\right) \leq \left(\lceil \log_{\rho} M^{-1} \rceil + \frac{1}{1-\rho}\right) \max_{s \in \mathcal{S}} \mathsf{TV}\left(p^{(k)}(\cdot|s), p^{(k')}(\cdot|s)\right)$$

⁷Recall that the Markov chain with stationary distribution π and transition matrix P is uniformly ergodic if there exists $\rho \in (0,1)$ and M>0 such that $\max_{s\in\mathcal{S}}\left\|P^H(s,\cdot),\pi\right\|_1 \leq M\rho^H$ for all $H\in\mathbb{N}$.

$$\leq \left(\lceil \log_{\rho} M^{-1} \rceil + \frac{1}{1-\rho} \right) \sqrt{\frac{1}{2} \max_{s \in \mathcal{S}} \mathsf{KL} \left(p^{(k)}(\cdot|s), p^{(k')}(\cdot|s) \right)}$$
 (Pinsker's inequality
$$\leq \left(\lceil \log_{\rho} M^{-1} \rceil + \frac{1}{1-\rho} \right) \sqrt{\frac{1}{2\pi_{\min}} \sum_{s \in \mathcal{S}} \pi^{(k)}(s) \, \mathsf{KL} \left(p^{(k)}(\cdot|s), p^{(k')}(\cdot|s) \right)}$$

$$= \left(\lceil \log_{\rho} M^{-1} \rceil + \frac{1}{1-\rho} \right) \sqrt{\frac{1}{2\pi_{\min}} \mathcal{D}_{\pi}^{(k,k')}}.$$

As $\frac{2}{\log \frac{e}{2}} < 7$, we finally have that

$$\Delta_{\mathbf{W}}^{2} \leq 7 \min_{k \neq k'} \left\{ p_{\max} \mathcal{D}_{\pi}^{(k,k')} + \left(\lceil \log_{\rho} M^{-1} \rceil + \frac{1}{1-\rho} \right) \sqrt{\frac{1}{2\pi_{\min}}} \mathcal{D}_{\pi}^{(k,k')} \right\}$$
$$= 7 \left(p_{\max} \mathcal{D}_{\pi} + \left(\lceil \log_{\rho} M^{-1} \rceil + \frac{1}{1-\rho} \right) \sqrt{\frac{1}{2\pi_{\min}}} \mathcal{D}_{\pi} \right),$$

where the last equality follows from the fact that $z\mapsto c_1z+c_2\sqrt{z}$ is strictly increasing for z>0 and $c_1,c_2>0$.

D.1.3 (c) Relationship between $\Delta_{\mathbf{W}}$ and Kausik et al. (2023)'s α, Δ

Similarly, for each $s \in \mathcal{S}$,

$$\begin{split} & \left\| \sqrt{\pi^{(k)}(s)} p^{(k)}(\cdot|s) - \sqrt{\pi^{(k')}(s)} p^{(k')}(\cdot|s) \right\|_{2}^{2} \\ & = \left\| \sqrt{\pi^{(k)}(s)} \left(p^{(k)}(\cdot|s) - p^{(k')}(\cdot|s) \right) + \left(\sqrt{\pi^{(k)}(s)} - \sqrt{\pi^{(k')}(s)} \right) p^{(k')}(\cdot|s) \right\|_{2}^{2} \\ & \geq \frac{1}{2} \pi^{(k)}(s) \left\| p^{(k)}(\cdot|s) - p^{(k')}(\cdot|s) \right\|_{2}^{2} - \left(\sqrt{\pi^{(k)}(s)} - \sqrt{\pi^{(k')}(s)} \right)^{2} \left\| p^{(k')}(\cdot|s) \right\|_{2}^{2} \\ & \geq \frac{1}{2} \alpha \Delta^{2} - \pi^{(k)}(s) \left(1 - \sqrt{\frac{\pi^{(k')}(s)}{\pi^{(k)}(s)}} \right)^{2} \\ & \geq \frac{1}{2} \alpha \Delta^{2} - \pi^{(k)}(s) \left((\sqrt{\eta_{\pi}} - 1)^{2} \vee \left(1 - \frac{1}{\sqrt{\eta_{\pi}}} \right)^{2} \right). \end{split} \tag{Assumption 2}$$

Summing over $s \in \mathcal{S}$ and taking the min over $k \neq k'$, we have:

$$\Delta_{\mathbf{W}}^2 \ge \frac{1}{2}\alpha\Delta^2 - \left((\sqrt{\eta_{\pi}} - 1)^2 \vee \left(1 - \frac{1}{\sqrt{\eta_{\pi}}}\right)^2\right). \tag{49}$$

D.2 Proof of Proposition 5.2

We will construct an instance with K=2. For the state space $\mathcal{S}=[S]$ with $S\geq 2$, assume that S=2S' for some $S'\in\mathbb{N}$. Let the state space be partitioned as $\mathcal{S}=\mathcal{S}_+\dot{\cup}\mathcal{S}_-$ with $\mathcal{S}_+=[S']$ and $\mathcal{S}_-=[2S']\setminus[S']$.

The two Markov chains' transition kernels $p(\cdot|\cdot)$ and $p'(\cdot|\cdot)$ are defined as

$$p(s'|s) = \begin{cases} \frac{3}{2S'}, & s' \in \mathcal{S}_+, \\ \frac{1}{2S'}, & s' \in \mathcal{S}_- \end{cases}, \quad p'(s'|s) = \begin{cases} \frac{1}{2S'}, & s' \in \mathcal{S}_+, \\ \frac{3}{2S'}, & s' \in \mathcal{S}_- \end{cases}$$
(50)

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Note that $p_{\max} \approx \frac{1}{S}$. Also, it is easy to check that their stationary distributions π and π' are given as

$$\pi(s) = \begin{cases} \frac{3}{4S'}, & s \in \mathcal{S}_+, \\ \frac{1}{4S'}, & s \in \mathcal{S}_- \end{cases}, \quad \pi'(s) = \begin{cases} \frac{1}{4S'}, & s \in \mathcal{S}_+, \\ \frac{3}{4S'}, & s \in \mathcal{S}_- \end{cases}$$
 (51)

Then, we can set $\alpha = \frac{1}{4S'}$ and $\Delta^2 = \frac{2}{S'}$, i.e., $\alpha \Delta^2 \asymp \frac{1}{S^2}$.

On the other hand, we have that

$$\begin{split} & \Delta_{\pmb{W}}^2 \\ & = \sum_{s \in \mathcal{S}_+} \left\| \sqrt{\pi(s)} p(\cdot|s) - \sqrt{\pi'(s)} p'(\cdot|s) \right\|_2^2 \\ & = \sum_{s \in \mathcal{S}_+} \left\| \sqrt{\pi(s)} p(\cdot|s) - \sqrt{\pi'(s)} p'(\cdot|s) \right\|_2^2 + \sum_{s \in \mathcal{S}_-} \left\| \sqrt{\pi(s)} p(\cdot|s) - \sqrt{\pi'(s)} p'(\cdot|s) \right\|_2^2 \\ & = S' \left\| \sqrt{3/(4S')} p(\cdot|s_+) - \sqrt{1/(4S')} p'(\cdot|s_+) \right\|_2^2 + S' \left\| \sqrt{1/(4S')} p(\cdot|s_-) - \sqrt{3/(4S')} p'(\cdot|s_-) \right\|_2^2 \\ & \qquad \qquad (s_+ \in \mathcal{S}_+ \text{ and } s_- \in \mathcal{S}_- \text{ are arbitrarily fixed.}) \\ & = \frac{1}{2} \sum_{s' \in \mathcal{S}} \left(\sqrt{3} p(s'|s_+) - p'(s'|s_+) \right)^2 + \frac{1}{2} \sum_{s' \in \mathcal{S}} \left(p(s'|s_+) - \sqrt{3} p'(s'|s_+) \right)^2 \\ & = \frac{S'}{2} \left(\sqrt{3} \frac{3}{2S'} - \frac{1}{2S'} \right)^2 + \frac{S'}{2} \left(\sqrt{3} \frac{1}{2S'} - \frac{3}{2S'} \right)^2 + \frac{S'}{2} \left(\frac{3}{2S'} - \sqrt{3} \frac{1}{2S'} \right)^2 + \frac{S'}{2} \left(\frac{1}{2S'} - \sqrt{3} \frac{3}{2S'} \right)^2 \\ & = \left\{ \left(\frac{3\sqrt{3} - 1}{2} \right)^2 + \left(\frac{3 - \sqrt{3}}{2} \right)^2 \right\} \frac{1}{S'} \times \frac{1}{S}. \end{split}$$