CLUSTERING IN BLOCK MARKOV CHAINS

BY JARON SANDERS*,† ALEXANDRE PROUTIÈRE* AND SE-YOUNG YUN‡

KTH Royal Institute of Technology**, Sweden*
Delft University of Technology†*, The Netherlands*
Korea Advanced Institute of Science and Technology‡*, South Korea*

This paper considers cluster detection in Block Markov Chains (BMCs). These Markov chains are characterized by a block structure in their transition matrix. More precisely, the n possible states are divided into a finite number of K groups or clusters, such that states in the same cluster exhibit the same transition rates to other states. One observes a trajectory of the Markov chain, and the objective is to recover, from this observation only, the (initially unknown) clusters. In this paper we devise a clustering procedure that accurately, efficiently, and provably detects the clusters. We first derive a fundamental information-theoretical lower bound on the detection error rate satisfied under any clustering algorithm. This bound identifies the parameters of the BMC, and trajectory lengths, for which it is possible to accurately detect the clusters. We next develop two clustering algorithms that can together accurately recover the cluster structure from the shortest possible trajectories, whenever the parameters allow detection. These algorithms thus reach the fundamental detectability limit, and are optimal in that sense.

1. Introduction. The ability to accurately discover all hidden relations between items that share similarities is of paramount importance to a wide range of disciplines. Clustering algorithms in particular are employed throughout social sciences, biology, computer science, economics, and physics. The reason these techniques have become prevalent is that once clusters of similar items have been identified, any subsequent analysis or optimization procedure benefits from a powerful reduction in dimensionality.

The canonical Stochastic Block Model (SBM), originally introduced in [1], has become the benchmark to investigate the performance of cluster detection algorithms. This model generates random graphs that contain groups of similar vertices. Vertices within the same group are similar in that they share the same average edge densities to the other vertices. More precisely, if the set of n vertices $\mathcal{V}$ is for example partitioned into two groups $\mathcal{V}_1$ and $\mathcal{V}_2$, an edge is drawn between two vertices $x, y \in \mathcal{V}$ with probability

MSC 2010 subject classifications: Primary 62H30, 60J10, 60J20
Keywords and phrases: clustering, Markov chains, mixing times, community detection, change of measure, asymptotic analysis, information theory

$p \in (0, 1)$ if they belong to the same group, and with probability $q \in (0, 1)$, $p \neq q$, if they belong to different groups. Edges are drawn independently of all other edges. Within the context of the SBM and its generalizations, the problem of cluster detection is to infer the clusters from observations of a realization of the random graph with the aforementioned structure.

This paper deviates by considering the problem of cluster detection when the observation is instead the sample path of a Markov chain over the set of vertices. Specifically, we introduce the Block Markov Chain (BMC), which is a Markov chain characterized by a block structure in its transition matrix. States that are in the same cluster are similar in the sense that they have the same transition rates. The goal is to detect the clusters from an observed sample path $X_0, X_1, \ldots, X_T$ of the Markov chain (Figure 1). This new clustering problem is mathematically more challenging because consecutive samples of the random walk are *not* independent: besides noise, there is bias in a sample path. Intuitively though there is hope for accurate cluster detection if the Markov chain can get close to stationarity within T steps. Indeed, as we will show, the mixing time [2] of the BMC plays a crucial role in the detectability of the clusters.

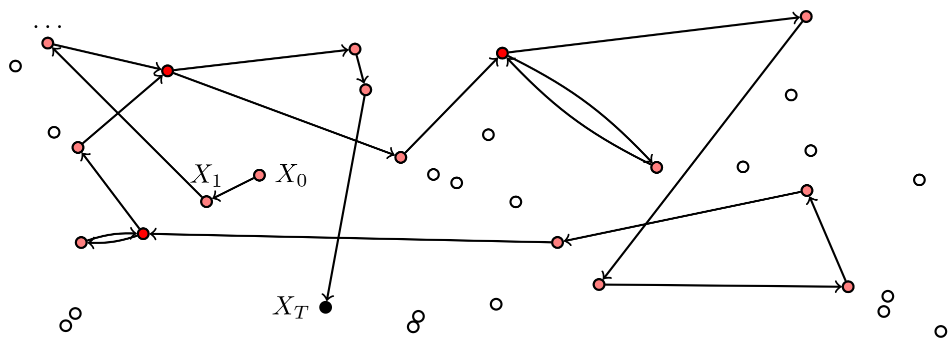


Fig 1: The goal of this paper is to infer the hidden cluster structure underlying a Markov chain $\{X_t\}_{t\geq 0}$, from one observation of a sample path $X_0, X_1, \ldots, X_T$ of length T.

Clustering in BMCs is motivated by Reinforcement Learning (RL) problems [3] with large state spaces. These problems have received substantial attention recently due to the wide spectrum of their applications in robotics, games, medicine, finance, etc. RL problems are concerned with the control of dynamical systems modeled as Markov chains whose transition kernels are initially unknown. The objective is to identify an optimal control policy as early as possible by observing the trajectory of a Markov chain generated under some known policy. The time it takes to learn efficient policies using standard algorithms such as Q-learning dramatically increases with the number of possible states, so that these algorithms become useless when the state space is prohibitively large. In most practical problems however, different states may yield similar reward and exhibit similar transition probabilities to other states, i.e., states can be grouped into clusters. In this scenario it becomes critical to learn and leverage this structure in order to speed up the learning process. In this paper we consider *uncontrolled* Markov chains, and we aim to identify clusters of states of quickly as possible. In the future we hope to extend the techniques developed here for an uncontrolled BMC to the more general case of controlled Markov chains, and hence to devise reinforcement learning algorithms that will efficiently exploit an underlying cluster structure. The idea of clustering states in reinforcement learning to speed up the learning process has been investigated in [4] and [5], but no theoretical guarantees were actually provided in these early papers.

This paper answers two major questions for the problem of cluster detection on BMCs. First, we derive a fundamental information-theoretical clustering error lower bound. The latter allows us to identify the parameters of the BMC and the sample path lengths T for which it is theoretically possible to accurately detect the underlying cluster structure. Second, we develop two clustering algorithms that when combined, are able to accurately detect the underlying cluster structure from the shortest possible sample paths, whenever the parameters of the BMC allow detection, and that provably work as $n \to \infty$. These algorithms thus reach the fundamental detectability limit, and are optimal in that sense.

1.1. *Related work.* Clustering in the SBM and the BMCs may be seen as similar problems: the objective in both cases consists in inferring the cluster structure from random observations made on the relationships between pair of vertices. However, the way these observations are gathered differ significantly in the SBM and the BMCs. In the SBM, these observations are independent random variables, which allows the use of theoretical developments in random matrices with independent entries. In the BMCs on the contrary, observations are successive states of a Markov chain and hence are not independent. Furthermore, observed edges in the SBM are scattered and undirected, whereas in a BMC, the observed path is a concatenation of directed edges. Generally the probabilities to move from state x to state y and from y to x are different. Finally, the sparsity of the observations in the BMC is controlled by the length T of the observed sample path, while it is hard-coded in the SBM. For all these reasons, it is difficult to quantitatively compare or relate the recovery rates in the two models. Nevertheless, techniques as those used in the SBM can be exploited in the analysis of the BMC if they are properly extended to handle the differences between the two models. For this reason, we now provide a brief survey of the techniques and results available for the SBM.

Significant advances have been made on cluster recovery within the context of the SBM and its generalizations. We defer the reader to [6] for an extensive overview. Substantial focus has in particular been on characterizing the set of parameters for which some recovery objectives can be met.

In the *sparse* regime, i.e., when the average degree of vertices is $O(1)$, necessary and sufficient conditions on the parameters have been identified under which it is possible to extract clusters that are positively correlated with the true clusters [7–9]. More precisely, for example if $p = a/n$ and $q = b/n$ and in the case of two clusters of equal sizes, it was conjectured in [7] that $a - b \geq \sqrt{2(a+b)}$ is a necessary and sufficient condition for the existence of algorithms that can *detect* the clusters (in the sense that they perform better than a random assignment of items to clusters). This result was established in [9] (necessary condition) and in [8] (sufficient condition).

In the *dense* regime, i.e., when the average degree is $\omega(1)$, it is possible to devise algorithms under which the proportion of misclassified vertices vanishes as the size of the graph grows large [10]. In this case, one may actually characterize the *minimal* asymptotic (as n grows large) classification error, and develop clustering algorithms achieving this fundamental limit [11]. We may further establish conditions under which asymptotic *exact* cluster recovery is possible [11–18].

This paper draws considerable inspiration from [10–12]. Over the course of these papers, the authors consider the problem of clustering in the Labeled Stochastic Block Model (LSBM), which is a generalization of the SBM. They identify the set of LSBM-parameters for which the clusters can be detected using change-of-measure arguments, and develop algorithms based on spectral methods that achieve this fundamental performance limit. Our contributions in this paper include the extension of the approaches to the context of Markov chains. This required us in particular to design novel changes-of-measure, carefully incorporate the effect of mixing, deal with new and non-convex log-likelihood functions, and widen the applicability of spectral methods to random matrices with bias. Note that we restrict the analysis in this paper to the case that the number of clusters K is known. This reduces the complexity of the analysis. Based on the findings in [10–12] however, we are confident that this assumption can be relaxed in future work.

1.2. *Methodology.* Similar to the extensive efforts for the SBM, we will first identify parameters of the BMC for which it is theoretically possible to detect the clusters. To this aim, we use techniques from information theory to derive a lower bound on the number of misclassified states that holds for any classification algorithm. This relies on a powerful change-of-measure argument, originally explored in [19] in the context of online stochastic optimization. First, we relate the probability of misclassifying a state in the BMC to a log-likelihood ratio that the sample path was generated by a perturbed Markov chain instead. Then, given any BMC, we show how to construct a perturbed Markov chain that assigns a nonzero probability to the event that all clustering algorithms misclassify at least one particular state. Finally, we maximize over all possible perturbations to get the best possible lower bound that holds for any algorithm.

We will further provide a clustering algorithm that achieves this fundamental limit. Specifically, the algorithm consists of two steps. The first step consists in applying a classical *Spectral Clustering Algorithm.* This algorithm essentially creates a rank-K approximation of a random matrix corresponding to the empirical transition rates between any pair of states, and then uses a K-means algorithm [20] to cluster all states. We show that this first step clusters the majority of states roughly correctly. Next, we introduce the *Cluster Improvement Algorithm.* This algorithm uses the rough structure learned from the Spectral Clustering Algorithm, together with the sample path, to move each individual state into the cluster the state most likely belongs to. This is achieved through a recursive, local maximization of a log-likelihood ratio.

The key difference between clustering in SBMs and clustering in BMCs is that instead of observing (the edges of) a random graph, we here try to infer the cluster structure from an as short as possible sample path of the Markov chain. This necessitates a careful analysis of the mixing time of the Markov chain [2], for which we use a rate of convergence result in terms of Dobrushin's ergodicity coefficient [21]. The observed sample path will be inherently noisy and biased by construction. The noise and bias within the sample path have to first be related to the spectrum of the random matrix recording the number of times transitions between any two states have been observed. This is done by using techniques from [22]. The spectrum of this random matrix has then to be analyzed which constitutes a major challenge. Indeed, most results investigating the spectrum of random matrices hold for matrices with independent and weakly dependent entries [23–28], or when the transition matrix of the Markov chain itself is random [29, 30]. Our random matrix has dependent entries, but by taking proof inspiration from

[31], using concentration results from [32], and smartly leveraging the way it is constructed from the observed sample path and Markov property, the analysis of its spectrum can be conducted.

1.3. *Overview.* This paper is structured as follows. We introduce the BMC in Section 2. Section 3 provides an overview of our results and our algorithms. We assess the performance of both algorithms, i.e., we quantify their asymptotic error rates. Section 4 discusses several numerical experiments designed to test the algorithms. We subsequently prove our results by first deriving an information lower bound and developing an optimal change-of-measure in Section 5, and then by developing the Spectral Clustering Algorithm in Section 6 and the Cluster Improvement Algorithm in Section 7.

Notation. For any two sets $\mathcal{A}, \mathcal{B} \subseteq \mathcal{V} \triangleq \{1, \ldots, n\}$ we define their symmetric difference by $\mathcal{A} \triangle \mathcal{B} = \{\mathcal{A} \backslash \mathcal{B}\} \cup \{\mathcal{B} \backslash \mathcal{A}\}$. For any two numbers $a, b \in \mathbb{R}$ we introduce the shorthand notations $a \wedge b = \min\{a, b\}$ and $a \vee b = \max\{a, b\}$. For any n-dimensional vector $x = (x_1, \ldots, x_n)^{\mathrm{T}} \in \mathbb{R}^n$, we define its l_p norms by

$$\|x\|_p = \Bigl(\sum_{r=1}^{n} |x_i|^p \Bigr)^{1/p} \quad \text{where} \quad p \in [1, \infty). \tag{1}$$

The n-dimensional unit vector of which the r-th component equals 1 will be denoted by $e_{n,r}$, and the n-dimensional vector for which all elements $r \in \mathcal{A} \subseteq \{1, \ldots, n\}$ equal 1 will be denoted by $1_{\mathcal{A}}$. For any $m \times n$ matrix $A \in \mathbb{R}^{m \times n}$, we indicate its rows by $A_{r,\cdot}$ for $r = 1, \ldots, m$ and its columns by $A_{\cdot,c}$ for $c = 1, \ldots, n$. We also introduce the short-hand notation $A_{\mathcal{A},\mathcal{B}} = \sum_{x \in \mathcal{A}} \sum_{y \in \mathcal{B}} A_{x,y}$ for all subsets $\mathcal{A}, \mathcal{B} \subseteq \mathcal{V}$. Its Frobenius norm and spectral norm are defined by

$$\|A\|_{\mathrm{F}} = \sqrt{\sum_{r=1}^{m} \sum_{c=1}^{n} A_{r,c}^2}, \quad \|A\| = \sup_{b \in \mathbb{S}^{n-1}} \{ \|Ab\|_2 \}, \tag{2}$$

respectively. Here, $\mathbb{S}^{n-1} = \{x = (x_1, \ldots, x_n) \in (0,1)^n : \|x\|_2 = 1\}$ denotes the n-dimensional unit sphere. We define the probability simplex of dimension $n-1$ by $\Delta^{n-1} = \bigl\{ x \in (0,1)^n : \|x\|_1 = 1 \bigr\}$ as well as the set of left stochastic matrices $\mathbb{\Delta}^{n \times (n-1)} = \bigl\{ ((x_{1,1}, \ldots, x_{1,n}), \ldots, (x_{n,1}, \ldots, x_{n,n})) \in [0,1]^{n \times n} : \sum_{c=1}^{n} x_{r,c} = 1 \text{ for } r = 1, \ldots, n \bigr\}$ similarly.

In our asymptotic analyses, we write $f(n) \sim g(n)$ if $\lim_{n \to \infty} f(n)/g(n) = 1$, $f(n) = o(g(n))$ if $\lim_{n \to \infty} f(n)/g(n) = 0$ and $f(n) = O(g(n))$ if $\limsup_{n \to \infty}$

$f(n)/g(n) < \infty$. Whenever $\{X_n\}_{n=1}^{\infty}$ is a sequence of real-valued random variables and $\{a_n\}_{n=1}^{\infty}$ a deterministic sequence, we write

(3)

$$X_n = o_{\mathbb{P}}(a_n) \Leftrightarrow \mathbb{P}\Big[\Big|\frac{X_n}{a_n}\Big| \geq \delta\Big] \to 0 \,\forall_{\delta>0} \Leftrightarrow \forall_{\varepsilon,\delta}\exists_{N_{\varepsilon,\delta}} : \mathbb{P}\Big[\Big|\frac{X_n}{a_n}\Big| \geq \delta\Big] \leq \varepsilon \,\forall_{n>N_{\varepsilon,\delta}},$$

$$\text{and} \quad X_n = O_{\mathbb{P}}(a_n) \Leftrightarrow \forall_{\varepsilon}\exists_{\delta_\varepsilon,N_\varepsilon} : \mathbb{P}\Big[\Big|\frac{X_n}{a_n}\Big| \geq \delta_\varepsilon\Big] \leq \varepsilon \,\forall_{n>N_\varepsilon}.$$

Similarly, $X_n = \Omega_{\mathbb{P}}(a_n)$ denotes $\forall_\varepsilon\exists_{\delta_\varepsilon,N_\varepsilon} : \mathbb{P}[|X_n/a_n| \leq \delta_\varepsilon] \leq \varepsilon \,\forall_{n>N_\varepsilon}$, and $X_n \asymp_{\mathbb{P}} (a_n)$ means $\forall_\varepsilon\exists_{\delta_\varepsilon^-,\delta_\varepsilon^+,N_\varepsilon} : \mathbb{P}[\delta_\varepsilon^- \leq |X_n/a_n| \leq \delta_\varepsilon^+] \geq 1-\varepsilon \,\forall_{n>N_\varepsilon}$.

2. Block Markov Chains (BMCs).

We assume that we have n states $\mathcal{V} = \{1,\ldots,n\}$, each of which is associated to one of K clusters. This means that the set of states is partitioned so that $\mathcal{V} = \cup_{k=1}^{K}\mathcal{V}_k$ with $\mathcal{V}_k \cap \mathcal{V}_l = \emptyset$ for all $k \neq l$. Let $\sigma(v)$ denote the cluster of a state $v \in \mathcal{V}$. We also assume that there exist constants $\alpha \in \Delta^{K-1}$ so that $\lim_{n\to\infty} |\mathcal{V}_k|/(n\alpha_k) = 1$.

For any $\alpha \in \Delta^{K-1}$ and $p \in \mathbb{\Delta}^{K\times(K-1)}$, we define the BMC $\{X_t\}_{t\geq 0}$ as follows. Its transition matrix $P \in \mathbb{\Delta}^{n\times(n-1)}$ will be defined as

$$P_{x,y} \triangleq \frac{p_{\sigma(x),\sigma(y)}}{|\mathcal{V}_{\sigma(y)}| - \mathbb{1}[\sigma(x)=\sigma(y)]}\mathbb{1}[x \neq y] \quad \text{for all} \quad x,y \in \mathcal{V}. \tag{4}$$

Note that this Markov chain is not necessarily reversible. Furthermore, note that in this paper we assume that K,α,p are fixed, and that we study the asymptotic regime $n \to \infty$. Finally, since we are interested in clustering of the states, we will assume that $\exists_{0<\eta\neq 1} : \max_{a,b,c}\{p_{b,a}/p_{c,a}, p_{a,b}/p_{a,c}\} \leq \eta$, which guarantees a minimum level of separability of the parameters.

2.1. *Equilibrium behavior.*

We assume that the stochastic matrix p is such that the equilibrium distribution of $\{X_t\}_{t\geq 0}$ exists, and we will denote it by Π_x for $x \in \mathcal{V}$. By symmetry, $\Pi_x = \Pi_y \triangleq \bar{\Pi}_k$ for any two states $x,y \in \mathcal{V}_k$ for all $k = 1,\ldots,K$. Consider the scaled quantity

$$\pi_k \triangleq \lim_{n\to\infty} \sum_{x\in\mathcal{V}_k} \Pi_x = \lim_{n\to\infty} |\mathcal{V}_k|\bar{\Pi}_k \quad \text{for} \quad k = 1,\ldots,K. \tag{5}$$

Proposition 1's proof can be found in §SM2.1, and follows from the symmetries between the states within the same clusters and the specific scalings of P's elements.

Proposition 1. *The quantity π solves $\pi^{\mathrm{T}}p = \pi^{\mathrm{T}}$, and is therefore the equilibrium distribution of a Markov chain with transition matrix p and state space $\Omega = \{1,\ldots,K\}$.*

2.2. *Mixing time.* Proposition 2 gives a bound on the mixing time $t_{\text{mix}} \in (0, \infty)$, which is defined by $d(t) \triangleq \sup_{x \in \mathcal{V}} \{ d_{\text{TV}}(P_{x,\cdot}^t, \Pi) \}$ and $t_{\text{mix}}(\varepsilon) \triangleq \min\{t \geq 0 : d(t) \leq \varepsilon\}$, where

$$d_{\text{TV}}(\mu, \nu) \triangleq \frac{1}{2} \sum_{x \in \mathcal{V}} |\mu_x - \nu_x|. \tag{6}$$

The proof of Proposition 2 is deferred to §SM2.2. The result follows after bounding Dobrushin's ergodicity coefficient [21] using P's structure, and invoking a convergence rate result in terms of Dobrushin's coefficient.

PROPOSITION 2. *There exists a strictly positive absolute constant c_{mix} such that $t_{\text{mix}}(\varepsilon) \leq -c_{\text{mix}} \ln \varepsilon$, for every BMC of finite size $n \geq K$.*

Proposition 2 implies that the mixing times are short enough so that our results will hold *irrespective* of whether we assume that the Markov chain is initially in equilibrium. We will show in Section 5.3 that what is important is that the chain reaches stationarity *within* T steps (the length of the observed trajectory), and consequentially, T needs to be chosen sufficiently large with respect to n to ensure that this occurs. Throughout this paper we therefore assume for simplicity that the chain is started from equilibrium. This eliminates the need of tracking higher order correction terms.

Examples. Figure 2 illustrates the structure of a BMC when there are $K = 2$ groups. We find after solving the balance equations that the limiting equilibrium behavior is given by $\pi_1 = p_{21}/(p_{12}+p_{21})$ and $\pi_2 = p_{12}/(p_{12}+p_{21})$.

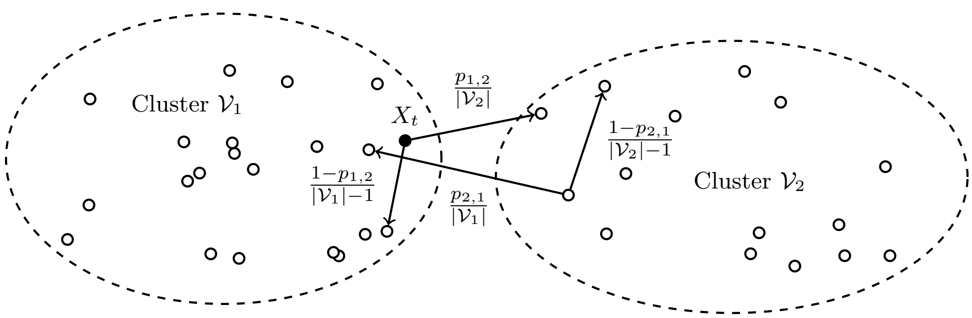


Fig 2: In the BMC with $K = 2$ groups $\mathcal{V}_1 \cup \mathcal{V}_2 = \mathcal{V}$, whenever the Markov chain is at some state $X_t \in \mathcal{V}_1$, it will next jump with probability $p_{1,2}$ to cluster $\mathcal{V}_2$, and with probability $1 - p_{1,2}$ to some other state in cluster $\mathcal{V}_1$. Similarly, if $X_t \in \mathcal{V}_2$, it would next jump to cluster $\mathcal{V}_1$ with probability $p_{2,1}$, or stay within its own cluster with probability $1 - p_{2,1}$.

For $K = 3$, we find after solving the balance equations that the limiting equilibrium behavior is given by

$$\pi_1 = \frac{p_{23}p_{31} + p_{21}(p_{31} + p_{32})}{Z(p)}, \quad \pi_2 = \frac{p_{13}p_{32} + p_{12}(p_{31} + p_{32})}{Z(p)}, \tag{7}$$

$\pi_3 = 1 - \pi_1 - \pi_2$, with $Z(p) = (p_{21} + p_{23})(p_{13} + p_{31}) + (p_{13} + p_{21})p_{32} + p_{12}(p_{23} + p_{31} + p_{32})$. Let us also illustrate the structure of the transition matrix when $\alpha = (2/10, 3/10, 5/10)$ and $n = 10$:

$$P = \left(\begin{array}{cc|ccc|ccccc}
0 & p_{1,1} & \frac{p_{1,2}}{3} & \frac{p_{1,2}}{3} & \frac{p_{1,2}}{3} & \frac{p_{1,3}}{5} & \frac{p_{1,3}}{5} & \frac{p_{1,3}}{5} & \frac{p_{1,3}}{5} & \frac{p_{1,3}}{5} \\
p_{1,1} & 0 & \frac{p_{1,2}}{3} & \frac{p_{1,2}}{3} & \frac{p_{1,2}}{3} & \frac{p_{1,3}}{5} & \frac{p_{1,3}}{5} & \frac{p_{1,3}}{5} & \frac{p_{1,3}}{5} & \frac{p_{1,3}}{5} \\
\hline
\frac{p_{2,1}}{2} & \frac{p_{2,1}}{2} & 0 & \frac{p_{2,2}}{2} & \frac{p_{2,2}}{2} & \frac{p_{2,3}}{5} & \frac{p_{2,3}}{5} & \frac{p_{2,3}}{5} & \frac{p_{2,3}}{5} & \frac{p_{2,3}}{5} \\
\frac{p_{2,1}}{2} & \frac{p_{2,1}}{2} & \frac{p_{2,2}}{2} & 0 & \frac{p_{2,2}}{2} & \frac{p_{2,3}}{5} & \frac{p_{2,3}}{5} & \frac{p_{2,3}}{5} & \frac{p_{2,3}}{5} & \frac{p_{2,3}}{5} \\
\frac{p_{2,1}}{2} & \frac{p_{2,1}}{2} & \frac{p_{2,2}}{2} & \frac{p_{2,2}}{2} & 0 & \frac{p_{2,3}}{5} & \frac{p_{2,3}}{5} & \frac{p_{2,3}}{5} & \frac{p_{2,3}}{5} & \frac{p_{2,3}}{5} \\
\hline
\frac{p_{3,1}}{2} & \frac{p_{3,1}}{2} & \frac{p_{3,2}}{3} & \frac{p_{3,2}}{3} & \frac{p_{3,2}}{3} & 0 & \frac{p_{3,3}}{4} & \frac{p_{3,3}}{4} & \frac{p_{3,3}}{4} & \frac{p_{3,3}}{4} \\
\frac{p_{3,1}}{2} & \frac{p_{3,1}}{2} & \frac{p_{3,2}}{3} & \frac{p_{3,2}}{3} & \frac{p_{3,2}}{3} & \frac{p_{3,3}}{4} & 0 & \frac{p_{3,3}}{4} & \frac{p_{3,3}}{4} & \frac{p_{3,3}}{4} \\
\frac{p_{3,1}}{2} & \frac{p_{3,1}}{2} & \frac{p_{3,2}}{3} & \frac{p_{3,2}}{3} & \frac{p_{3,2}}{3} & \frac{p_{3,3}}{4} & \frac{p_{3,3}}{4} & 0 & \frac{p_{3,3}}{4} & \frac{p_{3,3}}{4} \\
\frac{p_{3,1}}{2} & \frac{p_{3,1}}{2} & \frac{p_{3,2}}{3} & \frac{p_{3,2}}{3} & \frac{p_{3,2}}{3} & \frac{p_{3,3}}{4} & \frac{p_{3,3}}{4} & \frac{p_{3,3}}{4} & 0 & \frac{p_{3,3}}{4} \\
\frac{p_{3,1}}{2} & \frac{p_{3,1}}{2} & \frac{p_{3,2}}{3} & \frac{p_{3,2}}{3} & \frac{p_{3,2}}{3} & \frac{p_{3,3}}{4} & \frac{p_{3,3}}{4} & \frac{p_{3,3}}{4} & \frac{p_{3,3}}{4} & 0
\end{array} \right) \tag{8}$$

3. Main results.

In this paper we obtain quantitative statements on the set of misclassified states,

$$\mathcal{E} \triangleq \bigcup_{k=1}^{K} \hat{\mathcal{V}}_{\gamma^{\mathrm{opt}}(k)} \backslash \mathcal{V}_k \quad \text{where} \quad \gamma^{\mathrm{opt}} \in \arg \min_{\gamma \in \mathrm{Perm}(K)} \Big| \bigcup_{k=1}^{K} \hat{\mathcal{V}}_{\gamma(k)} \backslash \mathcal{V}_k \Big|. \tag{9}$$

Here, the sets $\hat{\mathcal{V}}_1, \dots, \hat{\mathcal{V}}_K$ will always denote an approximate cluster assignment obtained from some clustering algorithm. For notational convenience we will always number the approximate clusters so as to minimize the number of misclassifications, allowing us to forego defining it formally via a permutation.

3.1. *Information theoretical lower bound.*

Our results identify an important information quantity $I(\alpha, p) \geq 0$ that measures how difficult it is to cluster in a BMC. Its role will become clear in Theorem 1. The reason we call it an information quantity stems from fact that we have derived it as the leading coefficient in an asymptotic expansion of a log-likelihood function. Note that while it resembles one, this information quantity is not a Kullback–Leibler divergence. The individual terms are weighted according to the equilibrium distribution π, and there are two extra terms.

DEFINITION. *For $\alpha \in \Delta^{K-1}$ and $p \in \mathbb{\Delta}^{(K-1)\times K}$, let*

$$I(\alpha,p) \triangleq \min_{a\neq b}\Big\{\sum_{k=1}^{K}\frac{1}{\alpha_a}\Big(\pi_a p_{a,k}\ln\frac{p_{a,k}}{p_{b,k}}+\pi_k p_{k,a}\ln\frac{p_{k,a}\alpha_b}{p_{k,b}\alpha_a}\Big)+\Big(\frac{\pi_b}{\alpha_b}-\frac{\pi_a}{\alpha_a}\Big)\Big\}. \tag{10}$$

Here π denotes the solution to $\pi^{\mathrm{T}}p = \pi^{\mathrm{T}}$.

THEOREM 1. *Assume that $T = \omega(n)$. Then there exists a strictly positive and finite constant C independent of n such that: for any clustering algorithm*

$$\mathbb{E}_P[|\mathcal{E}|] \geq Cn\exp\Big(-I(\alpha,p)\frac{T}{n}(1+o(1))\Big). \tag{11}$$

Theorem 1 allows us to state necessary conditions for the existence of clustering algorithms that either detect clusters *asymptotically accurately*, namely with $\mathbb{E}_P[|\mathcal{E}|] = o(n)$, or recover clusters *asymptotically exactly*, i.e., with $\mathbb{E}_P[|\mathcal{E}|] = o(1)$.

Conditions for asymptotically accurate detection. In view of the lower bound derived above, there may exist asymptotically accurate clustering algorithms only if $I(\alpha,p) > 0$ and $T = \omega(n)$.

Conditions for asymptotically exact detection. Necessary conditions for the existence of an asymptotically exact algorithm are $I(\alpha,p) > 0$ and $T - \frac{n\ln(n)}{I(\alpha,p)} = \omega(1)$. In particular, T must be larger than $n\ln(n)$. We refer to the scenario where T is of the order $n\ln(n)$ as the *critical regime*. In this regime when $T = n\ln(n)$, the necessary condition for exact recovery is $I(\alpha,p) > 1$.

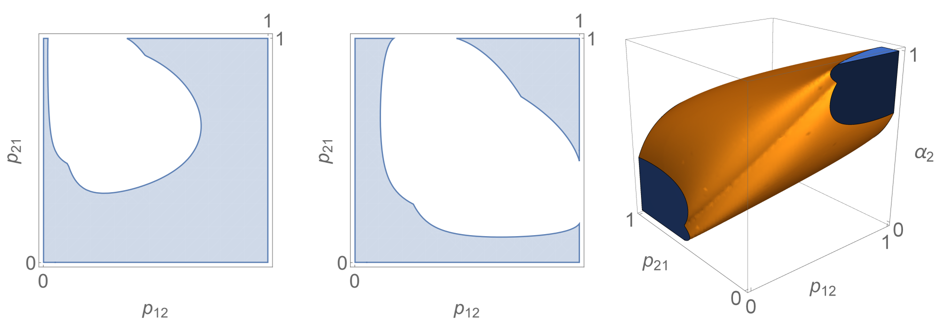
Note that qualitatively, the above conditions on the number of observations for accurate and exact recovery are similar to those in the SBMs. In the latter, for accurate detection, the average degrees of vertices should be such that the average total number of edges is $\omega(n)$ [10], whereas for exact recovery, this average must be at least $cn\ln(n)$ [13] (where c is known and depends on the parameters of the SBMs).

The information quantity $I(\alpha,p)$ for $K = 2$ clusters. In the case of two clusters, we study the set of parameters (α,p) of the BMCs for which $I(\alpha,p) > 0$ and $I(\alpha,p) > 1$, the latter condition being necessary in the critical regime when $T = n\ln(n)$.

A system with two clusters can be specified entirely with three parameters: α_2, $p_{1,2}$, and $p_{2,1}$. Examining the explicit expression for (10) in this case, we can conclude that $I(\alpha,p) = 0$ if and only if $\alpha_2 = p_{1,2} = 1 - p_{2,1}$. Asymptotic accurate (resp. exact) recovery seems thus possible as soon as

$T = \omega(n)$ (resp. $T = \omega(n \ln(n))$) for almost any BMC with two clusters – the only exception are BMCs with parameters on this line. Note that if we did not have the information quantity at our disposal, it would be challenging to give a heuristic argument whether a specific BMC allows for asymptotic exact recovery. Consider for instance a BMC with $\alpha_1 = \alpha_2 = \frac{1}{2}$ and $p_{1,2} = 1 - p_{2,1} \neq \frac{1}{2}$ and $p_{1,2} > p_{2,1}$ w.l.o.g. In this scenario, $P_{x,z} = P_{y,z}$ for all $x, y, z \in \mathcal{V}$, that is, every row of the kernel is identical to any other row. Looking at this kernel, we would not expect to be able to cluster. However here $\pi_2 > \pi_1$, and we could cluster based on the equilibrium distribution as $T \to \infty$. The information quantity takes the fact that we are dealing with a Markov chain appropriately into account, and correctly asserts for this case that asymptotic recovery is possible.

Figure 3 illustrates for which parameters one can possibly recover the two clusters asymptotically exactly when $T = n \ln n$. Specifically, it depicts all parameters $\alpha_2, p_{1,2}, p_{2,1} \in (0, 1)$ for which $I(\alpha, p) > 1$. If we fix α_2, note that when $p_{1,2}, p_{2,1} \downarrow 0$ (bottom left), the Markov chain tends to stay within the current cluster for a substantial time. Similarly when $p_{1,2}, p_{2,1} \uparrow 1$ (top right), the Markov chain tends to jump into the other cluster every time. In both scenarios, the states are relatively easy to cluster. This draws parallels with the SBM. When either $p_{1,2} \downarrow 0$ (left) or $p_{2,1} \downarrow 0$ (bottom), clustering is again doable: in these scenarios, the Markov chain tends to stay in the cluster of the starting state – and the fact that you never see the other vertices suggests that they have other transitions rates and therefore belong to the other cluster.



$\alpha_2 = 1/4$ $\alpha_2 = 1/2$ Region where $I(\alpha, p) < 1$.

Fig 3: (left, middle) The parameters $(p_{1,2}, p_{2,1})$ in blue for which asymptotic exact recovery should be possible in the critical regime $T = n \ln n$ for $K = 2$ clusters. (right) The parameters $(\alpha_2, p_{1,2}, p_{2,1})$ for which asymptotic exact recovery is likely not possible, i.e., $I(\alpha, p) < 1$.

3.2. *Procedure for cluster recovery.* Theorem 1 has established necessary conditions for asymptotically accurate and exact recovery, and has identified performance limits satisfied by any clustering algorithm. In this section, we devise a clustering procedure that reaches these limits order-wise. The proposed procedure proceeds in two steps: The first step performs a spectral decomposition of the random matrix $\hat{N}$ corresponding to the empirical transition rates between any pair of states, and defined by

$$\hat{N}_{x,y} \triangleq \sum_{t=0}^{T-1} \mathbb{1}[X_t = x, X_{t+1} = y] \quad \text{for} \quad x, y \in \mathcal{V}. \tag{12}$$

The rank-K approximation of $\hat{N}$ is used to get initial estimates of the clusters. The second step sequentially improves the cluster estimates. In each iteration, the parameters of the BMCs are inferred from the previous cluster estimates, and states are re-assigned to clusters based on these estimated parameters and the observed trajectory (by maximizing a log-likelihood).

3.2.1. *Spectral Clustering Algorithm.* The first step of our procedure is the Spectral Clustering Algorithm, presented in Algorithm 1. It leverages the spectral decomposition of $\hat{N}$ to estimate the clusters.

Before applying a singular value decomposition (SVD) to $\hat{N}$, we first need to trim the matrix so as to remove states that have been visited abnormally often. These states would namely perturb the spectral decomposition of $\hat{N}$. More precisely, we define the set Γ of states obtained from $\mathcal{V}$ by removing the $\lfloor n \exp(-(T/n) \ln(T/n)) \rfloor$ states with the highest numbers of visits in the observed sample path of length T. The spectral decomposition is applied to the matrix $\hat{N}_\Gamma$ obtained from $\hat{N}$ by setting all entries on the rows and columns corresponding to states not in Γ to zero.

The SVD of $\hat{N}_\Gamma$ is $U\Sigma V^{\mathrm{T}}$, from which we deduce $\hat{R}$ the best rank-K approximation of $\hat{N}_\Gamma$: $\hat{R} \triangleq \sum_{k=1}^{K} \sigma_k U_{\cdot,k} V_{\cdot,k}{}^{\mathrm{T}}$, where the values $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0$ denote the singular values of $\hat{N}_\Gamma$ in decreasing order. We apply a clustering algorithm to the rows and columns of $\hat{R}$ to determine the clusters. While in practice you may choose to use a different algorithm, for the analysis we use the following: first we calculate the *neighborhoods*

$$\mathcal{N}_x \triangleq \Big\{ y \in \mathcal{V} \Big| \sqrt{\|\hat{R}_{x,\cdot} - \hat{R}_{y,\cdot}\|_2^2 + \|\hat{R}_{\cdot,x} - \hat{R}_{\cdot,y}\|_2^2} \leq \frac{1}{n} \cdot \Big(\frac{T}{n}\Big)^{3/2} \Big(\ln \frac{T}{n}\Big)^{4/3} \Big\} \tag{13}$$

for $x \in \mathcal{V}$. Then we initialize $\hat{\mathcal{V}}_k \leftarrow \emptyset$ for $k = 1, \ldots, K$ and sequentially select K *centers* $z_1^*, \ldots, z_K^* \in \mathcal{V}$ from which we construct approximate clusters.

Specifically, we iterate for $k = 1, \dots K$:

$$\hat{\mathcal{V}}_k \leftarrow \mathcal{N}_{z_k^*} \backslash \{\cup_{l=1}^{k-1} \hat{\mathcal{V}}_l\} \quad \text{where} \quad z_k^* \triangleq \arg\max_{x \in \mathcal{V}} |\mathcal{N}_x \backslash \{\cup_{l=1}^{k-1} \hat{\mathcal{V}}_l\}|. \tag{14}$$

Any remaining state is finally associated to the center closest to it, i.e., we iterate for $y \in \{\cup_{k=1}^K \hat{\mathcal{V}}_k\}^{\mathrm{c}}$

$$\hat{\mathcal{V}}_{k_y^*} \leftarrow \hat{\mathcal{V}}_{k_y^*} \cup \{y\} \quad \text{with} \quad k_y^* \triangleq \arg\min_{k=1,\dots,K} \sqrt{\|\hat{R}_{z_k^*,\cdot} - \hat{R}_{y,\cdot}\|_2^2 + \|\hat{R}_{\cdot,z_k^*} - \hat{R}_{\cdot,y}\|_2^2}. \tag{15}$$

Finally, the Spectral Clustering Algorithm outputs $\hat{\mathcal{V}}_k$ for $k = 1, \dots, K$. The following theorem provides an upper bound on the number of misclassified states after executing the algorithm.

```
Input: n, K, and a trajectory X_0, X_1, ..., X_T
Output: An approximate cluster assignment V̂_1^[0], ..., V̂_K^[0], and matrix N̂
begin
    for x ← 1 to n do
        for y ← 1 to n do
            N̂_{x,y} ← ∑_{t=0}^{T−1} 𝟙[X_t = x, X_{t+1} = y];
        end
    end
    Calculate the trimmed matrix N̂_Γ;
    Calculate the Singular Value Decomposition (SVD) UΣV^T of N̂_Γ;
    Order U, Σ, V s.t. the singular values σ_1 ≥ σ_2 ≥ ... ≥ σ_n ≥ 0 are in descending
      order;
    Construct the rank-K approximation R̂ = ∑_{k=1}^K σ_k U_{·,k} V_{·,k}^T;
    Apply a K-means algorithm to [R̂, R̂^⊤] to determine V̂_1^[0], ..., V̂_K^[0];
end
```

Algorithm 1: Pseudo-code for the Spectral Clustering Algorithm.

THEOREM 2. *Assume that $T = \omega(n)$ and $I(\alpha, p) > 0$. Then the proportion of misclassified states after the Spectral Clustering Algorithm satisfies:*

$$\frac{|\mathcal{E}|}{n} = O_{\mathbb{P}}\Big(\frac{n}{T} \ln \frac{T}{n}\Big) = o_{\mathbb{P}}(1). \tag{16}$$

From the above theorem, we conclude that the first step of our recovery procedure (i.e., the Spectral Clustering Algorithm) alone achieves an asymptotically accurate detection whenever this is at all possible, say when $I(\alpha, p) > 0$ and $T = \omega(n)$. However, it fails at ensuring asymptotic exact recovery, even in certain cases of $T = \omega(n \ln(n))$, and we cannot guarantee that its recovery rate approaches the fundamental limit identified in Theorem 1.

3.2.2. *Cluster Improvement Algorithm.* The second step of our clustering procedure, referred to as Cluster Improvement Algorithm, aims at sequentially improving the cluster estimates obtained from the Spectral Clustering Algorithm until the recovery rate approaches the limits predicted in Theorem 1. The pseudo-code of the Cluster Improvement Algorithm is presented in Algorithm 2.

The Cluster Improvement Algorithm works as follows. Given a cluster assignment $\{\hat{\mathcal{V}}_k^{[t]}\}_{k=1,\dots,K}$ obtained after the t-th iteration, it first calculates the estimates

$$\hat{p}_{a,b} = \hat{N}_{\hat{\mathcal{V}}_a^{[t]},\hat{\mathcal{V}}_b^{[t]}} / \hat{N}_{\hat{\mathcal{V}}_a^{[t]},\mathcal{V}} \quad \text{for} \quad a,b = 1,\dots,K,$$

$$\hat{\pi}_k = \frac{1}{T} \sum_{x \in \hat{\mathcal{V}}_k^{[t]}} \sum_{y \in \mathcal{V}} \hat{N}_{x,y} \quad \text{and} \quad \hat{\alpha}_k = \frac{|\hat{\mathcal{V}}_k^{[t]}|}{n} \quad \text{for} \quad k = 1,\dots,K. \tag{17}$$

It then initializes $\hat{\mathcal{V}}_k^{[t+1]} = \emptyset$ for $k = 1,\dots,K$, and assigns each state $x = 1,\dots,n$ to $\mathcal{V}_{c_x^{\mathrm{opt}}}^{[t+1]} \leftarrow \mathcal{V}_{c_x^{\mathrm{opt}}}^{[t+1]} \cup \{x\}$, where $c_x^{\mathrm{opt}} \triangleq \arg\max_{c=1,\dots,K} u_x^{[t]}(c)$, and

$$u_x^{[t]}(c) \triangleq \Big\{ \sum_{k=1}^{K} \big(\hat{N}_{x,\hat{\mathcal{V}}_k^{[t]}} \ln \hat{p}_{c,k} + \hat{N}_{\hat{\mathcal{V}}_k^{[t]},x} \ln \frac{\hat{p}_{k,c}}{\hat{\alpha}_c} \big) - \frac{T}{n} \cdot \frac{\hat{\pi}_c}{\hat{\alpha}_c} \Big\}. \tag{18}$$

This results in a new cluster assignment $\{\hat{\mathcal{V}}_k^{[t+1]}\}_{k=1,\dots,K}$. Note that the algorithm works by placing each state in the cluster it most likely belongs to, based on the known structure and the sample path. This can be seen by noting that the objective function in (18) is the difference between two log-likelihood functions, which we discuss further in §SM6.3.

The second step of our clustering procedure applies the Cluster Improvement Algorithm several times, using as the initial input the cluster assignment $\{\hat{\mathcal{V}}_k^{[0]}\}_{k=1,\dots,K}$ obtained from the Spectral Clustering Algorithm. We denote by $\mathcal{E}^{[t]}$ the set of misclassified state after the t-th iteration of the Clustering Improvement Algorithm. The overall performance of the clustering procedure is quantified in the following theorem.

THEOREM 3. *Assume that $T = \omega(n)$ and $I(\alpha,p) > 0$. Then there exists a constant $C > 0$ such that for any $t \geq 1$, after t iterations of the Clustering Improvement Algorithm, initially applied to the output of the Spectral Clustering Algorithm, we have:*

$$\frac{|\mathcal{E}^{[t]}|}{n} = O_{\mathbb{P}}\Big(\mathrm{e}^{-t\left(\ln \frac{T}{n} - \ln\ln \frac{T}{n}\right)} + \mathrm{e}^{-C \frac{T}{n} I(\alpha,p)} \Big) \tag{19}$$

Input: An approximate assignment $\hat{\mathcal{V}}_1^{[t]}, \dots, \hat{\mathcal{V}}_K^{[t]}$, and matrix $\hat{N}$
Output: A revised assignment $\hat{\mathcal{V}}_1^{[t+1]}, \dots, \hat{\mathcal{V}}_K^{[t+1]}$

begin
  $n \leftarrow \dim(\hat{N})$, $\mathcal{V} \leftarrow \{1, \dots, n\}$, $T \leftarrow \sum_{x\in\mathcal{V}} \sum_{y\in\mathcal{V}} \hat{N}_{x,y}$;
  for $a \leftarrow 1$ **to** K **do**
    $\hat{\pi}_a \leftarrow \hat{N}_{\hat{\mathcal{V}}_a^{[t]},\mathcal{V}}/T$, $\hat{\alpha}_a \leftarrow |\hat{\mathcal{V}}_a^{[t]}|/n$, $\hat{\mathcal{V}}_a^{[t+1]} \leftarrow \emptyset$;
    for $b \leftarrow 1$ **to** K **do**
      $\hat{p}_{a,b} \leftarrow \hat{N}_{\hat{\mathcal{V}}_a^{[t]},\hat{\mathcal{V}}_b^{[t]}}/\hat{N}_{\hat{\mathcal{V}}_a^{[t]},\mathcal{V}}$;
    end
  end
  for $x \leftarrow 1$ **to** n **do**
    $c_x^{\mathrm{opt}} \leftarrow \arg\max_{c=1,\dots,K}\left\{\sum_{k=1}^K \left(\hat{N}_{x,\hat{\mathcal{V}}_k^{[t]}} \ln \hat{p}_{c,k} + \hat{N}_{\hat{\mathcal{V}}_k^{[t]},x} \ln \frac{\hat{p}_{k,c}}{\hat{\alpha}_c}\right) - \frac{T}{n}\cdot\frac{\hat{\pi}_c}{\hat{\alpha}_c}\right\}$;
    $\hat{\mathcal{V}}_{c_x^{\mathrm{opt}}}^{[t+1]} \leftarrow \hat{\mathcal{V}}_{c_x^{\mathrm{opt}}}^{[t+1]} \cup \{x\}$;
  end
end

Algorithm 2: Pseudo-code for the Cluster Improvement Algorithm.

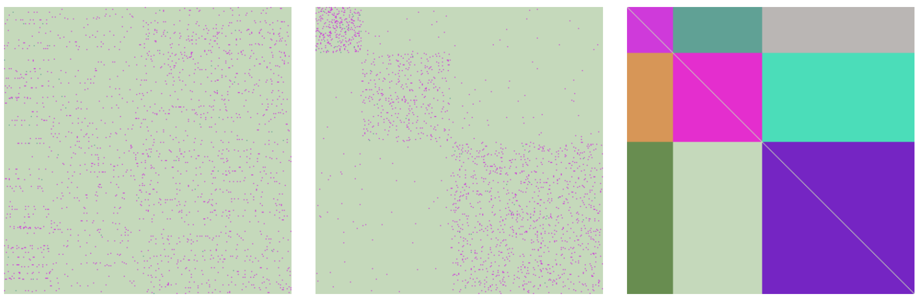
Observe now that for $t = \ln n$, the above theorem states that the number of misclassified implies after applying t times the Clustering Improvement Algorithm is at most of the order $n \exp\left(-C(T/n)I(\alpha, p)\right)$. Up to the constant C, this corresponds to the fundamental recovery rate limit identified in Theorem 1. In particular, our clustering procedure achieves asymptotically exact detection under the following nearly tight sufficient condition: $I(\alpha, p) > 0$ and $T - \frac{n \ln n}{C\cdot I(\alpha,p)} = \omega(1)$.

4. Numerical experiments. In this section, we numerically assess the performance of our algorithms. We first investigate a simple illustrative example. Then we study the sensitivity of the error rate of the Spectral Clustering Algorithm w.r.t. the number of states and the length of the observed trajectory. Finally we show the performance of the Cluster Improvement Algorithm depending on the number of times it is applied to the output of the Spectral Clustering Algorithm.

4.1. *An example.* Consider $n = 300$ states grouped into three clusters of respective relative sizes $\alpha = (0.15, 0.35, 0.5)$, i.e., the cluster sizes are cluster sizes $|\mathcal{V}_1| = 48$, $|\mathcal{V}_2| = 93$ and $|\mathcal{V}_3| = 159$. The transition rates between these clusters are defined by: $p = \big(0.9200, 0.0450, 0.0350;\ 0.0125, 0.8975, 0.0900;\ 0.0175, 0.0200, 0.9625\big)$.

We generate a sample path of the Markov chain of length $T = n^{1.025} \ln n \approx 1973$ and calculate $\hat{N}$. A density plot of a typical sample of $\hat{N}$ is shown in

Figure 4a. The same density plot is presented in Figure 4b where the states have been sorted so as states in the same cluster are neighbors. It is important to note that the algorithms are of course not aware of the structure initially – sorting states constitutes their objective. Next in Figure 4c, we show a color representation of the kernel P with sorted rows and columns, in which we can clearly see the groups. Note that the specific colors have no meaning, except for the fact that within the same image two entries with the same color have the same numerical value.

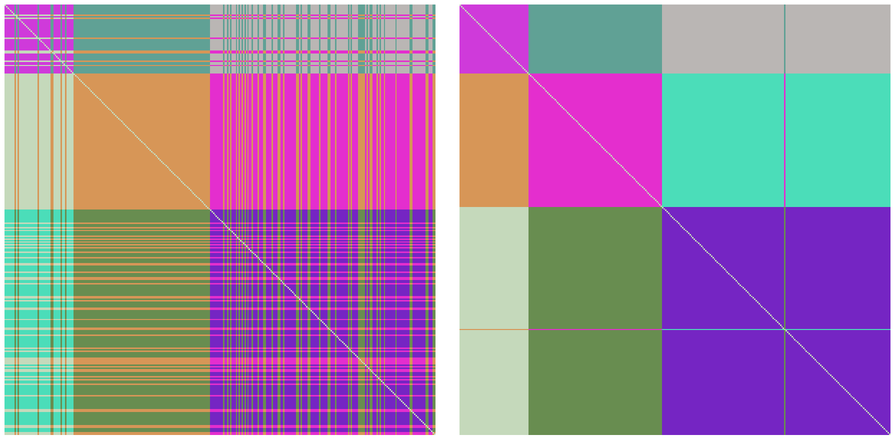


(a) $\hat{N}$, unsorted (b) $\hat{N}$, sorted (c) P, sorted

Fig 4: A sample path of length $T = n^{1.025} \ln n \approx 1973$ was generated, from which $\hat{N}$ is calculated. If we sort the states according to the clusters they belong to, we can see that states within the same cluster share similar dynamics.

Next we apply the Spectral Clustering Algorithm. This generates an initial approximate clustering $\hat{\mathcal{V}}_1^{[0]}, \hat{\mathcal{V}}_2^{[0]}, \hat{\mathcal{V}}_3^{[0]}$ of the states. We generate a visual representation of this clustering by constructing $\hat{N}^{[0]}$ from the approximate cluster structure and the estimate $\hat{p}^{[0]}$. This represents the belief that the algorithm has at this point of the true BMC kernel P. A color representation of this kernel is shown in Figure 5a. We finally execute the Cluster Improvement Algorithm. After 3 iterations, it has settled on a final clustering. We generate a color representation of the clustering similar to before, resulting in Figure 5b. The algorithms achieved a 99.7% accuracy: all but one state have been accurately clustered.

4.2. *Performance sensitivity of the Spectral Clustering Algorithm.* In this section, we examine the dependency of the number of misclassified states on the size of the kernel n, when we only apply the Spectral Clustering Algorithm. We choose $\alpha = (0.15, 0.35, 0.5)$, and set $p = (0.50, 0.20, 0.30;\ 0.10, 0.70, 0.20;\ 0.35, 0.05, 0.60)$. These parameters imply that $I(\alpha, p) \approx 0.88 > 0$. This



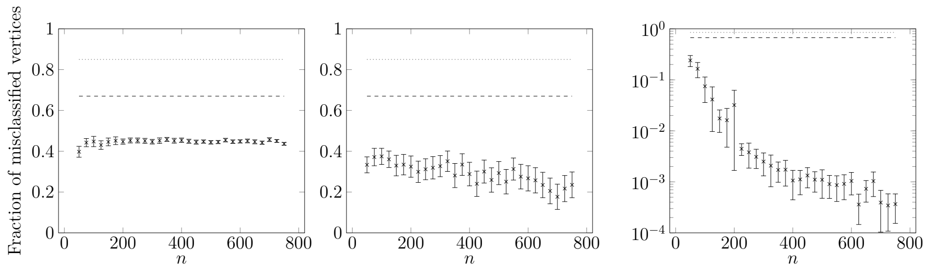
(a) Initial clustering. (b) Final clustering.

Fig 5: (a) Result after applying the Spectral Clustering Algorithm to the approximation $\hat{N}$. (b) Result after applying 3 iterations of the Cluster Improvement Algorithm. 99.7% of all states were accurately clustered.

value for $I(\alpha, p)$ is lower than in the case examined in Section 4.1, so we expect clustering to be more difficult. We have selected a more challenging model so that the initial number of misclassified states will be large and the asymptotics clear.

Figure 6 displays the error rate of the Spectral Clustering algorithm as a function of n, for different trajectory lengths T. As benchmarks, we include a dashed line that indicates the error rate obtained by assigning states to clusters uniformly at random, i.e., $\mathbb{P}[v \notin \mathcal{V}_{\sigma(v)}] = \sum_{k=1}^{K} \mathbb{P}[v \notin \mathcal{V}_k | \sigma(v) = k]\alpha_k = 1 - 1/K$, as well as a dotted line that indicates the error rate when assigning all states to the smallest cluster, i.e., $1 - \min_k\{\alpha_k\}$. For the K-means step of the algorithms, we use Mathematica's default implementation for convenience. Observe that when $T = n \ln n$, the fraction of misclassified states hardly decrease as a function of n. This is in line with our lower bound. When T gets larger, the error converges to zero faster. Note that the Spectral Clustering Algorithm recovers the clusters exactly when the sample path is sufficiently long.

4.3. *Performance sensitivity of the Cluster Improvement algorithm.* We now examine the number of misclassified states as a function of T, when we apply the Spectral Clustering Algorithm and a certain number of iterations of the Cluster Improvement Algorithm. We choose $\alpha = (1/3, 1/3, 1/3)$, and



(a) $T = n \ln n$ (b) $T = n(\ln n)^{3/2}$ (c) $T = n(\ln n)^2$

Fig 6: The error rate of the Spectral Clustering Algorithm as function of n, for different scalings of T. Every point is the average result of 40 simulations, and the bars indicate a 95%-confidence interval.

set $p = \big(0.1, 0.4, 0.5;\ 0.7, 0.1, 0.2;\ 0.6, 0.3, 0.1\big)$. Different from the previous experiments, the clusters are now of equal size and the off-diagonal entries of p are dominant. These parameters imply that $I(\alpha, p) \approx 0.27 > 0$, so the cluster algorithms should work, but the situation is again more challenging than in Section 4.1 and Section 4.2.

Figure 7 depicts the error after applying the Spectral Clustering Algorithm and subsequently the Cluster Improvement Algorithm up to two times, as a function of T. We have chosen both n, T relatively small so that the inputs are significantly noisy. For short sample paths, $T \lesssim 15000$, the data is so noisy that the Cluster Improvement Algorithm does not provide any improvement over the Spectral Clustering Algorithm. For $T \gtrsim 15000$, the Spectral Clustering Algorithm provides a sufficiently accurate initial clustering for the Cluster Improvement Algorithm to work. Because marks 1 and 2 overlap in almost all cases, we can conclude that there is (on average, and in the present situation) no benefit in running the Clustering Improvement Algorithm more than once. There is no mark 2 at $T = 30000$ in this logarithmic plot, because the Cluster Improvement Algorithm achieved 100% accurate detection after 2 iterations in *all* 200 simulations.

4.4. *Critical regime where* $T = n \ln(n)$. We now study how well our clustering procedure performs in the critical regime $T = n \ln n$. Here, we will consider $K = 2$ clusters of equal size: $\alpha_1 = \alpha_2 = \frac{1}{2}$. Recall that every such BMC can then be completely parameterized by $(p_{1,2}, p_{2,1}) \in (0,1)^2$. Our goal in this section is to numerically evaluate

$$\hat{\mathcal{F}}_1(\varepsilon) = \Big\{ (p_{1,2}, p_{2,1}) \in (0,1)^2 \Big| \mathbb{E}_P \Big[\frac{|\mathcal{E}^{[t]}|}{n} \Big] \geq \varepsilon \Big\}. \tag{20}$$

We rasterized $(0,1)^2$ and ran our clustering procedure for $n = 300$ with $t = 6$ improvement steps for each parameter pair $(p_{1,2}, p_{2,1})$. The results are shown in Figure 8. Note that the sample means at each rasterpoint was calculated from 10 independent runs.

5. The information bound and the change-of-measure. In this section, we prove Theorem 1. To this aim, we first prove, using a change-of-measure argument, that if $T = \omega(n)$ and $I(\alpha, p) > 0$, then there exists a strictly positive and finite constant C independent of n such that: for any clustering algorithm

$$\mathbb{E}_P[|\mathcal{E}|] \geq C \exp\Big(\ln n - J(\alpha, p)\frac{T}{n} + o\Big(\frac{T}{n}\Big)\Big), \tag{21}$$

where

$$0 < J(\alpha, p) \triangleq \min_{k \neq l} \min_{q \in \mathcal{Q}(k,l)} \Big(\frac{\alpha_k}{\alpha_k + \alpha_l} I_k(q||p) + \frac{\alpha_l}{\alpha_k + \alpha_l} I_l(q||p)\Big). \tag{22}$$

Here

$$I_c(q||p) \triangleq \sum_{k=1}^{K} \Big((\sum_{l=1}^{K} \pi_l q_{l,0}) q_{0,k} \ln \frac{q_{0,k}}{p_{c,k}} + \pi_k q_{k,0} \ln \frac{q_{k,0}\alpha_c}{p_{k,c}} \Big) + \Big(\frac{\pi_c}{\alpha_c} - \sum_{k=1}^{K} \pi_k q_{k,0} \Big) \tag{23}$$

for $c = 1, \ldots, K$, and

$$\mathcal{Q}(k,l) \triangleq \{q \in \mathcal{Q} \big| I_k(q||p) = I_l(q||p)\} \neq \emptyset \quad \text{for all} \quad k \neq l, \tag{24}$$

$$\mathcal{Q} \triangleq \big\{(q_{k,0}, q_{0,k})_{k=0,\ldots,K} \in (0,\infty) \big| q_{0,0} = 0, \sum_{l=1}^{K} q_{0,l} = 1\big\}. \tag{25}$$

The above quantities, e.g. q and $I_k(q||p)$, naturally arise in the change-of-measure argument developed in this section. In this argument, we isolate a state in a separate cluster, and pretend that the observations come from this perturbed model. q denotes the transition kernel in this perturbed model, and $I_k(q||p)$ appears when computing the log-likelihood ratio of the observations when generated from the initial and perturbed models.

The proof of Theorem 1 is then completed by establishing that $J(\alpha, p) \leq I(\alpha, p)$ and $I(\alpha, p) = 0$ if and only if there exists $i \neq j$ such that $p_{i,c} = p_{j,c}$ and $p_{c,i}/\alpha_i = p_{c,j}/\alpha_j$ for all $c \in \{1, \ldots, K\}$. When $I(\alpha, p) = 0$, thus, it is impossible to discriminate $\mathcal{V}_i$ and $\mathcal{V}_j$.

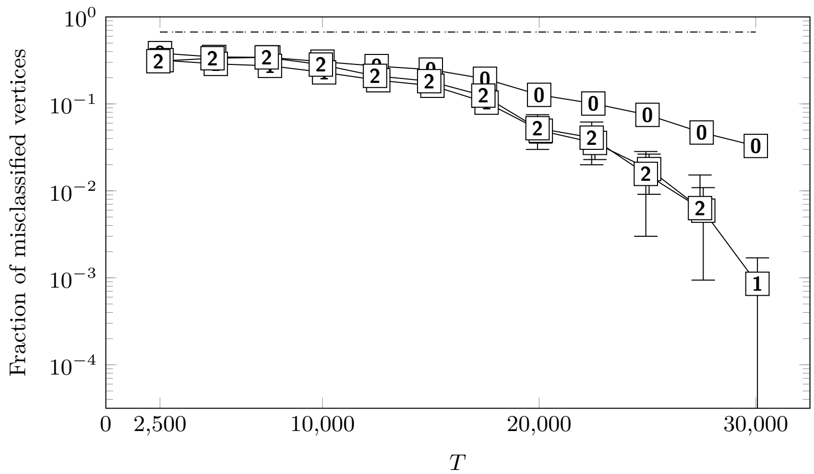
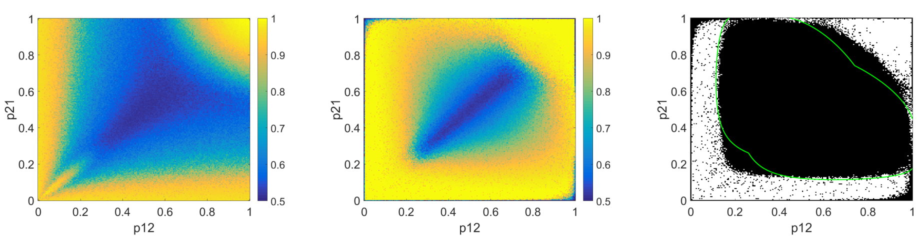


Fig 7: The error after applying the Spectral Clustering Algorithm (mark 0), and subsequently the Cluster Improvement Algorithm (marks $1, 2$) several times, as a function of T. Each number represents the number of improvement steps. Here, $n = 240$. Every point is the average result of 200 simulations, and the bars indicate a 95%-confidence interval. We have minorly offset marks $1, 2$ to the right and left for readability, respectively. At $T = 30000$, the Cluster Improvement Algorithm achieved 100% accurate detection after 2 iterations in *all* 200 instances.



After the SCA. After the CIA. $\hat{\mathcal{F}}_1(\varepsilon = 0.027)$

Fig 8: The average proportion of well-classified states for each rasterpoint $(p_{1,2}, p_{2,1}) \in (0,1)^2$ after the Spectral Clustering Algorithm (left) and Cluster Improvement Algorithm (middle), and numerical feasibility region of our clustering procedure (right), both in the critical regime $T = n \ln n$. The line outlines the theoretical region $I(\alpha, p) \leq 1$ within which no algorithm exists able to asymptotically recover the clusters exactly.

5.1. *Change-of-measure argument.* We start with a change-of-measure argument. Our argument consists in considering that the observations X_0, $\dots, X_T$ are generated by a slightly different stochastic model than the true model defined by the clusters and the transition matrix P. We denote by Φ (resp. by Ψ) the true (resp. modified) model, and by $\mathbb{P}_\Phi$ (resp. by $\mathbb{P}_\Psi$) the probability measure corresponding to Φ (resp. Ψ). The modified model is obtained by randomly choosing a state V^* (this choice will be made precise later on) and by constructing a transition matrix Q depending on V^* that is slightly different from P.

Given a sample path $X_0, X_1, \dots, X_T \in \mathcal{V}$, the argument revolves around the following log-likelihood ratio:

$$L \triangleq \ln \frac{\mathbb{P}_Q[X_0, X_1, \dots, X_T]}{\mathbb{P}_P[X_0, X_1, \dots, X_T]}. \tag{26}$$

Here,

$$\mathbb{P}_P[X_0, X_1, \dots, X_T] = \prod_{t=1}^{T} P_{X_{t-1},X_t}, \text{ and } \mathbb{P}_Q[X_0, X_1, \dots, X_T] = \prod_{t=1}^{T} Q_{X_{t-1},X_t} \tag{27}$$

so that $L = \sum_{t=1}^{T} \ln\left(Q_{X_{t-1},X_t}/P_{X_{t-1},X_t}\right)$. Note that L is random because it depends on the observations, but also on V^*. In §SM3.1, we prove the following information bound. The proof utilizes state symmetry, the change of measure's form, and Chebyshev's inequality.

PROPOSITION 3. *If V^* is chosen uniformly at random from two clusters $a \neq b$, and if*

$$\exists \text{ an absolute constant } \delta \text{ s.t. } \mathbb{P}_\Psi[V^* \in \mathcal{E}] \geq \delta > 0 \,\forall \text{classification algorithm}, \tag{28}$$

then there exists a strictly positive constant $C > 0$ independent of n such that

$$\frac{\mathbb{E}_\Phi[|\mathcal{E}|]}{n} \geq C \exp\left(-\mathbb{E}_\Psi[L] - \sqrt{\frac{2}{\delta}}\sqrt{\mathrm{Var}_\Psi[L]}\right) \tag{29}$$

for any clustering algorithm.

Preparing for the application of Proposition 3 to prove Theorem 1, we now proceed by constructing a change of measure that satisfies condition (28), and we then calculate the leading order behavior of $\mathbb{E}_\Psi[L|\sigma(V^*)]$ and upper bound $\mathrm{Var}_\Psi[L|\sigma(V^*)]$.

5.2. *The perturbed BMC given V^* and $q \in \mathcal{Q}$.* We now construct a transition matrix Q that resembles P, but differs in that V^* is placed in its own cluster with its own specific intra-cluster jump rates. We will label this extra cluster by 0 to indicate its special status. Asymptotically Q will resemble P as we are going to move probability mass away from and towards the other entries. While most entries will individually be perturbed slightly only, we still need to carefully analyze their collective contribution as this will be significant.

Define

$$q_{k,l} \triangleq p_{k,l} - \frac{q_{k,0}}{Kn} \quad \text{for} \quad k,l = 1,\dots,K, \tag{30}$$

and assume that $n > \lceil \max_{k,l=1,\dots,K} \{ q_{k,0}/(Kp_{k,l}) \} \rceil$ so that the entries of (30) are strictly positive. This assumption is not restrictive because the right-hand side is independent of n and finite. Note that the collection $\{q_{k,l}\}_{k,l \in \{0,1,\dots,K\}}$ does *not* constitute a stochastic matrix, but does resemble the transition matrix p for sufficiently large n. Now define component-wise

$$Q_{x,y} \triangleq \frac{q_{\omega(x),\omega(y)} \mathbb{1}[x \neq y]}{|\mathcal{W}_{\omega(y)}| - \mathbb{1}[\omega(x) = \omega(y)]}, \quad Q_{x,V^*} \triangleq \frac{q_{\omega(x),0}}{n} \quad \text{for} \quad x \in \mathcal{V}, y \neq V^*, \tag{31}$$

where

$$\omega(x) \triangleq \begin{cases} 0 & \text{if } x = V^*, \\ \sigma(x) & \text{if } x \neq V^*, \end{cases} \quad \text{and} \quad \mathcal{W}_k \triangleq \begin{cases} \{V^*\} & \text{if } k = 0, \\ \mathcal{V}_k \backslash \{V^*\} & \text{if } k = 1,\dots,K, \end{cases} \tag{32}$$

for notational convenience. This has the added benefit of giving (31) a similar form as (4).

Q is by construction a stochastic matrix (see §SM3.2). Note furthermore that because Q is constructed from P, which by assumption describes an irreducible Markov chain, and because the entries $\{q_{k,0}, q_{0,k}\}_{k=1,\dots,K}$ are all strictly positive, Q also describes an irreducible Markov chain.

5.2.1. *Asymptotic behavior of the equilibrium distribution.* Let $\Pi^{(Q)}$ denote the equilibrium distribution of a Markov chain with transition matrix Q, i.e., the solution to $\Pi^{(Q)\mathrm{T}} Q = \Pi^{(Q)\mathrm{T}}$. By symmetry of states in the same cluster $\Pi_x^{(Q)} = \Pi_y^{(Q)} \triangleq \bar{\Pi}_k^{(Q)}$ for any two states $x, y \in \mathcal{W}_k$ and all $k \in \{1,\dots,K,0\}$. Define

$$\gamma_k^{[0]} \triangleq \lim_{n\to\infty} \sum_{x \in \mathcal{W}_k} \Pi_x^{(Q)} = \lim_{n\to\infty} |\mathcal{W}_k| \bar{\Pi}_k^{(Q)} \quad \text{for} \quad k \in \{0,1,\dots,K\}. \tag{33}$$

We can expect $\gamma_0^{[0]}$ to be zero, because by our construction of Q we can expect that $\Pi_x^{(Q)} = O(1/n)$ for all $x \in \mathcal{V}$ (including V^*). We therefore also define its higher order statistic

$$\gamma_0^{[1]} \triangleq \lim_{n\to\infty} n\Pi_{V^*}^{(Q)}. \tag{34}$$

The following proposition relates these scaled quantities to the parameters of our BMC $\{X_t\}_{t\geq 0}$. The proof is deferred to §SM3.3, and relies on several applications of the balance equations and a subsequent asymptotic analysis.

Proposition 4. *For $k = 1, \ldots, K$, $\gamma_k^{[0]} = \pi_k$. Furthermore $\gamma_0^{[0]} = 0$ and $\gamma_0^{[1]} = \sum_{k=1}^K \pi_k q_{k,0}$.*

5.2.2. *Mixing time.* We now crucially note that Proposition 2 holds for a Markov chain with Q as its transition matrix as well. This follows when applying the exact same proof.

Example. It is illustrative to explicitly write down at least one example kernel Q. For $K = 3$, $\alpha = (2/10, 3/10, 5/10)$ and $n = 10$, $V^* = 7$, it is given by

$$Q = \left(\begin{array}{cc|ccc|ccccc}
0 & p_{1,1} & \frac{p_{1,2}}{3} & \frac{p_{1,2}}{3} & \frac{p_{1,2}}{3} & \frac{p_{1,3}}{4} & \frac{q_{1,0}}{10} & \frac{p_{1,3}}{4} & \frac{p_{1,3}}{4} & \frac{p_{1,3}}{4} \\
p_{1,1} & 0 & \frac{p_{1,2}}{3} & \frac{p_{1,2}}{3} & \frac{p_{1,2}}{3} & \frac{p_{1,3}}{4} & \frac{q_{1,0}}{10} & \frac{p_{1,3}}{4} & \frac{p_{1,3}}{4} & \frac{p_{1,3}}{4} \\
\hline
\frac{p_{2,1}}{2} & \frac{p_{2,1}}{2} & 0 & \frac{p_{2,2}}{2} & \frac{p_{2,2}}{2} & \frac{p_{2,3}}{4} & \frac{q_{2,0}}{10} & \frac{p_{2,3}}{4} & \frac{p_{2,3}}{4} & \frac{p_{2,3}}{4} \\
\frac{p_{2,1}}{2} & \frac{p_{2,1}}{2} & \frac{p_{2,2}}{2} & 0 & \frac{p_{2,2}}{2} & \frac{p_{2,3}}{4} & \frac{q_{2,0}}{10} & \frac{p_{2,3}}{4} & \frac{p_{2,3}}{4} & \frac{p_{2,3}}{4} \\
\frac{p_{2,1}}{2} & \frac{p_{2,1}}{2} & \frac{p_{2,2}}{2} & \frac{p_{2,2}}{2} & 0 & \frac{p_{2,3}}{4} & \frac{q_{2,0}}{10} & \frac{p_{2,3}}{4} & \frac{p_{2,3}}{4} & \frac{p_{2,3}}{4} \\
\hline
\frac{p_{3,1}}{2} & \frac{p_{3,1}}{2} & \frac{p_{3,2}}{3} & \frac{p_{3,2}}{3} & \frac{p_{3,2}}{3} & 0 & \frac{q_{3,0}}{10} & \frac{p_{3,3}}{3} & \frac{p_{3,3}}{3} & \frac{p_{3,3}}{3} \\
\frac{q_{0,1}}{2} & \frac{q_{0,1}}{2} & \frac{q_{0,2}}{3} & \frac{q_{0,2}}{3} & \frac{q_{0,2}}{3} & \frac{q_{0,3}}{4} & 0 & \frac{q_{0,3}}{4} & \frac{q_{0,3}}{4} & \frac{q_{0,3}}{4} \\
\frac{p_{3,1}}{2} & \frac{p_{3,1}}{2} & \frac{p_{3,2}}{3} & \frac{p_{3,2}}{3} & \frac{p_{3,2}}{3} & \frac{p_{3,3}}{3} & \frac{q_{3,0}}{10} & 0 & \frac{p_{3,3}}{3} & \frac{p_{3,3}}{3} \\
\frac{p_{3,1}}{2} & \frac{p_{3,1}}{2} & \frac{p_{3,2}}{3} & \frac{p_{3,2}}{3} & \frac{p_{3,2}}{3} & \frac{p_{3,3}}{3} & \frac{q_{3,0}}{10} & \frac{p_{3,3}}{3} & 0 & \frac{p_{3,3}}{3} \\
\frac{p_{3,1}}{2} & \frac{p_{3,1}}{2} & \frac{p_{3,2}}{3} & \frac{p_{3,2}}{3} & \frac{p_{3,2}}{3} & \frac{p_{3,3}}{3} & \frac{q_{3,0}}{10} & \frac{p_{3,3}}{3} & \frac{p_{3,3}}{3} & 0
\end{array}\right)$$

$$- \frac{1}{3\cdot 10}\left(\begin{array}{cc|ccc|ccccc}
0 & q_{1,0} & \frac{q_{1,0}}{3} & \frac{q_{1,0}}{3} & \frac{q_{1,0}}{3} & \frac{q_{1,0}}{4} & 0 & \frac{q_{1,0}}{4} & \frac{q_{1,0}}{4} & \frac{q_{1,0}}{4} \\
q_{1,0} & 0 & \frac{q_{1,0}}{3} & \frac{q_{1,0}}{3} & \frac{q_{1,0}}{3} & \frac{q_{1,0}}{4} & 0 & \frac{q_{1,0}}{4} & \frac{q_{1,0}}{4} & \frac{q_{1,0}}{4} \\
\hline
\frac{q_{2,0}}{2} & \frac{q_{2,0}}{2} & 0 & \frac{q_{2,0}}{2} & \frac{q_{2,0}}{2} & \frac{q_{2,0}}{4} & 0 & \frac{q_{2,0}}{4} & \frac{q_{2,0}}{4} & \frac{q_{2,0}}{4} \\
\frac{q_{2,0}}{2} & \frac{q_{2,0}}{2} & \frac{q_{2,0}}{2} & 0 & \frac{q_{2,0}}{2} & \frac{q_{2,0}}{4} & 0 & \frac{q_{2,0}}{4} & \frac{q_{2,0}}{4} & \frac{q_{2,0}}{4} \\
\frac{q_{2,0}}{2} & \frac{q_{2,0}}{2} & \frac{q_{2,0}}{2} & \frac{q_{2,0}}{2} & 0 & \frac{q_{2,0}}{4} & 0 & \frac{q_{2,0}}{4} & \frac{q_{2,0}}{4} & \frac{q_{2,0}}{4} \\
\hline
\frac{q_{3,0}}{2} & \frac{q_{3,0}}{2} & \frac{q_{3,0}}{3} & \frac{q_{3,0}}{3} & \frac{q_{3,0}}{3} & 0 & 0 & \frac{q_{3,0}}{3} & \frac{q_{3,0}}{3} & \frac{q_{3,0}}{3} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{q_{3,0}}{2} & \frac{q_{3,0}}{2} & \frac{q_{3,0}}{3} & \frac{q_{3,0}}{3} & \frac{q_{3,0}}{3} & \frac{q_{3,0}}{3} & 0 & 0 & \frac{q_{3,0}}{3} & \frac{q_{3,0}}{3} \\
\frac{q_{3,0}}{2} & \frac{q_{3,0}}{2} & \frac{q_{3,0}}{3} & \frac{q_{3,0}}{3} & \frac{q_{3,0}}{3} & \frac{q_{3,0}}{3} & 0 & \frac{q_{3,0}}{3} & 0 & \frac{q_{3,0}}{3} \\
\frac{q_{3,0}}{2} & \frac{q_{3,0}}{2} & \frac{q_{3,0}}{3} & \frac{q_{3,0}}{3} & \frac{q_{3,0}}{3} & \frac{q_{3,0}}{3} & 0 & \frac{q_{3,0}}{3} & \frac{q_{3,0}}{3} & 0
\end{array}\right). \tag{35}$$

Here, we have indicated the original cluster structure in dashed lines, and we have colored the row and column corresponding to the modified cluster behavior of state V^*. Comparing (35) to (8) helps understanding how Q is constructed and how Q compares to P. Note in particular the minor changes in the normalizations of all entries.

5.3. *Leading order behavior of* $\mathbb{E}_Q[L|\sigma(V^*)]$ *and* $\mathrm{Var}_Q[L|\sigma(V^*)]$. Having constructed the transition matrix Q, we now calculate the leading order behavior of $\mathbb{E}_Q[L|\sigma(V^*)]$ in Proposition 5. The proof in §SM3.4 relies on asymptotic expansions and the fact that the element-wise similarity of P and Q allows for term neglection.

PROPOSITION 5. *For any given* $V^* \in \mathcal{V}$ *and* $q \in \mathcal{Q}$, $\mathbb{E}_Q[L|\sigma(V^*)] = (T/n)I_{\sigma(V^*)}(q||p) + o(T/n)$. *Here,* $I_{\sigma(V^*)}(q||p)$ *is defined in* (23).

With Proposition 6, we next establish that $\sqrt{\mathrm{Var}_Q[L|\sigma(V^*)]}$ is asymptotically negligible when compared to $\mathbb{E}_Q[L|\sigma(V^*)]$ whenever $T = \omega(n)$. The crux of the proof is to relate the covariances *between* the T steps of the sample path $\{X_1, X_2, \ldots, X_T\}$ to the mixing time of the underlying Markov chain. The mixing time result of Proposition 2 then allows us to bound variance. The detailed proof is relegated to §SM3.5.

PROPOSITION 6. *For any given* $V^* \in \mathcal{V}$ *and* $q \in \mathcal{Q}$, *it holds that if* $T = \omega(1)$, *then* $\mathrm{Var}_Q[L|\sigma(V^*)] = O(T/n)$. *As a consequence if* $T = \omega(n)$, *then* $\mathrm{Var}_Q[L|\sigma(V^*)] = o(T^2/n^2)$.

5.4. *Appropriateness, deconditioning, and bound optimization.* Recall that the transition matrix Q is constructed given a state $V^* \in \mathcal{V}$. This implies in particular that Proposition 5 and Proposition 6 have determined the asymptotic behavior of the conditional expectation $\mathbb{E}_Q[L|\sigma(V^*)]$ and conditional variance $\mathrm{Var}_Q[L|\sigma(V^*)]$. The information bound Proposition 3 requires us however to analyze their unconditioned counterparts, which is the subject of this section. Importantly, we can limit the variance introduced by a random state selection by choosing $q \in \mathcal{Q}$ appropriately.

5.4.1. *Appropriateness.*

LEMMA 1. *For any two clusters* $a \neq b$ *there exists at least one finite point* $\bar{q} \in \mathcal{Q}$ *such that* $I_a(\bar{q}||p) = I_b(\bar{q}||p)$.

Lemma 1's proof is deferred to §SM3.6. It leverages that the objective function can to leading order be related to a KL-divergence.

In §SM3.7 we prove that the change of measure Ψ satisfies condition (28), as summarized in Lemma 2. The proof follows from the fact that, with respect to the transition matrix Q, the state V^* behaves differently from any state in *either* cluster a or b: as a consequence, no algorithm can correctly assign V^* with certainty to either of the two cluster it possibly originated from.

LEMMA 2. *For any two clusters $a \neq b$, if Q is constructed using any $\bar{q} \in \mathcal{Q}(a,b)$, recall its definition in* (25)*, then there exists an absolute constant δ such that $\mathbb{P}_\Psi[V^* \in \mathcal{E}] \geq \delta > 0$.*

One difficulty encountered in Lemma 2's proof is that given $a \neq b$ and $\bar{q} \in \mathcal{Q}(a,b)$ with which Q is constructed, this does *not* imply that e.g. $\mathbb{P}_Q[V^* \in \hat{\mathcal{V}}_a | \sigma(V^*) = a]$ equals $\mathbb{P}_Q[V^* \in \hat{\mathcal{V}}_a | \sigma(V^*) = b]$ for any clustering algorithm when n is finite. This is because the rows of the transition matrix are normalized. In particular, depending on which cluster V^* originated from, the transition probabilities from/to the originating cluster differ on the order of $O(1/n^2)$.

5.4.2. *Deconditioning.* Lemma 3 now revisits Proposition 3 and accounts for the specific choices made in the change-of-measure. See §SM3.8 for its proof, which essentially applies the laws of total probability and variance to decondition our earlier conditional statements.

LEMMA 3. *If $T = \omega(n)$, then for any two clusters $a \neq b$, there exists a strictly positive constant $c > 0$ independent of n such that*

$$\frac{\mathbb{E}_P[|\mathcal{E}|]}{n} \geq c \exp\Big(-\frac{T}{n} I_{a,b}(\bar{q}||p) + o\Big(\frac{T}{n}\Big)\Big). \tag{36}$$

Here,

$$I_{a,b}(\bar{q}||p) = \frac{\alpha_a}{\alpha_a + \alpha_b} I_a(\bar{q}||p) + \frac{\alpha_b}{\alpha_a + \alpha_b} I_b(\bar{q}||p) \tag{37}$$

for any point $\bar{q}$ selected from the set $\mathcal{Q}(a,b)$.

5.4.3. *Bound optimization.* We now optimize the bound in (36). This is straightforward: build the change of measure using the parameters

$$(k^{\text{opt}}, l^{\text{opt}}, q^{\text{opt}}) \in \arg\min_{k \neq l} \min_{q \in \mathcal{Q}(k,l)} \Big\{ \frac{\alpha_k}{\alpha_k + \alpha_l} I_k(q||p) + \frac{\alpha_l}{\alpha_k + \alpha_l} I_l(q||p) \Big\}. \tag{38}$$

Then by construction $\mathbb{E}_\Psi[L] = (T/n) J(\alpha, p) + o(T/n)$, and since $q^{\text{opt}} \in Q(k^{\text{opt}}, l^{\text{opt}})$, we have $0 < J(\alpha, p) < \infty$.

Finally, we provide the upper bound for $J(\alpha, p)$. Its proof relies on identifying a concatenation of line segments *along* which two particular functions $I_c(q||p)$ are convex – recall that $I_c(q||p)$ is not convex on its entire domain. The proof is given in §SM3.9. This completes the proof of Theorem 1.

LEMMA 4. *For any BMC, $J(\alpha, p) \leq I(\alpha, p)$. Furthermore, $I(\alpha, p) = 0$ if and only if there exists $i \neq j$ such that $p_{i,c} = p_{j,c}$ and $p_{c,i}/\alpha_i = p_{c,j}/\alpha_j$ for all $c \in \{1, \ldots, K\}$.*

6. Performance of the Spectral Clustering Algorithm. This section is devoted to the proof of Theorem 2. The Spectral Clustering Algorithm relies on a spectral decomposition of the trimmed matrix $\hat{N}_\Gamma$. Hence in the proof, we will leverage concentration inequalities for Markov chains which is provided in §SM1 and a spectral analysis for $\hat{N}$ or $\hat{N}_\Gamma$ which we present in the next subsection. Throughout the section we use the following notation: $N_{x,y} \triangleq \mathbb{E}_P[\hat{N}_{x,y}] = T\Pi_x P_{x,y} N_{x,y}$ for $x, y \in \mathcal{V}$, $\hat{R}^0 = [\hat{R}, \hat{R}^\top]$, $N^0 = [N, N^\top]$, and $\hat{N}^0 = [\hat{N}_\Gamma, \hat{N}_\Gamma^\top]$.

6.1. *Spectral analysis.* The performance analysis of the Spectral Clustering Algorithm relies on a concentration bound on the spectral norm of the matrix $\hat{N}_\Gamma$ centered around its mean, i.e., on $\|\hat{N}_\Gamma - N\|$. The tighter such a bound one can obtain, the tighter our performance analysis will be. Note that the concentration of the spectral norm holds for the trimmed matrix, i.e., a matrix whose rows and columns in $\hat{N}$ corresponding to states visited too often are set to 0. In particular, in the spectral analysis, we use the following concentration result, upper bounding the entries of $\hat{N}_\Gamma$: there exists an absolute constant $c > 0$ such that

$$\max_{y \in \Gamma} \{\hat{N}_{\Gamma,y} \vee \hat{N}_{y,\Gamma}\} \leq c\frac{T}{n} \ln \frac{T}{n} \quad \text{with probability} \quad 1 - \mathrm{e}^{-\frac{T}{n} \ln \frac{T}{n}}. \tag{39}$$

This concentration result is a direct consequence of the concentration inequality in (56) and of Markov's inequality. The proof of the following proposition is presented in §SM4.1.

PROPOSITION 7. *For any BMC, $\|\hat{N}_\Gamma - N\| = O_{\mathbb{P}}\Big(\sqrt{\frac{T}{n} \ln \frac{T}{n}}\Big)$.*

This bound is sufficiently tight for the purposes of this paper, but can be improved up to logarithmic terms. The primary challenge one encounters in establishing this bound is that $\hat{N}$ is a random matrix with stochastic *dependent* entries, as explained in the introduction. The concentration of the entire spectrum spectrum of $\hat{N}_\Gamma$ would be an intriguing topic for future study.

6.2. *Proof of Theorem 2.* For this proof, we introduce the quantity

$$D_N(\alpha,p) \triangleq \min_{a,b:a\neq b} \sum_{k=1}^{K} \Big(\big(\frac{\pi_a p_{a,k}}{\alpha_k\alpha_a} - \frac{\pi_b p_{b,k}}{\alpha_k\alpha_b}\big)^2 + \big(\frac{\pi_k p_{k,a}}{\alpha_k\alpha_a} - \frac{\pi_k p_{k,b}}{\alpha_k\alpha_b}\big)^2 \Big) > 0. \tag{40}$$

Note that $D_N(\alpha,p)=0$ if and only if there exist a,b such that (C1) $p_{a,k}=p_{b,k}$ for all k, (C2) $p_{k,a}/\alpha_a = p_{k,b}/\alpha_b$ for all k, and (C3) $\pi_a/\alpha_a = \pi_b/\alpha_b$. Under (C1)–(C3), $I(\alpha,p)=0$. Thus, $D(\alpha,p)>0$ when $I(\alpha,p)>0$.

The proof of Theorem 2 consists of four steps.

Step 1. We show that N^0 satisfies a *separability property*: i.e., if two states $x,y\in\mathcal{V}$ do not belong to the same cluster, the l_2-distance between their respective rows $N^0_{x,\cdot}$, $N^0_{y,\cdot}$ is at least $\Omega(\sqrt{T^2 D_N(\alpha,p)/n^3})$.

Step 2. We upper bound the error $\|\hat{R}^0 - N^0\|_{\mathrm{F}}$ using $\|\hat{N}_\Gamma - N\|$.

Step 3. We prove that $\hat{R}$ also satisfies the separability property if $\|\hat{N}_\Gamma - N\| \to 0$, as suggested by Step 1 and Step 2.

Step 4. Because of $\hat{R}^0$'s separability property, we must conclude that the number of misclassified states satisfies Theorem 2. Otherwise the separability property of Step 3 would contradict with Step 2.

Step 1 is formalized in Lemma 5, and proven in §SM4.2. It is a consequence of the block structure of matrix N.

LEMMA 5. *For any $x,y\in\mathcal{V}$ for which $\sigma(x)\neq\sigma(y)$,*

$$\|N^0_{x,\cdot} - N^0_{y,\cdot}\|_2 = \Omega\Big(\sqrt{\frac{T^2 D_N(\alpha,p)}{n^3}}\Big). \tag{41}$$

Step 2. Lemma 6 shows that the error $\|\hat{R}^0 - N^0\|_{\mathrm{F}}$ is asymptotically bounded by $\|\hat{N}_\Gamma - N\|$, and is proven in §SM4.3. The proof relies on a powerful bound relating decompositions of random matrices and their spectra [22].

LEMMA 6. $\|\hat{R}^0 - N^0\|_{\mathrm{F}} \le \sqrt{16K}\|\hat{N}_\Gamma - N\|$.

Step 3. The fact that $\hat{R}^0$ also satisfies a separability property, is stated in Lemma 7. Its proof, presented in §SM4.4, requires a bound on the spectral concentration rate of $\hat{N}_\Gamma$'s noise matrix, relies on Lemmas 5, 6, and exploits the design of the K-means algorithm used after the spectral decomposition.

LEMMA 7. *If $\|\hat{N}_\Gamma - N\| = o_{\mathbb{P}}(f(n,T))$ for some $f(n,T)=o(T/n)$ and $h(n,T)$ is s.t. $\omega((f(n,T))^2/n) = \big(h(n,T)\big)^2 = o(T^2 D_N(\alpha,p)/n^3)$, then*

$$\|\hat{R}^0_{x,\cdot} - N^0_{x,\cdot}\|_2 = \Omega_{\mathbb{P}}\Big(\sqrt{\frac{T^2 D_N(\alpha,p)}{n^3}}\Big) \quad \text{for any misclassified vertex} \quad x\in\mathcal{E}. \tag{42}$$

In view of Proposition 7, the conditions of the above lemma are satisfied for the following choices: $f(n,T) = ((T/n)\ln(T/n))^{\frac{1}{2}+\zeta}$ and $h(n,T) = (f(n,T)/\sqrt{n}) \cdot (T/n)^{\zeta}$ for $0 < \zeta \ll 1$.

Step 4. The final step is almost immediate. Gathering the arguments of the previous steps, we have:

$$\Omega_{\mathbb{P}}\Big(|\mathcal{E}|\frac{T^2 D_N(\alpha,p)}{n^3}\Big) \overset{\text{(i)}}{=} \|\hat{R}^0 - N^0\|_{\mathrm{F}}^2 \overset{\text{(ii)}}{\leq} 16K\|\hat{N}_\Gamma - N\|^2 \overset{\text{(iii)}}{=} O_{\mathbb{P}}\Big(\frac{T}{n}\ln\frac{T}{n}\Big), \tag{43}$$

where (i) stems from Lemma 7 (the terms $\|\hat{R}^0_{x,\cdot} - N^0_{x,\cdot}\|_2^2$ for $x \in \mathcal{V} \setminus \mathcal{E}$ can be added to form the Frobenius norm), (ii) comes from Lemma 6, and (iii) is from Proposition 7. We deduce that $|\mathcal{E}|/n = O_{\mathbb{P}}((n/T)\ln(T/n))$: see Lemma 18 in §SM6.5 for a precise justification. This concludes the proof.

7. Performance of the Cluster Improvement Algorithm.

7.1. *Proof of Theorem 3.* To establish Theorem 3, we give an asymptotic upper bound on the number of states in $\mathcal{E}_{\mathcal{H}}^{[t]} = \mathcal{E}^{[t]} \cap \mathcal{H}$, where $\mathcal{H}$ is the largest set of states $x \in \Gamma$ that satisfy the following two properties:

(H1) When $x \in \mathcal{V}_i$, for all $j \neq i$,

$$\sum_{k=1}^{K}\Big(\hat{N}_{x,\mathcal{V}_k}\ln\frac{p_{i,k}}{p_{j,k}} + \hat{N}_{\mathcal{V}_k,x}\ln\frac{p_{k,i}\alpha_j}{p_{k,j}\alpha_i}\Big) + \Big(\frac{\hat{N}_{\mathcal{V}_j,\mathcal{V}}}{\alpha_j n} - \frac{\hat{N}_{\mathcal{V}_i,\mathcal{V}}}{\alpha_i n}\Big) \geq \frac{T}{2n}I(\alpha,p). \tag{44}$$

(H2) $\hat{N}_{x,\mathcal{V}\setminus\mathcal{H}} + \hat{N}_{\mathcal{V}\setminus\mathcal{H},x} \leq 2\ln((T/n)^2)$.

In the following, we specifically consider $f(n,T) = \sqrt{(T/n)\ln(T/n)}$. We can then show that:

THEOREM 4. *If $I(\alpha,p) > 0$ and $T = \omega(n)$, and $|\mathcal{E}_{\mathcal{H}}^{[t]}| = O_{\mathbb{P}}(e_n^{[t]})$ for some $0 < e_n^{[t]} = o(n)$, then*

$$|\mathcal{E}_{\mathcal{H}}^{[t+1]}| \asymp_{\mathbb{P}} e_n^{[t+1]} = O\Big(e_n^{[t]}\Big(\frac{n}{T}f(n,T)\Big)^2\Big) = o(e_n^{[t]}). \tag{45}$$

Furthermore, there exists a strictly positive absolute constant C such that

$$|\mathcal{E}_{\mathcal{H}^{\mathrm{c}}}^{[t]}| \leq |\mathcal{H}^{\mathrm{c}}| = O_{\mathbb{P}}\Big(n\exp\Big(-C\frac{T}{n}I(\alpha,p)\Big) + n\exp\Big(-\frac{T}{n}\ln\frac{T}{n}\Big)\Big) \tag{46}$$

for all $t \in \mathbb{N}_0$.

If we initiate the Cluster Improvement Algorithm using the cluster assignment provided by the Spectral Clustering Algorithm when $T = \omega(n)$, we satisfy the initial condition $|\mathcal{E}_{\mathcal{H}}^{[0]}| = o_{\mathbb{P}}(n)$. We are now able to iterate the bound in (45). Furthermore, since $|\mathcal{E}^{[t]}| = |\mathcal{E}_{\mathcal{H}}^{[t]}| + |\mathcal{E}_{\mathcal{H}^{\mathrm{c}}}^{[t]}|$, we conclude that after $t \in \mathbb{N}_0$ improvement steps the Cluster Improvement Algorithm

$$|\mathcal{E}^{[t]}| = O_{\mathbb{P}}\Bigl(\mathrm{e}^{\ln n - t\left(\ln \frac{T}{n} - \ln\ln \frac{T}{n}\right)} + \mathrm{e}^{\ln n - C\frac{T}{n}I(\alpha,p)} + \mathrm{e}^{\ln n - \frac{T}{n}\ln\frac{T}{n}}\Bigr). \tag{47}$$

This completes the proof of Theorem 3.

7.2. *Proof of Theorem 4.*

Proof of (46). This is relegated to §SM5.1.

Proof of (45). First observe that after the $(t+1)$-st iteration, for any misclassified state x, its true cluster $\sigma(x)$ does not maximize the objective function $u_x^{[t]}(c)$. Hence summing over all misclassified states that also belong to the set $\mathcal{H}$, i.e., $\mathcal{E}_{\mathcal{H}}^{[t+1]} \triangleq \mathcal{E}^{[t+1]} \cap \mathcal{H}$, we obtain

$$E \triangleq \sum_{x \in \mathcal{E}_{\mathcal{H}}^{[t+1]}} \bigl(u_x^{[t]}(\sigma^{[t+1]}(x)) - u_x^{[t]}(\sigma(x))\bigr) \geq 0. \tag{48}$$

Next the proof proceed in two steps.

Step 1. We show through concentration arguments that asymptotically $E \approx -(T/n)I(\alpha,p)|\mathcal{E}_{\mathcal{H}}^{[t+1]}| + \|\hat{N}_\Gamma - N\|\sqrt{|\mathcal{E}_{\mathcal{H}}^{[t+1]}||\mathcal{E}_{\mathcal{H}}^{[t]}|}$.

Step 2. For sufficiently large n, T, putting the result of Step 1 together with the aforementioned suboptimality $E \geq 0$ yields Theorem 4.

Proof. For *Step 1* we first substitute $u_x^{[t]}$'s definition from (18), and we obtain after simplifying

$$\begin{aligned} E = \sum_{x \in \mathcal{E}_{\mathcal{H}}^{[t+1]}} \Bigl[\sum_{k=1}^{K} \Bigl(\hat{N}_{x,\hat{\mathcal{V}}_k^{[t]}} \ln \frac{\hat{p}_{\sigma^{[t+1]}(x),k}}{\hat{p}_{\sigma(x),k}} + \hat{N}_{\hat{\mathcal{V}}_k^{[t]},x} \ln \frac{\hat{p}_{k,\sigma^{[t+1]}(x)}}{\hat{p}_{k,\sigma(x)}} \Bigr) \\ + \Bigl(\frac{\hat{N}_{\hat{\mathcal{V}}_{\sigma(x)}^{[t]},\mathcal{V}}}{|\hat{\mathcal{V}}_{\sigma(x)}^{[t]}|} - \frac{\hat{N}_{\hat{\mathcal{V}}_{\sigma^{[t+1]}(x)}^{[t]},\mathcal{V}}}{|\hat{\mathcal{V}}_{\sigma^{[t+1]}(x)}^{[t]}|} \Bigr) \Bigr]. \end{aligned} \tag{49}$$

Next, we split $E = E_1 + E_2 + U$, where the terms E_1, E_2 center around different objects that are expected to concentrate and U denotes the remainder.

Specifically, we define $E_1 = E_1^{\mathrm{out}} + E_1^{\mathrm{in}} + E_1^{\mathrm{cross}}$ with

$$E_1^{\mathrm{out}} = \sum_{x \in \mathcal{E}_{\mathcal{H}}^{[t+1]}} \sum_{k=1}^{K} \hat{N}_{x,\mathcal{V}_k} \ln \frac{p_{\sigma^{[t+1]}(x),k}}{p_{\sigma(x),k}}, \quad E_1^{\mathrm{in}} = \sum_{x \in \mathcal{E}_{\mathcal{H}}^{[t+1]}} \sum_{k=1}^{K} \hat{N}_{\mathcal{V}_k,x} \ln \frac{p_{k,\sigma^{[t+1]}(x)}}{p_{k,\sigma(x)}},$$

$$E_1^{\mathrm{cross}} = \sum_{x \in \mathcal{E}_{\mathcal{H}}^{[t+1]}} \Big(\frac{\hat{N}_{\mathcal{V}_{\sigma(x)},\mathcal{V}}}{|\mathcal{V}_{\sigma(x)}|} - \frac{\hat{N}_{\mathcal{V}_{\sigma^{[t+1]}(x)},\mathcal{V}}}{|\mathcal{V}_{\sigma^{[t+1]}(x)}|} \Big) \tag{50}$$

as well as $E_2 = E_2^{\mathrm{out}} + E_2^{\mathrm{in}}$ with

$$E_2^{\mathrm{out}} = \sum_{x \in \mathcal{E}_{\mathcal{H}}^{[t+1]}} \sum_{k=1}^{K} (\hat{N}_{x,\hat{\mathcal{V}}_k^{[t]}} - \hat{N}_{x,\mathcal{V}_k}) \ln \frac{p_{\sigma^{[t+1]}(x),k}}{p_{\sigma(x),k}},$$

$$E_2^{\mathrm{in}} = \sum_{x \in \mathcal{E}_{\mathcal{H}}^{[t+1]}} \sum_{k=1}^{K} (\hat{N}_{\hat{\mathcal{V}}_k^{[t]},x} - \hat{N}_{\mathcal{V}_k,x}) \ln \frac{p_{k,\sigma^{[t+1]}(x)}}{p_{k,\sigma(x)}}. \tag{51}$$

We then bound E_1, E_2 and U. Lemma 8 holds the precise statements, and the proof is in §SM5.2. The proof relies on asymptotic expansions, concentration bounds, our mixing time bound, and general properties of matrix multiplication, set construction, and stochastic boundedness.

LEMMA 8. *If $T = \omega(n)$, $|\mathcal{E}_{\mathcal{H}}^{[t]}| = O_{\mathbb{P}}(e_n^{[t]})$, and $|\mathcal{E}_{\mathcal{H}}^{[t+1]}| \asymp_{\mathbb{P}} e_n^{[t+1]}$, then*

$$-E_1 = \Omega_{\mathbb{P}}\Big(I(\alpha,p) \frac{T}{n} e_n^{[t+1]} \Big), \quad |U| = O_{\mathbb{P}}\Big(\sqrt{\frac{T}{n}} \Big(\ln \frac{T}{n} \Big) e_n^{[t+1]} \Big), \quad \textit{and} \tag{52}$$

$$|E_2| = O_{\mathbb{P}}\Big(\frac{T}{n} \frac{e_n^{[t]}}{n} e_n^{[t+1]} + f(n,T) \sqrt{e_n^{[t]} e_n^{[t+1]}} + \Big(\ln \frac{T}{n} \Big) e_n^{[t+1]} \Big). \tag{53}$$

Finally, we execute *Step 2*: Note that $E = E_1 + E_2 + U \geq 0$ so that $-E_1 \leq |E_2| + |U|$ almost surely. Together with Lemma 8, the prerequisites of Lemma 18, see §SM6.5, are met, so necessarily

$$I(\alpha,p) e_n^{[t+1]} = O\Big(\frac{n}{T} f(n,T) \sqrt{e_n^{[t]} e_n^{[t+1]}} \Big).$$

Note that equality holds when $e_n^{[t+1]} = 0$. When $e_n^{[t+1]} > 0$, and recall that $e_n^{[t]} > 0$ by assumption, we can divide by $(e_n^{[t]} e_n^{[t+1]})^{1/2}$ to obtain

$$\sqrt{\frac{e_n^{[t+1]}}{e_n^{[t]}}} = O\Big(\frac{n}{T} f(n,T) \Big). \tag{54}$$

This completes the proof of Theorem 4. □

8. Acknowledgments. We thank Pascal Lagerweij for having conducted the numerical experiment in Section 4.4.

Bibliography.

[1] P. W. Holland, K. B. Laskey, and S. Leinhardt. "Stochastic blockmodels: First steps". In: *Social networks* 5.2 (1983), pp. 109–137.

[2] D. A. Levin, Y. Peres, and E. L. Wilmer. *Markov Chains and Mixing Times*. en. American Mathematical Soc., 2009.

[3] R. S. Sutton and A. G. Barto. *Introduction to Reinforcement Learning*. 1st. Cambridge, MA, USA: MIT Press, 1998.

[4] S. P. Singh, T. Jaakkola, and M. I. Jordan. "Reinforcement Learning with Soft State Aggregation". In: *Advances in Neural Information Processing Systems 7*. Ed. by G. Tesauro, D. S. Touretzky, and T. K. Leen. MIT Press, 1995, pp. 361–368. URL: `http://papers.nips.cc/paper/981-reinforcement-learning-with-soft-state-aggregation.pdf`.

[5] R. Ortner. "Adaptive aggregation for reinforcement learning in average reward Markov decision processes". In: *Annals OR* 208.1 (2013), pp. 321–336.

[6] C. Gao, Z. Ma, A. Y. Zhang, and H. H. Zhou. "Achieving optimal misclassification proportion in stochastic block model". In: *arXiv preprint arXiv:1505.03772* (2015).

[7] A. Decelle, F. Krzakala, C. Moore, and L. Zdeborová. "Inference and phase transitions in the detection of modules in sparse networks". In: *Physical Review Letters* 107.6 (2011), p. 065701.

[8] L. Massoulié. "Community detection thresholds and the weak Ramanujan property". In: *Proceedings of the forty-sixth annual ACM symposium on Theory of computing*. ACM. 2014, pp. 694–703.

[9] E. Mossel, J. Neeman, and A. Sly. "Reconstruction and estimation in the planted partition model". In: *Probability Theory and Related Fields* 162.3-4 (2015), pp. 431–461.

[10] S.-Y. Yun and A. Proutiere. "Community Detection via Random and Adaptive Sampling." In: *COLT*. 2014, pp. 138–175.

[11] S.-Y. Yun and A. Proutiere. "Optimal cluster recovery in the labeled stochastic block model". In: *Advances in Neural Information Processing Systems*. 2016, pp. 965–973.

[12] S.-Y. Yun and A. Proutiere. "Accurate community detection in the stochastic block model via spectral algorithms". In: *arXiv preprint arXiv:1412.7335* (2014).

[13] E. Abbe and C. Sandon. "Community detection in general stochastic block models: Fundamental limits and efficient algorithms for recovery". In: *Foundations of Computer Science (FOCS), 2015 IEEE 56th Annual Symposium on*. IEEE. 2015, pp. 670–688.

[14] E. Abbe and C. Sandon. "Recovering communities in the general stochastic block model without knowing the parameters". In: *Advances in neural information processing systems*. 2015, pp. 676–684.

[15] V. Jog and P.-L. Loh. "Information-theoretic bounds for exact recovery in weighted stochastic block models using the Renyi divergence". In: *arXiv preprint arXiv:1509.06418* (2015).

[16] E. Mossel, J. Neeman, and A. Sly. "Consistency thresholds for the planted bisection model". In: *Proceedings of the forty-seventh annual ACM symposium on Theory of computing*. ACM. 2015, pp. 69–75.

[17] E. Abbe, A. S. Bandeira, and G. Hall. "Exact recovery in the stochastic block model". In: *IEEE Transactions on Information Theory* 62.1 (2016), pp. 471–487.

[18] B. Hajek, Y. Wu, and J. Xu. "Achieving exact cluster recovery threshold via semidefinite programming". In: *IEEE Transactions on Information Theory* 62.5 (2016), pp. 2788–2797.

[19] T. Lai and H. Robbins. "Asymptotically efficient adaptive allocation rules". In: *Advances in Applied Mathematics* 6.1 (1985), pp. 4 –22. DOI: https://doi.org/10.1016/0196-8858(85)90002-8. URL: http://www.sciencedirect.com/science/article/pii/0196885885900028.

[20] S. Lloyd. "Least squares quantization in PCM". In: *IEEE transactions on information theory* 28.2 (1982), pp. 129–137.

[21] P. Bremaud. *Markov Chains: Gibbs Fields, Monte Carlo Simulation, and Queues*. en. Springer, May 1999.

[22] N. Halko, P. G. Martinsson, and J. A. Tropp. "Finding Structure with Randomness: Probabilistic Algorithms for Constructing Approximate Matrix Decompositions". In: *SIAM Review* 53.2 (2011), pp. 217–288. DOI: 10.1137/090771806. URL: http://dx.doi.org/10.1137/090771806.

[23] E. P. Wigner. "On the distribution of the roots of certain symmetric matrices". In: *Annals of Mathematics* (1958), pp. 325–327.

[24] T. Tao. *Topics in random matrix theory*. Vol. 132. American Mathematical Society Providence, RI, 2012.

[25] J. A. Tropp et al. "An introduction to matrix concentration inequalities". In: *Foundations and Trends® in Machine Learning* 8.1-2 (2015), pp. 1–230.

[26] W. Hochstättler, W. Kirsch, and S. Warzel. "Semicircle law for a matrix ensemble with dependent entries". In: *Journal of Theoretical Probability* 29.3 (2016), pp. 1047–1068.

[27] W. Kirsch and T. Kriecherbauer. "Sixty years of moments for random matrices". In: *arXiv preprint arXiv:1612.06725* (2016).

[28] W. Kirsch and T. Kriecherbauer. "Semicircle law for generalized Curie-Weiss matrix ensembles at subcritical temperature". In: *arXiv preprint arXiv:1703.05183* (2017).

[29] C. Bordenave, P. Caputo, and D. Chafai. "Spectrum of large random reversible Markov chains: two examples". In: *ALEA: Latin American Journal of Probability and Mathematical Statistics* 7 (2010), pp. 41–64.

[30] C. Bordenave, P. Caputo, D. Chafai, et al. "Spectrum of large random reversible Markov chains: heavy-tailed weights on the complete graph". In: *The Annals of Probability* 39.4 (2011), pp. 1544–1590.

[31] U. Feige and E. Ofek. "Spectral techniques applied to sparse random graphs". In: *Random Structures & Algorithms* 27.2 (2005), pp. 251–275.

[32] D. Paulin. "Concentration inequalities for Markov chains by Marton couplings and spectral methods". In: *Electron. J. Probab.* 20 (2015), 32 pp. DOI: 10.1214/EJP.v20-4039. URL: https://doi.org/10.1214/EJP.v20-4039.

SUPPLEMENTARY MATERIAL

SM1. Concentration inequalities for BMCs. Recall the notation $\hat{N}_{\mathcal{A},\mathcal{B}} = \sum_{x\in\mathcal{A}}\sum_{y\in\mathcal{B}} \hat{N}_{x,y}$ for any subsets $\mathcal{A},\mathcal{B} \subseteq \mathcal{V}$.

PROPOSITION 8. *For $k = 1, \dots, K$,*

$$\mathbb{P}[|\hat{N}_{\mathcal{V},\mathcal{V}_k} - N_{\mathcal{V},\mathcal{V}_k}| \geq c_1\sqrt{T\ln n}] \leq \frac{1}{n^2}. \tag{55}$$

For $x \in \mathcal{V}$,

$$\mathbb{P}\Big[\Big|\hat{N}_{\mathcal{V},x} - N_{\mathcal{V},x}\Big| \geq c_2\frac{T}{n}\ln\frac{T}{n}\Big] \leq \mathrm{e}^{-2\frac{T}{n}\ln\frac{T}{n}},$$

$$\mathbb{P}\Big[\Big|\hat{N}_{\mathcal{V},x} - N_{\mathcal{V},x}\Big| \geq c_2\sqrt{\frac{T}{n}}\ln n\Big] \leq \frac{1}{n^2}, \tag{56}$$

and hence $\max_{y,z\in\mathcal{V}_k}|\hat{N}_{\mathcal{V},y} - \hat{N}_{\mathcal{V},z}| = O_{\mathbb{P}}(\sqrt{(T/n)}\ln n)$.

For any subset $\mathcal{S} \subset \mathcal{V}$ of size $|\mathcal{S}| = \lfloor n\exp\left(-(T/n)\ln(T/n)\right)\rfloor$,

$$\mathbb{P}[|\hat{N}_{\mathcal{V},\mathcal{S}} - N_{\mathcal{V},\mathcal{S}}| \geq c_3 n] \leq \mathrm{e}^{-4n}. \tag{57}$$

For any $i, j \in \{1, \dots, K\}$,

$$\mathbb{P}\Big[\Big|\sum_{t=1}^{T} f(\tilde{X}_t) - \mathbb{E}_\pi(f(\tilde{X}_t))\Big| \geq \frac{1}{2}\frac{T}{n}I(\alpha,p)\Big] \leq \mathrm{e}^{-c_5\frac{T}{n}I(\alpha,p)} \tag{58}$$

with $I(\alpha,p)$ as in (10)*, and* $f(\tilde{X}_t) = \sum_{k=1}^{K}(\mathbb{1}[X_{t-1} = x, X_t \in \mathcal{V}_k]\ln(p_{i,k}/p_{j,k}) + \mathbb{1}[X_{t-1} \in \mathcal{V}_k, X_t = x]\ln((p_{k,i}\alpha_j)/(p_{k,j}\alpha_i))) + (1/n)(\mathbb{1}[X_{t-1} \in \mathcal{V}_j]/\alpha_j - \mathbb{1}[X_{t-1} \in \mathcal{V}_i]/\alpha_i)$.

The concentration inequalities in Proposition 8 can all be shown using [32, Thm. 3.10], which we reproduce here for your convenience:

THEOREM 5 (Daniel Paulin, 2015). *Let $f \in L^2(\pi)$ with $|f(x) - \mathbb{E}_\pi(f)| \leq C$ for every $x \in \Omega$. Let V_f be the variance of $f(X)$ when X follows the stationary distribution π. Then,*

$$\mathbb{P}_\pi\Big[\Big|\sum_{t=1}^{T} f(X_t) - \mathbb{E}_\pi\Big[\sum_{t=1}^{T} f(X_t)\Big]\Big| \geq x\Big] \leq 2\exp\Big(-\frac{x^2\gamma_{ps}}{8(T+1/\gamma_{ps})V_f + 20xC}\Big). \tag{59}$$

In order to be able to apply Theorem 5, we also utilize [32, Prop. 3.4], which states that the pseudo spectral gap satisfies

(60)
$$\gamma_{\text{ps}} \triangleq \max_{i \geq 1} \frac{1 - \lambda\big((P^*)^i P^i\big)}{i} \geq \frac{1 - \varepsilon}{t_{\text{mix}}(\varepsilon)} \quad \text{with} \quad P^*(x, y) \triangleq \frac{P(x, y)}{\Pi(x)} \Pi(y).$$

Next it is important to note that Proposition 2 also holds for the Markov chain induced by the *transitions* of the BMC. To see this, define $\tilde{X}_t \triangleq (X_{t-1}, X_t)$ such that $\{\tilde{X}_t\}_{t \geq 0}$ denotes a Markov process describing the transitions of $\{X_t\}_{t \geq 0}$. Let $\tilde{P}$ and $\tilde{\Pi}$ be the transition kernel and the stationary distribution of $\tilde{X}_t$, respectively. Note now that $d_{\text{TV}}(P^t_{x,\cdot}, \Pi) = d_{\text{TV}}(\tilde{P}^t_{(y,x),\cdot}, \tilde{\Pi})$ for all $x, y \in \mathcal{V}$, $t \in \mathbb{N}_+$ and $r \in [1, \infty)$. Both processes $\{\tilde{X}_t\}_{t \geq 0}$ and $\{X_t\}_{t \geq 0}$ therefore share the same mixing time. As a consequence of Proposition 2, we have for both of our Markov processes $\{X_t\}_{t \geq 0}$, $\{\tilde{X}_t\}_{t \geq 0}$ that $\gamma_{ps} \geq 1/(2c_{\mathtt{mix}} \ln(2))$.

Example 1. Let $f(X_t) = \mathbb{1}[X_t \in \mathcal{V}_k]$ such that $\sum_{t=1}^T f(X_t) = \hat{N}_{\mathcal{V}, \mathcal{V}_k}$ and $V_f \leq \pi_k$. From Theorem 5, there exists a constant c_1 such that

$$\mathbb{P}[|\hat{N}_{\mathcal{V}, \mathcal{V}_k} - N_{\mathcal{V}, \mathcal{V}_k}| \geq c_1 \sqrt{T \ln n}] \leq \frac{1}{n^2}. \tag{61}$$

Example 2. Let $f(X_t) = \mathbb{1}[X_t = x]$ such that $\sum_{t=1}^T f(X_t) = \hat{N}_{\mathcal{V}, x}$ and $V_f \leq \pi_k / \alpha_k n$. From Theorem 5, it follows that there exists a constant c_2 such that

$$\mathbb{P}\Big[\Big|\hat{N}_{\mathcal{V}, x} - N_{\mathcal{V}, x}\Big| \geq c_2 \frac{T}{n} \ln \frac{T}{n}\Big] \leq \exp\Big(-2 \frac{T}{n} \ln \frac{T}{n}\Big) \tag{62}$$

and

$$\mathbb{P}\Big[\Big|\hat{N}_{\mathcal{V}, x} - N_{\mathcal{V}, x}\Big| \geq c_2 \sqrt{\frac{T}{n}} \ln n\Big] \leq \frac{1}{n^2}. \tag{63}$$

From the union bound, it follows that for $k \in \{1, \ldots, K\}$,

$$\max_{y, z \in \mathcal{V}_k} |\hat{N}_{\mathcal{V}, y} - \hat{N}_{\mathcal{V}, z}| = O_{\mathbb{P}}\Big(\sqrt{\frac{T}{n}} \ln n\Big). \tag{64}$$

Example 3. Consider any set $\mathcal{S} \subset \mathcal{V}$ with $|S| = \lfloor n \exp(-\frac{T}{n} \ln \frac{T}{n}) \rfloor$. Let $f(X_t) = \mathbb{1}[X_t \in \mathcal{S}]$ such that $\sum_{t=1}^T f(X_t) = \hat{N}_{\mathcal{V}, S}$ and $V_f = O(\exp(-\frac{T}{n} \ln \frac{T}{n}))$. Use Theorem 5 to conclude that there exists a constant c_3 such that

$$\mathbb{P}\Big[\Big|\hat{N}_{\mathcal{V}, \mathcal{S}} - N_{\mathcal{V}, \mathcal{S}}\Big| \geq c_3 n\Big] \leq \exp(-4n). \tag{65}$$

Example 4. Consider $f(\tilde{X}_t) = \sum_{k=1}^K (\mathbb{1}[X_{t-1} = x, X_t \in \mathcal{V}_k] \ln(p_{i,k}/p_{j,k}) + \mathbb{1}[X_{t-1} \in \mathcal{V}_k, X_t = x] \ln((p_{k,i}\alpha_j)/(p_{k,j}\alpha_i))) + (1/n)(\mathbb{1}[X_{t-1} \in \mathcal{V}_j]/\alpha_j - \mathbb{1}[X_{t-1} \in \mathcal{V}_i]/\alpha_i)$ such that $V_f = O(1/n)$. It follows from Theorem 5 that there exists a constant $c_4 > 0$ such that

$$\mathbb{P}\Big[\Big|\sum_{t=1}^T f(\tilde{X}_t) - \mathbb{E}_\pi(f(\tilde{X}_t))\Big| \geq \frac{1}{2}\frac{T}{n} I(\alpha, p)\Big] \leq \exp\Big(-c_4 \frac{T}{n} I(\alpha, p)\Big). \tag{66}$$

Example 5. Consider any set $\mathcal{A}, \mathcal{B} \subset \mathcal{V}$ and consider $f(\tilde{X}_t) = \mathbb{1}[X_{t-1} \in \mathcal{A}_a, X_t \in \mathcal{B}_b]$. For this function, $V_f = O(1)$. It follows from Theorem 5 that there exists a constant $c_5 > 0$ such that

$$\mathbb{P}\Big[\Big|\hat{N}_{\mathcal{A},\mathcal{B}} - N_{\mathcal{A},\mathcal{B}}\Big| \geq c_5\sqrt{nT}\Big] \leq \exp(-4n).$$

Since $\mathcal{V}$ has 2^n subsets, with probability $1 - \exp(-(4 - \ln 4)n)$,

$$\max_{\mathcal{A},\mathcal{B}} \Big|\hat{N}_{\mathcal{A},\mathcal{B}} - N_{\mathcal{A},\mathcal{B}}\Big| \leq c_5\sqrt{nT}. \tag{67}$$

SM2. Proofs of Chapter 2.

SM2.1. *Proof of Proposition 1.*

PROOF. We first prove that π is a probability distribution. This follows by (i) definition of π, (ii) symmetry of all states in the same cluster, and (iii) because Π is a probability distribution:

$$\sum_{k=1}^K \pi_k \overset{\text{(i)}}{=} \sum_{k=1}^K \lim_{n\to\infty} \bar{\Pi}_k |\mathcal{V}_k| \overset{\text{(ii)}}{=} \lim_{n\to\infty} \sum_{k=1}^K \sum_{x\in\mathcal{V}_k} \Pi_x = \lim_{n\to\infty} \sum_{x\in\mathcal{V}} \Pi_x \overset{\text{(iii)}}{=} 1. \tag{68}$$

Next, we show that the balance equations hold. For $k = 1, \ldots, K$ it follows by symmetry of any two states $x, z \in \mathcal{V}_k$ that $\Pi_x = \Pi_z = \bar{\Pi}_k$. Hence for any $y \in \mathcal{V}_l$, by (iv) global balance

$$\Pi_y = \bar{\Pi}_l \overset{\text{(iv)}}{=} \sum_{k=1}^K \sum_{x\in\mathcal{V}_k} \Pi_x P_{x,y} = \sum_{k=1}^K \bar{\Pi}_k (|\mathcal{V}_k| - \mathbb{1}[k = l]) \frac{p_{k,l}}{|\mathcal{V}_l| - \mathbb{1}[k = l]}. \tag{69}$$

Letting $n \to \infty$, we find that $\pi_l = \sum_{k=1}^K \pi_k p_{k,l}$ for all k, l. This completes the proof. $\square$

SM2.2. *Proof of Proposition 2.*

PROOF. We will use Dobrushin's ergodic coefficient, which is defined for any stochastic matrix P by [21, Definition 7.1]

$$\delta(P) \triangleq \tfrac{1}{2} \sup_{x,y\in\mathcal{V}} \sum_{z\in\mathcal{V}} |P_{x,z} - P_{y,z}|. \tag{70}$$

Moreover, Dobrushin's coefficient satisfies $\delta(P) = 1 - \inf_{x,y\in\mathcal{V}} \sum_{z\in\mathcal{V}} (P_{x,z} \wedge P_{y,z})$, see [21, Eq. (7.3)]. Recalling our assumption $\exists_{0<\eta\neq 1} : \max_{a,b,c}\{p_{b,a}/p_{c,a}, p_{a,b}/p_{a,c}\} \leq \eta$, this implies that $\delta(P) < 1$ strictly.

Next [21, Thm. 7.2] gives us the convergence rate in terms of Dobrushin's coefficient. Specifically,

$$d_{\mathrm{TV}}(P^t_{x,\cdot}, \Pi) \leq \big(\delta(P)\big)^t d_{\mathrm{TV}}(P^0_{x,\cdot}, \Pi) \quad \text{for} \quad x \in \mathcal{V}. \tag{71}$$

As a consequence

$$d_{\mathrm{TV}}(P^t_{x,\cdot}, \Pi) \leq \varepsilon \quad \text{whenever} \quad t \geq \frac{\ln \varepsilon}{\ln\big(\delta(P)\big)}. \tag{72}$$

This completes the proof. □

SM3. Proofs of Chapter 5.

SM3.1. *Proof of Proposition 3.*

PROOF. Select a state V^* uniformly at random from any two specific clusters $a, b \in \{1, \ldots, K\}$, $a \neq b$. We are going to bound

$$\mathbb{P}_\Psi[L \leq f(n,T)] = \mathbb{P}_\Psi[L \leq f(n,T), V^* \in \mathcal{E}] + \mathbb{P}_\Psi[L \leq f(n,T), V^* \notin \mathcal{E}]. \tag{73}$$

for any function $f : \mathbb{N}^2_+ \to \mathbb{R}$.

The first term of (73) can be bounded using our change of measure formula (26). Namely,

$$\begin{aligned} \mathbb{P}_\Psi[L \leq f(n,T), V^* \in \mathcal{E}] &\overset{(26)}{\leq} \mathrm{e}^{f(n,T)} \mathbb{P}_\Phi[L \leq f(n,T), V^* \in \mathcal{E}] \\ &\leq \mathrm{e}^{f(n,T)} \mathbb{P}_\Phi[V^* \in \mathcal{E}]. \end{aligned} \tag{74}$$

Because V^* is selected from $\mathcal{V}_a \cup \mathcal{V}_b$ uniformly at random, we have by Lemma 11, see §SM6.1, that for any V selected uniformly at random from *all* vertices $\mathcal{V}$,

$$\mathbb{P}_\Phi[V^* \in \mathcal{E}] = \mathbb{P}_\Phi[V \in \mathcal{E} | V \in \mathcal{V}_a \cup \mathcal{V}_b] = \frac{\mathbb{P}_\Phi[V \in \mathcal{E}, V \in \mathcal{V}_a \cup \mathcal{V}_b]}{\mathbb{P}_\Phi[V \in \mathcal{V}_a \cup \mathcal{V}_b]} \leq \frac{\mathbb{P}_\Phi[V \in \mathcal{E}]}{\alpha_a + \alpha_b}. \tag{75}$$

Subsequently by Lemma 12, see §SM6.1,

$$\mathbb{P}_\Phi[V^* \in \mathcal{E}] \leq \frac{\mathbb{E}_\Phi[|\mathcal{E}|]}{(\alpha_a + \alpha_b)n}. \tag{76}$$

Substituting (76) into (74), we obtain

$$\mathbb{P}_\Psi[L \leq f(n,T), V^* \in \mathcal{E}] \leq \mathrm{e}^{f(n,T)} \frac{\mathbb{E}_\Phi[|\mathcal{E}|]}{(\alpha_a + \alpha_b)n}. \tag{77}$$

The second term of (73) can be bounded using Assumption (28):

$$\mathbb{P}_\Psi[L \leq f(n,T), V^* \notin \mathcal{E}] \leq \mathbb{P}_\Psi[V^* \notin \mathcal{E}] = 1 - \mathbb{P}_\Psi[V^* \in \mathcal{E}] \leq 1 - \delta < 1. \tag{78}$$

Now using (77) and (78) to bound (73), we arrive at

$$\mathbb{P}_\Psi[L \leq f(n,T)] \leq \mathrm{e}^{f(n,T)} \frac{\mathbb{E}_\Phi[|\mathcal{E}|]}{(\alpha_a + \alpha_b)n} + 1 - \delta \tag{79}$$

with $\delta > 0$. This strict separation will become important in a moment.

We now prepare for an application of Chebyshev's inequality. First note using (79) that

$$\mathbb{P}_\Psi[L \geq f(n,T)] = 1 - \mathbb{P}_\Psi[L \leq f(n,T)] \geq \delta - \mathrm{e}^{f(n,T)} \frac{\mathbb{E}_\Phi[|\mathcal{E}|]}{(\alpha_a + \alpha_b)n}. \tag{80}$$

Specify $f(n,T) = \ln(\delta/2) + \ln((\alpha_a + \alpha_b)n / \mathbb{E}_\Phi[|\mathcal{E}|])$, so that

$$\mathbb{P}_\Psi\Big[L \geq \ln \frac{\delta}{2} + \ln \frac{(\alpha_a + \alpha_b)n}{\mathbb{E}_\Phi[|\mathcal{E}|]}\Big] \geq \frac{\delta}{2}. \tag{81}$$

Since $\delta > 0$, we can apply (i) Chebyshev's inequality and (ii) Eq. (80) to conclude

$$\mathbb{P}_\Psi\Big[L \geq \mathbb{E}_\Psi[L] + \sqrt{\frac{2}{\delta}}\sqrt{\mathrm{Var}_\Psi[L]}\Big] \overset{\text{(i)}}{\leq} \frac{\delta}{2} \overset{\text{(ii)}}{\leq} \mathbb{P}_\Psi\Big[L \geq \ln \frac{\delta}{2} + \ln \frac{(\alpha_a + \alpha_b)n}{\mathbb{E}_\Phi[|\mathcal{E}|]}\Big]. \tag{82}$$

Comparing the events in the left member and the right member, we then must have

$$\ln \frac{\delta}{2} + \ln \frac{(\alpha_a + \alpha_b)n}{\mathbb{E}_\Phi[|\mathcal{E}|]} \leq \mathbb{E}_\Psi[L] + \sqrt{\frac{2}{\delta}}\sqrt{\mathrm{Var}_\Psi[L]}. \tag{83}$$

Rearranging gives (29) with $C = (\alpha_a + \alpha_b)\delta/2 > 0$. This completes the proof. □

SM3.2. *Q is a stochastic matrix.* To see this, observe that for $x \in \mathcal{V}\backslash\{V^*\}$,

$$\sum_{y\in\mathcal{V}} Q_{x,y} = \frac{q_{\omega(x),0}}{n} + \sum_{y\in\mathcal{W}_{\omega(x)}\backslash\{x\}} \frac{q_{\omega(x),\omega(x)}}{|\mathcal{W}_{\omega(x)}|-1} + \sum_{k=1}^{K} \mathbb{1}[k\neq\omega(x)] \sum_{y\in\mathcal{W}_k} \frac{q_{\omega(x),k}}{|\mathcal{W}_k|}$$

$$= \frac{q_{\omega(x),0}}{n} + \sum_{k=1}^{K} q_{\omega(x),k} \overset{(30)}{=} \frac{q_{\omega(x),0}}{n} + \sum_{k=1}^{K}\Big(p_{\omega(x),k} - \frac{q_{\omega(x),0}}{Kn}\Big) = 1. \tag{84}$$

Similarly for $x = V^*$

$$\sum_{y\in\mathcal{V}} Q_{V^*,y} = \sum_{k=1}^{K}\sum_{y\in\mathcal{W}_k} \frac{q_{0,k}}{|\mathcal{W}_k|} = \sum_{k=1}^{K} q_{0,k} \overset{(25)}{=} 1. \tag{85}$$

SM3.3. *Proof of Proposition 4.*

PROOF. We first show that $(\gamma_1^{[0]},\dots,\gamma_K^{[0]},\gamma_0^{[0]})$ is a probability distribution. Since (i) $\Pi^{(Q)}$ is a probability distribution

$$\sum_{k=1}^{K}\gamma_k + \gamma_0 = \lim_{n\to\infty}\Big(\sum_{k=1}^{K}|\mathcal{W}_k|\bar{\Pi}_k^{(Q)} + \Pi_{V^*}^{(Q)}\Big) = \lim_{n\to\infty}\Big(\sum_{k=1}^{K}\sum_{x\in\mathcal{W}_k}\Pi_x^{(Q)} + \Pi_{V^*}^{(Q)}\Big)$$

$$= \lim_{n\to\infty}\sum_{x\in\mathcal{V}}\Pi_x^{(Q)} \overset{\text{(i)}}{=} 1. \tag{86}$$

Next we show that (ii) by the global balance equations for $\Pi^{(Q)}$

$$\gamma_0^{[0]} = \lim_{n\to\infty}\Pi_{V^*}^{(Q)} \overset{\text{(ii)}}{=} \lim_{n\to\infty}\sum_{x\in\mathcal{V}}\Pi_x^{(Q)}Q_{x,V^*} \overset{(31)}{=} \lim_{n\to\infty}\sum_{k=1}^{K}\sum_{x\in\mathcal{W}_k}\bar{\Pi}_k^{(Q)}\frac{q_{k,0}}{n}$$

$$= \lim_{n\to\infty}\sum_{k=1}^{K}\gamma_k^{[0]}\frac{q_{k,0}}{n} = 0. \tag{87}$$

Now we establish that the vector $(\gamma_1^{[0]},\dots,\gamma_K^{[0]})^{\mathrm{T}}$ satisfies the balance equations $(\gamma_1^{[0]},\dots,\gamma_K^{[0]})p = (\gamma_1^{[0]},\dots,\gamma_K^{[0]})$. For $l = 1,\dots,K$

$$\gamma_l^{[0]} = \lim_{n\to\infty}|\mathcal{W}_l|\bar{\Pi}_l^{(Q)} = \lim_{n\to\infty}\sum_{y\in\mathcal{W}_l}\Pi_y^{(Q)} \overset{\text{(ii)}}{=} \lim_{n\to\infty}\sum_{y\in\mathcal{W}_l}\sum_{x\in\mathcal{V}}\Pi_x^{(Q)}Q_{x,y} \tag{88}$$

$$\overset{(31)}{=} \lim_{n\to\infty}\sum_{y\in\mathcal{W}_l}\Big(\sum_{k=1}^{K}\sum_{x\in\mathcal{W}_k\backslash\{y\}}\bar{\Pi}_k^{(Q)}\frac{q_{k,l}}{|\mathcal{W}_l|-\mathbb{1}[k=l]} + \Pi_{V^*}^{(Q)}\frac{q_{0,l}}{|\mathcal{W}_l|}\Big)$$

$$= \lim_{n\to\infty}\Big(\sum_{k=1}^{K}(|\mathcal{W}_k| - \mathbb{1}[k=l])\bar{\Pi}_k^{(Q)}\frac{|\mathcal{W}_l|}{|\mathcal{W}_l| - \mathbb{1}[k=l]}q_{k,l} + \Pi_{V^*}^{(Q)}q_{0,l}\Big)$$
$$\overset{(30)}{=} \sum_{k=1}^{K}\gamma_k^{[0]}p_{k,l},$$

where we also recalled (33). This proves the first two assertions.

The third assertion follows from (87) when multiplying the intermediate steps by n, i.e.,

$$\gamma_0^{[1]} \overset{(87)}{=} \lim_{n\to\infty} n\sum_{k=1}^{K}\gamma_k^{[0]}q_{k,0}\frac{1}{n} = \sum_{k=1}^{K}\gamma_k^{[0]}q_{k,0}. \tag{89}$$

Together with the first assertion, this completes the proof. □

SM3.4. *Proof of Proposition 5.*

PROOF. Define $R_{x,y} \triangleq \ln(Q_{x,y}/P_{x,y})$ for notational convenience: we refer to §SM6.2 for its asymptotic behavior. Since the Markov chain is started from equilibrium,

$$\mathbb{E}_Q[L|\sigma(V^*)] = T\sum_{x\in\mathcal{V}}\sum_{y\in\mathcal{V}}\Pi_x^{(Q)}Q_{x,y}\ln R_{x,y}. \tag{90}$$

The largest individual contributions to the expectation in (90) are by jumps to and from V^*, since this is where the change of measure is modified most. Jumps not involving V^* contribute less individually, but there are many of such jumps. We therefore separate out the jumps to and from V^*, i.e.,

$$\begin{aligned}\frac{\mathbb{E}_Q[L|\sigma(V^*)]}{T} &= \sum_{y\neq V^*}\Pi_{V^*}^{(Q)}Q_{V^*,y}\ln R_{V^*,y} + \sum_{x\neq V^*}\Pi_x^{(Q)}Q_{x,V^*}\ln R_{x,V^*}\\ &\quad+\sum_{x,y\neq V^*}\Pi_x^{(Q)}Q_{x,y}\ln R_{x,y}.\end{aligned} \tag{91}$$

We now calculate the leading order behavior of each term.

For the first term in (91) we have by (i) Lemma 13 in §SM6.2 and Q's definition, see (31), and (ii) Proposition 4,

$$\begin{aligned}\sum_{y\neq V^*}\Pi_{V^*}^{(Q)}Q_{V^*,y}\ln R_{V^*,y} &\overset{(i)}{\sim} \sum_{k=1}^{K}\sum_{y\in\mathcal{W}_k}\Pi_{V^*}^{(Q)}\frac{q_{0,k}}{|\mathcal{W}_k|}\ln\frac{q_{0,\omega(y)}}{p_{\sigma(V^*),\omega(y)}}\\ &\overset{(ii)}{\sim} \frac{1}{n}\sum_{k=1}^{K}\gamma_0^{[1]}q_{0,k}\ln\frac{q_{0,k}}{p_{\sigma(V^*),k}}.\end{aligned} \tag{92}$$

The second term in (91) handles similarly:

$$\sum_{x\neq V^*} \Pi_x^{(Q)} Q_{x,V^*} \ln R_{x,V^*} \overset{\text{(i)}}{\sim} \sum_{k=1}^{K} \sum_{x\in\mathcal{W}_k\setminus\{V^*\}} \bar{\Pi}_k^{(Q)} \frac{q_{k,0}}{n} \ln \frac{q_{k,0}\alpha_{\sigma(V^*)}}{p_{k,\sigma(V^*)}}$$

$$\overset{\text{(ii)}}{\sim} \frac{1}{n} \sum_{k=1}^{K} \gamma_k^{[0]} q_{k,0} \ln \frac{q_{k,0}\alpha_{\sigma(V^*)}}{p_{k,\sigma(V^*)}}. \tag{93}$$

The third term in (91) requires (iii) a Taylor expansion of $\ln(1+x) = x + O(x^2)$ for $x \approx 0$ and (iv) the balance equations (88)–(89), so that

$$\sum_{x,y\neq V^*} \Pi_x^{(Q)} Q_{x,y} \ln R_{x,y} \overset{\text{(iii)}}{\sim} \sum_{k,l\neq 0} \sum_{x\in\mathcal{W}_k} \sum_{y\in\mathcal{W}_l\setminus\{x\}} \bar{\Pi}_k^{(Q)} \frac{q_{k,l}}{|\mathcal{W}_l| - \mathbb{1}[k=l]} \times$$

$$\cdots \times \frac{1}{n}\Big(\frac{\mathbb{1}[l=\sigma(V^*)]}{\alpha_l} - \frac{q_{k,0}}{p_{k,l}K}\Big) \overset{(30)}{\sim} \frac{1}{n}\sum_{k=1}^{K} \gamma_k^{[0]} \Big(\frac{q_{k,\sigma(V^*)}}{\alpha_{\sigma(V^*)}} - \sum_{l=1}^{K} \frac{1}{K} q_{k,0}\Big)$$

$$\overset{\text{(iv)}}{=} \frac{1}{n}\Big(\frac{\gamma_{\sigma(V^*)}^{[0]}}{\alpha_{\sigma(V^*)}} - \gamma_0^{[1]}\Big). \tag{94}$$

Substituting (92)–(94) into (91) gives

$$\mathbb{E}_Q[L|\sigma(V^*)] \sim \frac{T}{n} \sum_{k=1}^{K} \Big(\gamma_0^{[1]} q_{0,k} \ln \frac{q_{0,k}}{p_{\sigma(V^*),k}} + \gamma_k^{[0]} q_{k,0} \ln \frac{q_{k,0}\alpha_{\sigma(V^*)}}{p_{k,\sigma(V^*)}}\Big)$$

$$+ \frac{T}{n}\Big(\frac{\gamma_{\sigma(V^*)}^{[0]}}{\alpha_{\sigma(V^*)}} - \gamma_0^{[1]}\Big). \tag{95}$$

By now applying Proposition 4, we complete the proof. □

SM3.5. *Proof of Proposition 6.*

PROOF. Define $L_t \triangleq \ln(Q_{X_{t-1},X_t}/P_{X_{t-1},X_t})$. Expanding, we obtain

$$\mathrm{Var}_Q[L|\sigma(V^*)] = \mathrm{Var}_Q\Big[\sum_{t=1}^{T} L_t \Big| \sigma(V^*)\Big] = \sum_{t=1}^{T}\sum_{s=1}^{T} \mathrm{Cov}_Q[L_t, L_s|\sigma(V^*)]. \tag{96}$$

We now consider the cases $|t-s| \geq 2$ and $|t-s| \leq 1$, in that order. The idea is that we bound relatively crudely in the latter cases since there are only $O(T)$ such terms that contribute to the sum, and the former cases more sharply. Applying one rough bound on all terms of the former cases would not suffice, because there are as many as $O(T^2)$ such terms. As we will show for the former cases, we can derive a sharper bound when $|t-s| \gg t_{\mathrm{mix}}(\varepsilon)$ because Proposition 2 implies that the covariances decay quickly.

First note that because (i) the process is started from equilibrium, we have for any $t, s \in \{1, \dots, T\}$ that

$$\begin{aligned} \mathrm{Cov}_Q[L_t, L_s|\sigma(V^*)] &= \mathbb{E}_Q[L_t L_s|\sigma(V^*)] - \mathbb{E}_Q[L_t|\sigma(V^*)]\mathbb{E}_Q[L_s|\sigma(V^*)] \\ &\overset{\text{(i)}}{=} \mathbb{E}_Q[L_t L_s|\sigma(V^*)] - \mathbb{E}_Q[L_t|\sigma(V^*)]^2. \end{aligned} \tag{97}$$

Now consider the case $|t-s| \geq 2$. Define $S_{x,y,u,v} \triangleq (\ln R_{x,y})(\ln R_{u,v})$ for notational convenience: we refer to §SM6.2 for its asymptotic behavior. In this case the first term of (97) evaluates as

$$\begin{aligned} &\mathbb{E}_Q[L_t L_s|\sigma(V^*)] \\ &= \sum_{x,y,u,v} \mathbb{P}_Q[X_{t\wedge s-1} = x, X_{t\wedge s} = y, X_{t\vee s-1} = u, X_{t\vee s} = v|\sigma(V^*)] S_{x,y,u,v} \\ &= \sum_{x,y,u,v} \Pi_x^{(Q)} Q_{x,y} \Big(\sum_{z_{t\wedge s+1},\dots,z_{t\vee s-2}} Q_{y,z_{t\wedge s+1}} Q_{z_{t\wedge s+2},z_{t\wedge s+2}} \cdots Q_{z_{t\vee s-2},u} \Big) Q_{u,v} S_{x,y,u,v} \end{aligned} \tag{98}$$

$$= \sum_{x,y,u,v} \Pi_x^{(Q)} Q_{x,y} Q_{y,u}^{|t-s|-1} Q_{u,v} S_{x,y,u,v}. \tag{99}$$

The second term of (97) expands as

$$\mathbb{E}_Q[L_t|\sigma(V^*)]^2 = \Big(\sum_{x,y} \Pi_x^{(Q)} Q_{x,y} \ln \frac{Q_{x,y}}{P_{x,y}} \Big)^2 = \sum_{x,y,u,v} \Pi_x^{(Q)} Q_{x,y} \Pi_u^{(Q)} Q_{u,v} S_{x,y,u,v}. \tag{100}$$

Substituting (98) and (100) into the last member of (97) gives

$$\mathrm{Cov}_Q[L_t, L_s|\sigma(V^*)] = \sum_{x,y,u,v} \Pi_x^{(Q)} Q_{x,y} (Q_{y,u}^{|t-s|-1} - \Pi_u^{(Q)}) Q_{u,v} S_{x,y,u,v}. \tag{101}$$

In order to bound (101), we need to take two effects into consideration: a filter effect that happens because the transition matrix Q is similar to the transition matrix P, and a concentration effect because the Markov chain moves closer to equilibrium as time progresses. The filter effect is quantified by Corollary 1 in §SM6.2, because the latter implies that $\sum_{x,y,u,v} S_{x,y,u,v} \leq c_1 n^2$ for some absolute constant c_1 (even though $\sum_{x,y,u,v} 1 = n^4$). We can use the effect by for example bounding $\Pi_x^{(Q)} Q_{x,y} (Q_{y,u}^m - \Pi_u^{(Q)}) Q_{u,v} \leq c_2/n^4$ uniformly using another absolute constant, and then concluding that $\mathrm{Cov}_Q[L_t, L_s|\sigma(V^*)] \leq$

$c_2(T^2/n^4)\sum_{x,y,u,v} S_{x,y,u,v} \le c_1c_2T^2/n^2$. However, this bound is not sufficiently sharp for our purposes: we need to provide a bound that is at least $o(T^2/n^2)$.

To arrive at a sharper bound, we use the concentration of the Markov chain. Apply the triangle inequality first, and then bound $\Pi_x^{(Q)}Q_{x,y}Q_{u,v} \le c_1/n^3$ uniformly using an absolute constant c_1 to obtain

$$\begin{aligned}&\Big|\sum_{t=1}^T\sum_{s=1}^T \mathbb{1}[|t-s|\ge 2]\mathrm{Cov}_Q[L_t,L_s|\sigma(V^*)]\Big|\\ &\le \frac{2c_1}{n^3}\sum_{t=1}^T\sum_{s=t+2}^T\sum_{x,y,u,v}|Q_{y,u}^{|t-s|-1}-\Pi_u^{(Q)}||S_{x,y,u,v}|. \end{aligned} \tag{102}$$

Now let $m\in\mathbb{N}_+$. By nonnegativity of the summands and (6), $|Q_{x,y}^m-\Pi_y^{(Q)}| \le \sum_y |Q_{x,y}^m - \Pi_y^{(Q)}| = 2d_{\mathrm{TV}}(Q_{x,\cdot}^m,\Pi^{(Q)})$. Recall furthermore from (71) and (72) combined that there exists a $\delta(Q)\in(0,1)$ such that $d_{\mathrm{TV}}(Q_{u,\cdot}^m,\Pi)\le(\delta(Q))^m d_{\mathrm{TV}}(Q_{u,\cdot}^0,\Pi)$ for $u\in\mathcal{V}$. We therefore have that there exists an absolute constant c_3 such that

$$\begin{aligned}&\Big|\sum_{t=1}^T\sum_{s=1}^T \mathbb{1}[|t-s|\ge 2]\mathrm{Cov}_Q[L_t,L_s|\sigma(V^*)]\Big|\\ &\le \frac{4c_1c_2\max_{u\in\mathcal{V}}\{d_{\mathrm{TV}}(Q_{u,\cdot}^0,\Pi)\}}{n^3}\sum_{t=1}^T\sum_{s=t+2}^T\big(\delta(Q)\big)^{|t-s|-1}\sum_{x,y,u,v}|S_{x,y,u,v}|\\ &\overset{\text{(i)}}{\le} \frac{c_3}{n}\sum_{t=1}^T\sum_{s=t+2}^T\big(\delta(Q)\big)^{|t-s|-1}, \end{aligned} \tag{103}$$

due to (i) the filter effect. By a continuous extension of the sum,

$$\sum_{t=1}^T\sum_{s=t+2}^T\big(\delta(Q)\big)^{|t-s|-1} \le \int_0^T\int_{t+1}^T\big(\delta(Q)\big)^{|t-s|-1}\,\mathrm{d}s\,\mathrm{d}t \sim -\frac{T}{\ln\big(\delta(Q)\big)}. \tag{104}$$

Since $\delta(Q)\in(0,1)$, there thus exists an absolute constant $c_4>0$ such that

$$\Big|\sum_{t=1}^T\sum_{s=1}^T \mathbb{1}[|t-s|\ge 2]\mathrm{Cov}_Q[L_t,L_s|\sigma(V^*)]\Big| \le c_4\frac{T}{n}. \tag{105}$$

Lastly we deal with the cases $|t-s|\le 1$. When $|t-s|=0$, or equivalently $t=s$, we have that (iv) because of Lemma 13 and Corollary 1 that there exist absolute constants $c_5, \dots, c_8$ such that

$$
\begin{aligned}
&\mathrm{Cov}[L_t, L_t|\sigma(V^*)] \overset{(97)}{\leq} \mathbb{E}_Q[L_t^2|\sigma(V^*)] = \sum_{x\in\mathcal{V}}\sum_{y\in\mathcal{V}} \Pi_x^{(Q)} Q_{x,y}(\ln R_{x,y})^2 \\
&\overset{(\mathrm{iv})}{\leq} \Pi_{V^*}^{(Q)} \sum_{y\neq V^*} Q_{V^*,y} c_5 + \sum_{x\neq V^*} \Pi_x^{(Q)} Q_{x,V^*} c_6 + \sum_{x\neq V^*}\sum_{y\neq V^*} \Pi_x^{(Q)} Q_{x,y} \frac{c_7}{n^2} \leq \frac{c_8}{n}
\end{aligned}
\tag{106}
$$

for all $t = 1, \dots, T$. Therefore

$$
\Big|\sum_{t=1}^T\sum_{s=1}^T \mathbb{1}[|t-s|=0]\mathrm{Cov}_Q[L_t, L_s|\sigma(V^*)]\Big| = \sum_{t=1}^T \mathrm{Var}_Q[L_t|\sigma(V^*)] = O\Big(\frac{T}{n}\Big).
\tag{107}
$$

When $|t-s| = 1$, there exists an absolute constant $c_9 > 0$ such that

$$
\begin{aligned}
&\mathrm{Cov}_Q[L_{t\wedge s}, L_{t\wedge s+1}|\sigma(V^*)] \overset{(97)}{\leq} \mathbb{E}_Q[L_{t\wedge s}L_{t\wedge s+1}|\sigma(V^*)] \\
&\leq \sum_{x,y,z} \Pi_x^{(Q)} Q_{x,y} Q_{y,z} S_{x,y,y,z} \leq \frac{c_9}{n^3}\sum_{x,y,z} S_{x,y,y,z}.
\end{aligned}
\tag{108}
$$

Invoking Corollary 1's filter effect implies that $\sum_{x,y,z} S_{x,y,y,z} = O(n^2)$. Therefore

$$
\Big|\sum_{t=1}^T\sum_{s=1}^T \mathbb{1}[|t-s|=1]\mathrm{Cov}[L_t, L_s|\sigma(V^*)]\Big| \leq 2\sum_{t=1}^T |\mathrm{Cov}_Q[L_t, L_{t+1}|\sigma(V^*)]| = O\Big(\frac{T}{n}\Big).
\tag{109}
$$

Splitting (96) into the respective cases and then (v) substituting (105), (107), and (109) gives

$$
\begin{aligned}
&\mathrm{Var}_Q[L|\sigma(V^*)] \\
&= \sum_{t=1}^T\sum_{s=1}^T (\mathbb{1}[t=s] + \mathbb{1}[|t-s|=1] + \mathbb{1}[|t-s|\geq 2])\mathrm{Cov}_Q[L_t, L_s|\sigma(V^*)] \\
&\overset{(\mathrm{v})}{=} O\Big(\frac{T}{n}\Big),
\end{aligned}
\tag{110}
$$

which completes the proof. □

SM3.6. *Proof of Lemma 1.*

PROOF. Consider the points

$$q_c = \Big(\frac{p_{1,c}}{\alpha_c}, \dots, \frac{p_{K,c}}{\alpha_c}; p_{c,1}, \dots, p_{c,K}; 0 \Big) \in \mathcal{Q} \quad \text{where} \quad c \in \{1, \dots, K\}. \tag{111}$$

Let $a \neq b$. The points q_a, q_b have the following properties: (i) $I_a(q_a||p) = I_b(q_b||p) = 0$, and (ii) $I(\alpha, p) \leq I_a(q_b||p) < \infty$ and $I(\alpha, p) \leq I_b(q_a||p) < \infty$ by definition of $I(\alpha, p)$. Together with the continuity of $I_c(q||p)$ w.r.t. $q \in \mathcal{Q}$, this implies that there exists a $\lambda \in (0, 1)$ such that

$$I_a(\lambda q_a + (1 - \lambda) q_b||p) = I_b(\lambda q_a + (1 - \lambda) q_b||p). \tag{112}$$

This establishes the existence. □

SM3.7. *Proof of Lemma 2.*

PROOF. Let $a \neq b$ denote any two distinct clusters, and construct Q using some $\bar{q} \in \mathcal{Q}(a, b)$. By (i) the law of total probability,

$$\mathbb{P}_\Psi[V^* \in \mathcal{E}] = 1 - \mathbb{P}_\Psi[V^* \notin \mathcal{E}] \overset{\text{(i)}}{=} 1 - \sum_{c=a,b} \frac{\alpha_c}{\alpha_a + \alpha_b} \mathbb{P}_Q[V^* \in \hat{\mathcal{V}}_{\gamma(c)} | \sigma(V^*) = c]. \tag{113}$$

Since $q_a, q_b \notin \mathcal{Q}(a, b)$, the state V^* behaves differently than any state in either cluster a or b. We must therefore have $0 \leq \mathbb{P}_Q[V^* \in \hat{\mathcal{V}}_{\gamma(c)} | \sigma(V^*) = c] < 1$ for $c = a, b$. When $x, y \in [0, 1]$, $\alpha_a x + \alpha_b y = \alpha_a + \alpha_b$ if and only if $x, y = 1$. This implies that there exists a $\delta > 0$ such that $\mathbb{P}_\Psi[V^* \in \mathcal{E}] \geq \delta > 0$. This completes the proof. □

SM3.8. *Proof of Lemma 3.*

PROOF. Let $a \neq b$ be any two distinct clusters. Choose $q = \bar{q} \in Q(a, b)$ such that $I_a(\bar{q}||p) = I_b(\bar{q}||p) \triangleq I_{a,b}(\bar{q}||p) \in (0, \infty)$. This is possible by Lemma 1. Select V^* uniformly at random in $\mathcal{V}_a \cup \mathcal{V}_b$. Then by (i) the law of total probability and (ii) Proposition 5

$$\begin{aligned} \mathbb{E}_\Psi[L] &\overset{\text{(i)}}{=} \frac{\alpha_a}{\alpha_a + \alpha_b} \mathbb{E}_Q[L | \sigma(V^*) = a] + \frac{\alpha_b}{\alpha_a + \alpha_b} \mathbb{E}_Q[L | \sigma(V^*) = b] \\ &\overset{\text{(ii)}}{=} \frac{T}{n} I_{a,b}(p) + o\Big(\frac{T}{n}\Big). \end{aligned} \tag{114}$$

By (iii) the law of total variance $\mathrm{Var}[X] = \mathbb{E}_Y[\mathrm{Var}[X|Y]] + \mathrm{Var}_Y[\mathbb{E}[X|Y]]$, we have

(115)

$$\mathrm{Var}_\Psi[L] \overset{\text{(iii)}}{=} \frac{\alpha_a}{\alpha_a + \alpha_b} \mathrm{Var}_Q[L | \sigma(V^*) = a] + \frac{\alpha_b}{\alpha_a + \alpha_b} \mathrm{Var}_Q[L | \sigma(V^*) = b]$$

$$+ \frac{\alpha_a}{\alpha_a + \alpha_b}\Big(\mathbb{E}_Q[L|\sigma(V^*) = a] - \mathbb{E}_\Psi[L]\Big)^2$$
$$+ \frac{\alpha_b}{\alpha_a + \alpha_b}\Big(\mathbb{E}_Q[L|\sigma(V^*) = b] - \mathbb{E}_\Psi[L]\Big)^2 \overset{\text{(iv)}}{=} o\Big(\frac{T^2}{n^2}\Big),$$

where for (iv) we have used Proposition 6 for the first two terms, and the fact that $\bar{q} \in Q(a,b)$ guarantees that $I_a(\bar{q}||p) = I_b(\bar{q}||p)$ for the last two terms. □

SM3.9. *Proof of Lemma 4.*

PROOF. Recall the points q_c for $c = 1, \ldots, K$ in (111). Let a^* and b^* be the indices such that

$$I(\alpha, p) = \sum_{k=1}^{K} \frac{1}{\alpha_{a^*}}\Big(\pi_{a^*} p_{a^*,k} \ln \frac{p_{a^*,k}}{p_{b^*,k}} + \pi_k p_{k,a^*} \ln \frac{p_{k,a^*}}{p_{k,b^*}} + \Big(\frac{\pi_{b^*}}{\alpha_{b^*}} - \frac{\pi_{a^*}}{\alpha_{a^*}}\Big)\Big). \tag{116}$$

From the definitions of $I(\alpha, p)$, $I_c(q\|p)$, and q_c, we have that (i) $I_{a^*}(q_{a^*}\|p) = 0$, $I_{a^*}(q_{b^*}\|p) = I(\alpha, p)$, and (ii) $I_{b^*}(q_{b^*}\|p) = 0$, $I_{b^*}(q_{a^*}\|p) \geq I(\alpha, p)$.

We are now going to show that there exists a path along which $I_{a^*}(q\|p)$ monotonically decreases from $I(\alpha, p)$ to 0, while at the same time the $I_{b^*}(q\|p)$ moves from initially 0 to eventually $I_{b^*}(q_{a^*}\|p) \geq I(\alpha, p)$. Since $I_c(q\|p)$ is continuous in q, this implies the existence of atleast one point $\bar{q}$ such that $0 \leq I_{a^*}(\bar{q}\|p) = I_{b^*}(\bar{q}\|p) \leq I(\alpha, p)$.

First, we will walk along the path

$$\begin{aligned} q^{(1)}(\lambda) &= (1-\lambda)\Big(\frac{p_{1,b^*}}{\alpha_{b^*}}, \ldots, \frac{p_{K,b^*}}{\alpha_{b^*}}; p_{b^*,1}, \ldots, p_{b^*,K}; 0\Big) \\ &\quad + \lambda\Big(\frac{p_{1,b^*}}{\alpha_{b^*}}, \ldots, \frac{p_{K,b^*}}{\alpha_{b^*}}; p_{a^*,1}, \ldots, p_{a^*,K}; 0\Big). \end{aligned} \tag{117}$$

parameterized by $\lambda \in [0,1]$. Specifically note that $I_{a^*}(q^{(1)}(\lambda)\|p)$ is convex and monotonically decreasing in λ. This is because λ only changes the convex summands $(\sum_{k=1}^{K} \pi_l q_{l,0})\mathrm{KL}(q_{0,\cdot}\|p_{c,\cdot})$ in (23), and additionally, $\mathrm{KL}(q_{0,\cdot}\|p_{c,\cdot})$ is minimized at $\lambda = 1$.

Next, starting from the end point $q^{(1)}(1)$, we will walk along the path

$$\begin{aligned} q^{(2)}(\eta) &= (1-\eta)\Big(\frac{p_{1,b^*}}{\alpha_{b^*}}, \ldots, \frac{p_{K,b^*}}{\alpha_{b^*}}; p_{a^*,1}, \ldots, p_{a^*,K}; 0\Big) \\ &\quad + \eta\Big(\frac{p_{1,a^*}}{\alpha_{a^*}}, \ldots, \frac{p_{K,a^*}}{\alpha_{a^*}}; p_{a^*,1}, \ldots, p_{a^*,K}; 0\Big) \end{aligned}$$

parameterized by $\eta \in [0,1]$. Similar to before $I_{a^*}(q^{(2)}(\lambda)\|p)$ is convex and monotonically decreasing in η, and tends to 0 as $\eta \to 1$. Note that we have that $I_{b^*}(q^{(1)}(0)\|p) = 0$ and $I_{b^*}(q^{(2)}(1)\|p) = I_{b^*}(q_{a^*}\|p) \geq I(\alpha, p)$.

Next we prove the second claim of the lemma. Recall that

$$\mathbb{E}_Q[L|\sigma(V^*)] = \sum_{\text{all sample paths } \chi} \mathbb{P}_Q[\chi|\sigma(V^*)] \ln \frac{\mathbb{P}_Q[\chi|\sigma(V^*)]}{\mathbb{P}_P[\chi]} \tag{118}$$

is a KL-divergence. As a consequence, $\mathbb{E}_Q[L] = 0$ if and only if

$$\mathbb{P}_Q[\chi|\sigma(V^*)] = \prod_{t=1}^{T} Q_{x_{t-1},x_t} = \prod_{t=1}^{T} P_{x_{t-1},x_t} = \mathbb{P}_P[\chi] \quad \text{for all sample paths } \chi. \tag{119}$$

Equivalently $\mathbb{E}_Q[L|\sigma(V^*)] = 0$ if and only if $Q_{x,y} = P_{x,y}$ for all $x, y \in \mathcal{V}$, which can be seen by considering the set of paths that disagree only on the last jump. Since

$$I_{\sigma(V^*)}(q||p) = \lim_{n\to\infty} \frac{n}{T}\Big(\mathbb{E}_Q[L|\sigma(V^*)] + o(1)\Big), \tag{120}$$

we obtain that $I_{\sigma(V^*)}(q||p) = 0$ if and only if $q = q_{\sigma(V^*)}$. Since there exists $\bar{q}$ such that $I_{a^*}(\bar{q}||p) = I_{b^*}(\bar{q}||p) = 0$, $q_{a^*} = q_{b^*}$. This completes the proof. $\square$

SM4. Proofs of Chapter 6.

SM4.1. *Proof of Proposition 7.*

Proof. Let $\mathrm{diag}(\Pi) \in [0,1]^{n\times n}$ denote the matrix whose diagonal entries correspond with the entries of Π. Then $N = T\mathrm{diag}(\Pi)P$ according to (12).

The Markov process $\{X_t\}_{0\le t\le T}$ generates $\hat{N}$. We can think of $\hat{N}$ as a sum of random matrices $\hat{N} = \sum_{t=0}^{T-1} \hat{N}(t)$, where all the elements of each t-th matrix $\hat{N}(t) \in \{0,1\}^{n\times n}$ are zero except for the one element $(\hat{N}(t))_{X_t,X_{t+1}} = 1$. It is important to note that matrices $\hat{N}(t)$ and $\hat{N}(t-1)$ are dependent. In particular, only the X_t-th row of $\hat{N}(t)$ can contain a nonzero value. These dependencies are what make the analysis challenging.

To circumvent the difficulties associated with the strong dependencies, we use the following trick. We split $\hat{N}$ into two parts, specifically, $\hat{N} = \hat{N}^{(0)} + \hat{N}^{(1)}$ with

$$\hat{N}^{(0)} = \sum_{t=0}^{\lceil T/2\rceil -1} \hat{N}(2t) \quad \text{and} \quad \hat{N}^{(1)} = \sum_{t=0}^{\lfloor T/2\rfloor -1} \hat{N}(2t+1). \tag{121}$$

This particular split ensures that the elements of $\hat{N}^{(0)}$ and $\hat{N}^{(1)}$ are almost independent. Consider for instance the dependency between a matrix $\hat{N}(t)$ and the matrix $\hat{N}(t-2)$. Note that $\hat{N}(t)$ can contain a nonzero element almost anywhere when comparing to $\hat{N}(t-2)$, and that the only exceptions are diagonal entries.

Let us introduce notation to explain this precisely. Define $\bar{N}(t) = \mathbb{E}_P[\hat{N}(t)|\hat{N}(t-2)]$ for $t \geq 2$ and $\bar{N}(t) = \operatorname{diag}(\Pi)P$ for $t = 1, 2$. Note that $\mathbb{E}_P[\hat{N}(t)|\hat{N}(t-2)] = \mathbb{E}_P[\hat{N}(t)|\hat{N}(t-2), \hat{N}(t-4), \ldots]$ for all $t \geq 2$ since $\{X_t\}_{0\leq t\leq T}$ is a Markov chain. We therefore have that $\bar{N}(t) = \operatorname{diag}(P_{X_{t-2},\cdot})P$. This trick of separating the original process into two processes each of which skips one unit of time ensures that almost all elements of $\bar{N}(t)$ are of order $1/n^2$. Note that there exists an absolute constant $p_{\max} > 0$ such that $(\operatorname{diag}(P_{x,\cdot})P)_{y,z} \leq p_{\max}/n^2$ for all $x, y, z \in \mathcal{V}$.

We now explain how to show $\|\hat{N}_\Gamma - N\|_2 = O_{\mathbb{P}}(\sqrt{(T/n)\log(n)})$. Using the triangle inequality, it follows that $\|\hat{N}_\Gamma - N\| \leq \|\hat{N}_\Gamma - \sum_{t=0}^{T-1}\bar{N}(t)\| + \|N - \sum_{t=0}^{T-1}\bar{N}(t)\|$. To prove the proposition, we will first show that

$$\Big\|N - \sum_{t=0}^{T-1}\bar{N}(t)\Big\| = O_{\mathbb{P}}\Big(\sqrt{\frac{T}{n}\ln\frac{T}{n}}\Big) \tag{122}$$

and then that

$$\Big\|\hat{N}_\Gamma - \sum_{t=0}^{T-1}\bar{N}(t)\Big\| = O_{\mathbb{P}}\Big(\sqrt{\frac{T}{n}\ln\frac{T}{n}}\Big). \tag{123}$$

Proof of (122). The Frobenius norm is a direct upper bound for the spectral norm, giving

$$\Big\|N - \sum_{t=0}^{T-1}\bar{N}(t)\Big\| \leq \Big\|\Big(\sum_{t=2}^{T-1}\big(\operatorname{diag}(\Pi) - \operatorname{diag}(P_{X_{t-2},\cdot})\big)\Big)P\Big\|_{\mathrm{F}}. \tag{124}$$

In order to prove (122), it is therefore sufficient to show that

$$\Big\|\sum_{t=2}^{T-1}(\Pi - P_{X_{t-2},\cdot})\Big\|_2 = O_{\mathbb{P}}\Big(\sqrt{T\ln\frac{T}{n}}\Big) \tag{125}$$

since $\|P_{\cdot,y}\|_2 = O(1/\sqrt{n})$ for all $y \in \mathcal{V}$.

In fact (125) can be verified immediately, since

$$\begin{aligned}
\text{LHS} &\leq \Big\|\sum_{t=2}^{T-1}\Pi - \sum_{i=1}^{K}\frac{\hat{N}_{\mathcal{V},\mathcal{V}_i}}{|\mathcal{V}_i|}\sum_{v\in\mathcal{V}_i}P_{v,\cdot}\Big\|_2 + \Big\|\sum_{i=1}^{K}\frac{\hat{N}_{\mathcal{V},\mathcal{V}_i}}{|\mathcal{V}_i|}\sum_{v\in\mathcal{V}_i}P_{v,\cdot} - \sum_{t=2}^{T-1}P_{X_{t-2},\cdot}\Big\|_2 \\
&\leq \sum_{i=1}^{K}|T\pi_i - \hat{N}_{\mathcal{V},\mathcal{V}_i}|\|\Pi\|_2 + \Big\|\sum_{i=1}^{K}\frac{\hat{N}_{\mathcal{V},\mathcal{V}_i}}{|\mathcal{V}_i|}\sum_{v\in\mathcal{V}_i}P_{v,\cdot} - \sum_{t=2}^{T-1}P_{X_{t-2},\cdot}\Big\|_2
\end{aligned}$$

(126)

$$\stackrel{\text{(i)}}{=} O_{\mathbb{P}}\Big(\sqrt{\frac{T\ln n}{n}}\Big) + \Big\|\sum_{i=1}^{K}\frac{\hat{N}_{\mathcal{V},\mathcal{V}_i}}{|\mathcal{V}_i|}\sum_{v\in\mathcal{V}_i}P_{v,\cdot} - \sum_{t=2}^{T-1}P_{X_{t-2},\cdot}\Big\|_2 \stackrel{\text{(ii)}}{=} O_{\mathbb{P}}\Big(\sqrt{\frac{T}{n}}\ln n\Big).$$

Here, (i) follows from (55) and (ii) follows from the fact that for $k = 1,\dots,K$, $\|(1/|\mathcal{V}_k|)\sum_{v\in\mathcal{V}_k}P_{v,\cdot} - P_{w,\cdot}\|_2 = O(1/n)$ for all $w\in\mathcal{V}_k$, and that $\max_{y,z\in\mathcal{V}_k}|\hat{N}_{\mathcal{V},y} - \hat{N}_{\mathcal{V},z}| = O_{\mathbb{P}}(\sqrt{(T/n)}\ln n)$ for $k = 1,\dots,K$. This concludes the proof.

Proof of (123). Using the triangle inequality, we obtain

$$\begin{aligned}\Big\|\hat{N}_\Gamma - \sum_{t=0}^{T-1}\bar{N}(t)\Big\| &\le \Big\|\sum_{t=0}^{\lceil T/2\rceil-1}\big(\hat{N}_\Gamma(2t) - \bar{N}(2t)\big)\Big\| \\ &\quad + \Big\|\sum_{t=0}^{\lfloor T/2\rfloor-1}\big(\hat{N}_\Gamma(2t+1) - \bar{N}(2t+1)\big)\Big\|. \qquad (127)\end{aligned}$$

We start by proving that $\|\sum_{t=0}^{\lceil T/2\rceil-1}(\hat{N}_\Gamma(2t)-\bar{N}(2t))\|_2$ is in fact $O_{\mathbb{P}}(\sqrt{T/n}\ \ln(T/n))$. The remaining member can be bounded using an analogous argument. Specifically, we will follow the proof strategy in [31] and prove that for all $x,y\in\mathbb{R}^n$ such that $\|x\|_2 = \|y\|_2 = 1$,

$$\Big|x^{\mathrm{T}}\Big(\sum_{t=0}^{\lceil T/2\rceil-1}\big(\hat{N}_\Gamma(2t) - \bar{N}(2t)\big)\Big)y\Big| = O_{\mathbb{P}}\Big(\sqrt{\frac{T}{n}\ln\frac{T}{n}}\Big). \qquad (128)$$

For any given $x,y\in\mathbb{R}^n$ such that $\|x\|_2 = \|y\|_2 = 1$, define $\mathcal{L} = \{(v,v')\in\mathcal{V}\times\mathcal{V} : |x_v y_{v'}| \le (1/n)\sqrt{T/n}\}$. Recall that $\mathcal{L}^{\mathrm{c}} \triangleq \mathcal{V}\backslash\Gamma$, and for notational convenience define $\mathcal{K}\triangleq\Gamma^{\mathrm{c}}\times\mathcal{V}\cup\mathcal{V}\times\Gamma^{\mathrm{c}}$. Furthermore let $A\triangleq\sum_{t=0}^{\lceil T/2\rceil-1}\hat{N}(2t)$, $M\triangleq\sum_{t=0}^{\lceil T/2\rceil-1}\bar{N}(2t)$, and A_Γ denote the matrix after trimming A. Then using the definition of $\mathcal{L}$ and the triangle inequality, we bound the summand as follows:

$$\begin{aligned}\Big|x^{\mathrm{T}}(A_\Gamma - M)\,y\Big| &\le \Big|\sum_{(v,v')\in\mathcal{L}}x_v(A_\Gamma)_{vv'}y_{v'} - x^{\mathrm{T}}My\Big| + \Big|\sum_{(v,v')\in\mathcal{L}^{\mathrm{c}}}x_v(A_\Gamma)_{vv'}y_{v'}\Big| \\ &\le \Big|\sum_{(v,v')\in\mathcal{K}\cap\mathcal{L}}x_vA_{vv'}y_{v'}\Big| + \Big|\sum_{(v,v')\in\mathcal{L}}x_vA_{vv'}y_{v'} - x^{\mathrm{T}}My\Big| + \Big|\sum_{(v,v')\in\mathcal{L}^{\mathrm{c}}}x_v(A_\Gamma)_{vv'}y_{v'}\Big| \\ &\le \frac{1}{n}\sqrt{\frac{T}{n}}\Big|\sum_{(v,v')\in\mathcal{K}\cap\mathcal{L}}A_{vv'}\Big| + \Big|\sum_{(v,v')\in\mathcal{L}}x_vA_{vv'}y_{v'} - x^{\mathrm{T}}My\Big| + \Big|\sum_{(v,v')\in\mathcal{L}^{\mathrm{c}}}x_v(A_\Gamma)_{vv'}y_{v'}\Big|. \qquad (129)\end{aligned}$$

We will prove (128) by showing that for $x, y \in \mathbb{S}^{n-1}$,

$$\frac{1}{n}\sqrt{\frac{T}{n}}\Big|\sum_{(v,v')\in\mathcal{K}\cap\mathcal{L}} A_{vv'}\Big| = O_{\mathbb{P}}\Big(\sqrt{\frac{T}{n}}\Big), \tag{130}$$

$$\Big|\sum_{(v,v')\in\mathcal{L}} x_v A_{vv'} y_{v'} - x^{\mathrm{T}} M y\Big| = O_{\mathbb{P}}\Big(\sqrt{\frac{T}{n}}\Big), \tag{131}$$

$$\text{and} \quad \Big|\sum_{(v,v')\in\mathcal{L}^{\mathrm{c}}} x_v (A_\Gamma)_{vv'} y_{v'}\Big| = O_{\mathbb{P}}\Big(\sqrt{\frac{T}{n}\ln\frac{T}{n}}\Big). \tag{132}$$

Proof of (130). Since the number of subsets of $\mathcal{V}$ is less than 2^n, from (57) and the union bound, it follows that

$$\sum_{(v,v')\in\mathcal{K}\cap\mathcal{L}} A_{vv'} \le 2\hat{N}_{\mathcal{V},\overline{\Gamma}} \le 2 \max_{\mathcal{S}:|\mathcal{S}|=\lfloor n\exp(-T/n)\rfloor} \hat{N}_{\mathcal{V},\mathcal{S}} = O_{\mathbb{P}}(n). \tag{133}$$

Thus, we have (130).
Proof of (131). For given $x, y \in \mathbb{S}^{n-1}$, with $\lambda = \frac{1}{2}n\sqrt{n/T}$, we have

$$\begin{aligned}
&\mathbb{P}\Big[\sum_{(v,v')\in\mathcal{L}} x_v A_{vv'} y_{v'} - x^{\mathrm{T}} M y \ge C\sqrt{\frac{T}{n}}\Big] \\
&\le \frac{\mathbb{E}\Big[\exp\big(\lambda\sum_{(v,v')\in\mathcal{L}} x_v A_{vv'} y_{v'} - \lambda x^\top M y\big)\Big]}{\exp\big(\lambda C\sqrt{T/n}\big)} \\
&\overset{\text{(i)}}{=} \mathbb{E}\Big[\frac{\prod_{t=0}^{\lceil T/2\rceil-1}\big(1+\sum_{(v,v')\in\mathcal{L}}\bar{N}(2t)_{v,v'}(\mathrm{e}^{\lambda x_v y_{v'}}-1)\big)}{\exp\big(\lambda C\sqrt{T/n}+\lambda x^\top M y\big)}\Big] \\
&\overset{\text{(ii)}}{\le} \mathbb{E}\Big[\frac{\prod_{t=0}^{\lceil T/2\rceil-1}\big(1+\sum_{(v,v')\in\mathcal{L}}\bar{N}(2t)_{v,v'}(\lambda x_v y_{v'}+2(\lambda x_v y_{v'})^2)\big)}{\exp\big(\lambda C\sqrt{T/n}+\lambda x^{\mathrm{T}} M y\big)}\Big] \\
&\overset{\text{(iii)}}{\le} \mathbb{E}\Big[\frac{\exp\big(\sum_{(v,v')\in\mathcal{L}} M_{vv'}(\lambda x_v y_{v'}+2(\lambda x_v y_{v'})^2)\big)}{\exp\big(\lambda C\sqrt{T/n}+\lambda x^{\mathrm{T}} M y\big)}\Big],
\end{aligned} \tag{134}$$

where we have used (i) the tower property, (ii) $e^x \le 1+x+2x^2$ for $|x|\le 1/2$, and (iii) $1+x\le e^x$.

We now bound the last term in (134). Note that $\sum_{(v,v')\in\mathcal{L}^{\mathrm{c}}}|x_v y_{v'}| \le n\sqrt{n/T}$ since $\sum_{v\in\mathcal{V}}\sum_{v'\in\mathcal{V}} x_v^2 y_{v'}^2 = 1$ and $|x_v y_{v'}| > (1/n)\sqrt{T/n}$ for all $(v,v')\in\mathcal{L}^{\mathrm{c}}$. This implies that

$$\exp\Big(\sum_{(v,v')\in\mathcal{L}}\lambda M_{vv'} x_v y_{v'} - \lambda x^{\mathrm{T}} M y\Big) = \exp\Big(-\sum_{(v,v)\in\mathcal{L}^{\mathrm{c}}}\lambda M_{vv'} x_v y_{v'}\Big)$$

$$\leq \exp\Big(\lambda \frac{p_{\max} T}{n^2} n \sqrt{\frac{n}{T}}\Big) = \exp\Big(\frac{n}{2} p_{\max}\Big). \tag{135}$$

If we in addition recall that $\sum_{v \in \mathcal{V}} \sum_{v' \in \mathcal{V}} x_v^2 y_{v'}^2 = 1$, it follows that

$$\exp\Big(\sum_{(v,v') \in \mathcal{L}} M_{vv'} 2(\lambda x_v y_{v'})^2\Big) \leq \exp\Big(\frac{n}{2} p_{\max}\Big). \tag{136}$$

Combining (134)–(136), we obtain

$$\mathbb{P}\Big[\sum_{(v,v') \in \mathcal{L}} x_v A_{vv'} y_{v'} - x^{\mathrm{T}} M y \geq C \sqrt{\frac{T}{n}}\Big] \leq \exp\Big(n p_{\max} - \frac{C}{2} n\Big). \tag{137}$$

In order to be able to deal with the issue that $x, y \in \mathbb{B}^n \triangleq \{x \in \mathbb{R}^n | \|x\|_2 \leq 1\}$ are in a continuous space, we can for instance use an ε-net. Specifically, we can use the union bound on the set

$$\mathbb{B}_\varepsilon^n \triangleq \Big\{x \in \Big(\frac{\varepsilon}{\sqrt{n}} \mathbb{Z}\Big)^n \Big| \|x\|_2 \leq 1\Big\} \quad \text{where} \quad 0 < \varepsilon < 1. \tag{138}$$

It follows from Claim 2.4 and Claim 2.9 of [31] that there exists an absolute constant c_ε such that $|\mathbb{B}_\varepsilon^n| \leq \mathrm{e}^{c_\varepsilon n}$ and

$$\max_{x,y \in \mathbb{B}^n} x^{\mathrm{T}} A y \leq \frac{1}{(1-\varepsilon)^2} \max_{x,y \in \mathbb{B}_\varepsilon^n} x^{\mathrm{T}} A y. \tag{139}$$

The union bound and (137) therefore imply that

$$\begin{aligned} &\max_{x,y \in \mathbb{B}^n} \sum_{(v,v') \in \mathcal{L}} x_v A_{vv'} y_{v'} - x^{\mathrm{T}} M y \\ &\leq 4 \max_{x,y \in \mathbb{B}_\varepsilon^n} \sum_{(v,v') \in \mathcal{L}} x_v A_{vv'} y_{v'} - x^{\mathrm{T}} M y = O\Big(\sqrt{n p_{\max}}\Big) \end{aligned} \tag{140}$$

with a probability of at least $1 - \exp\big(c_\varepsilon n + n + 5h^2 m/n - Cn/2\big)$. This in turn implies (131) when we choose a sufficiently large constant C.

Proof of (132). In order to prove (132), it suffices to extend the arguments in [31]. Introduce the quantity $e(\mathcal{A}, \mathcal{B}) \triangleq (A_\Gamma)_{\mathcal{A},\mathcal{B}}$. It is then explained in [31] that the discrepancy property is a sufficient condition for (132).

DEFINITION (Discrepancy property). *All $\mathcal{A}, \mathcal{B} \subset \mathcal{V}$ satisfy one of the following properties: for some constants c_2 and c_3,*

- $\frac{e(\mathcal{A},\mathcal{B}) n^2}{|\mathcal{A}||\mathcal{B}| T} \leq c_2 \ln \frac{T}{n}$

- $e(\mathcal{A},\mathcal{B}) \ln \frac{e(\mathcal{A},\mathcal{B})n^2}{|\mathcal{A}||\mathcal{B}|T} \leq c_3 \max\left(|\mathcal{A}|,|\mathcal{B}|\right) \ln \frac{n}{\max|\mathcal{A}|,|\mathcal{B}|}$.

We will therefore now establish that the discrepancy property holds with high probability. Let $\mathcal{A},\mathcal{B} \subset \mathcal{V}$ be two subsets such that $|\mathcal{A}| \leq |\mathcal{B}|$ w.l.o.g. Also let c_2, c_3 be two large constants (how large will be sufficient will become clear in a moment). We can now distinguish two cases:
Case 1: $|\mathcal{B}| \geq n/5$. The trimming step ensures that $e(v,\mathcal{V}) = O(T/n)$ for all $v \in \mathcal{V}$. We therefore have in this case that $e(\mathcal{A},\mathcal{B}) \leq c_2 \frac{|\mathcal{A}||\mathcal{B}|T}{n^2}$.
Case 2: $|\mathcal{B}| \leq n/5$. For this case, define the quantity $\eta(|\mathcal{A}|,|\mathcal{B}|) = \max\{\eta^0, (c_2|\mathcal{A}||\mathcal{B}|T\ln(T/n))/n^2\}$ with η^0 the constant that satisfies the relation $\eta^0 \ln\left((\eta^0 n^2)/(|\mathcal{A}||\mathcal{B}|T)\right) - c_3|\mathcal{B}|\ln(n/|\mathcal{B}|) = 0$. If all pairs of subsets $A, B \subset \mathcal{V}$ then satisfy $e(\mathcal{A},\mathcal{B}) \leq \eta(|\mathcal{A}|,|\mathcal{B}|)$, the discrepancy property holds. It therefore suffices to show that $e(\mathcal{A},\mathcal{B}) \leq \eta(|\mathcal{A}|,|\mathcal{B}|)$ with high probability for all $A, B \subset \mathcal{V}$.

We will first quantify the probability that $e(\mathcal{A},\mathcal{B}) \leq \eta(|\mathcal{A}|,|\mathcal{B}|)$ for any arbitrary subsets $A, B \subset \mathcal{V}$. Using Markov's inequality, we obtain

$$
\begin{aligned}
&\mathbb{P}[e(\mathcal{A},\mathcal{B}) > \eta(|\mathcal{A}|,|\mathcal{B}|)] \leq \inf_{h\geq 0} \frac{\mathbb{E}[\exp(h\cdot e(\mathcal{A},\mathcal{B}))]}{\exp(h\cdot\eta(|\mathcal{A}|,|\mathcal{B}|))} \\
&\leq \inf_{h\geq 0} \prod_{t=1}^{\lceil T/2\rceil -1} \frac{1+\frac{|\mathcal{A}||\mathcal{B}|p_{\max}}{2n^2}\mathrm{e}^h}{\exp(h\cdot\eta(|\mathcal{A}|,|\mathcal{B}|))} \leq \inf_{h\geq 0} \prod_{t=1}^{\lceil T/2\rceil -1} \frac{\exp\left(\frac{|\mathcal{A}||\mathcal{B}|p_{\max}}{2n^2}\mathrm{e}^h\right)}{\exp(h\cdot\eta(|\mathcal{A}|,|\mathcal{B}|))} \\
&\leq \inf_{h\geq 0} \exp\Big(\frac{|\mathcal{A}||\mathcal{B}|p_{\max}T}{4n^2}\mathrm{e}^h - h\eta(|\mathcal{A}|,|\mathcal{B}|)\Big) \\
&\leq \exp\Big(-\eta(|\mathcal{A}|,|\mathcal{B}|)\Big(\ln\frac{4n^2\eta(|\mathcal{A}|,|\mathcal{B}|)}{|\mathcal{A}||\mathcal{B}|p_{\max}T} - 1\Big)\Big),
\end{aligned} \tag{141}
$$

where, for the last inequality, we specify $h = \ln\left(4n^2\eta(|\mathcal{A}|,|\mathcal{B}|)\right)/(|\mathcal{A}||\mathcal{B}|p_{\max}T)\big)$.

As a last step, we compute the expected number of pairs $\mathcal{A},\mathcal{B} \subset \mathcal{V}$ such that $e(\mathcal{A},\mathcal{B}) > \eta(|\mathcal{A}|,|\mathcal{B}|)$. The number of possible pairs of sets $\mathcal{A}$ and $\mathcal{B}$ such that $|\mathcal{A}| = a$ and $|\mathcal{B}| = b$ is $\binom{n}{a}\binom{n}{b}$. Hence using (141),

$$
\begin{aligned}
&\mathbb{E}\Big[\Big|\Big\{(\mathcal{A},\mathcal{B})\Big|e(\mathcal{A},\mathcal{B}) > \eta(|\mathcal{A}|,|\mathcal{B}|), |\mathcal{A}| = a, |\mathcal{B}| = b, \mathcal{A},\mathcal{B} \subset \mathcal{V}\Big\}\Big|\Big] \\
&\leq \binom{n}{a}\binom{n}{b} \max_{\mathcal{A},\mathcal{B}\subset\mathcal{V} \text{ s.t. } |\mathcal{A}|=a,|\mathcal{B}|=b} \mathbb{P}[e(\mathcal{A},\mathcal{B}) > \eta(a,b)] \\
&\overset{\text{(i)}}{\leq} \Big(\frac{n\mathrm{e}}{b}\Big)^{2b} \max_{\mathcal{A},\mathcal{B}\subset\mathcal{V} \text{ s.t. } |\mathcal{A}|=a,|\mathcal{B}|=b} \mathbb{P}[e(\mathcal{A},\mathcal{B}) > \eta(\mathcal{A},\mathcal{B})] \\
&\overset{\text{(ii)}}{\leq} \exp\Big(4b\ln\frac{n}{b} - \eta(a,b)\Big(\ln\frac{4n^2\eta(a,b)}{abp_{\max}T} - 1\Big)\Big)
\end{aligned}
$$

$$\overset{\text{(iii)}}{\leq} \exp\Big(-3\ln n + 7b\ln\frac{n}{b} - \eta(a,b)\Big(\ln\frac{4n^2\eta(a,b)}{abp_{\max}T} - 1\Big)\Big)$$

$$\overset{\text{(iv)}}{\leq} \exp\Big(-3\ln n + 7b\ln\frac{n}{b} - \frac{\eta(a,b)}{2}\ln\frac{\eta(a,b)4n^2}{abp_{\max}T}\Big) \overset{\text{(v)}}{\leq} \frac{1}{n^3}. \tag{142}$$

Here, we have used that (i,ii) $a \leq b \leq n/5$, and (iii) $x\ln x$ is increasing in x. Inequality (iv) follows from $n^2 eta(\mathcal{A},\mathcal{B})/(abT) \geq c_2 \ln T/n$, and (v) follows from the definition of $\eta(a,b)$. We have therefore shown that when we sum the above inequality for all possible cardinalities a, b,

$$\mathbb{E}\Big[\Big|\Big\{(\mathcal{A},\mathcal{B})\Big|e(\mathcal{A},\mathcal{B}) > \eta(|\mathcal{A}|,|\mathcal{B}|), \mathcal{A},\mathcal{B} \subset V_1 \cap \Gamma\Big\}\Big|\Big] \leq \frac{1}{n}. \tag{143}$$

We can thus conclude that with probability $1 - 1/n$ the discrepancy property holds. □

SM4.2. *Proof of Lemma 5.*

PROOF. By (i) definition $N_{x,y} = T\Pi_x P_{x,y}$, and (ii) by the definition of $P_{x,y}$, recall (4),

$$\|N_{x,\cdot} - N_{y,\cdot}\|_2^2 = \sum_{z\in\mathcal{V}} |N_{x,z} - N_{y,z}|^2 \overset{\text{(i)}}{=} \sum_{z\in\mathcal{V}} |T\Pi_x P_{x,z} - T\Pi_y P_{y,z}|^2$$

$$\overset{\text{(ii)}}{=} T^2 \sum_{k=1}^{K}\sum_{z\in\mathcal{V}_k}\Big|\bar{\Pi}_{\sigma(x)}\frac{p_{\sigma(x),k}}{|\mathcal{V}_k| - \mathbb{1}[\sigma(x)=k]} - \bar{\Pi}_{\sigma(y)}\frac{p_{\sigma(y),k}}{|\mathcal{V}_k| - \mathbb{1}[\sigma(y)=k]}\Big|^2 \tag{144}$$

and

$$\|N_{\cdot,x} - N_{\cdot,y}\|_2^2 = \sum_{z\in\mathcal{V}} |N_{z,x} - N_{z,y}|^2 \overset{\text{(i)}}{=} \sum_{z\in\mathcal{V}} |T\Pi_z P_{z,x} - T\Pi_z P_{z,y}|^2$$

$$\overset{\text{(ii)}}{=} T^2 \sum_{k=1}^{K}\sum_{z\in\mathcal{V}_k}\Big|\bar{\Pi}_k\frac{p_{k,\sigma(x)}}{|\mathcal{V}_{\sigma(x)}| - \mathbb{1}[\sigma(x)=k]} - \bar{\Pi}_k\frac{p_{k,\sigma(y)}}{|\mathcal{V}_{\sigma(y)}| - \mathbb{1}[\sigma(y)=k]}\Big|^2. \tag{145}$$

Then, we have that

$$\begin{aligned}
&\|N^0_{x,\cdot} - N^0_{y,\cdot}\|_2^2 = \|N_{x,\cdot} - N_{y,\cdot}\|_2^2 + \|N_{\cdot,x} - N_{\cdot,y}\|_2^2 \\
&\sim \frac{T^2}{n^3}\sum_{k=1}^{K}\Bigg(\Big(\frac{\pi_{\sigma(x)}p_{\sigma(x),k}}{\alpha_k\alpha_{\sigma(x)}} - \frac{\pi_{\sigma(y)}p_{\sigma(y),k}}{\alpha_k\alpha_{\sigma(y)}}\Big)^2 + \Big(\frac{\pi_k p_{k,\sigma(x)}}{\alpha_k\alpha_{\sigma(x)}} - \frac{\pi_k p_{k,\sigma(y)}}{\alpha_k\alpha_{\sigma(y)}}\Big)^2\Bigg) \\
&\geq \frac{T^2}{n^3}D_N(\alpha,p)
\end{aligned} \tag{146}$$

asymptotically. This completes the proof. □

SM4.3. *Proof of Lemma 6.*

PROOF. Recall that for the Frobenius norm it holds for any matrix $A \in \mathbb{R}^{n\times n}$ that $\|A\|_{\mathrm{F}}^2 = \sum_{i=1}^n \sigma_i^2(A)$, and that for the spectral norm $\|A\| = \max_{i=1,\ldots,n}\{\sigma_i(A)\}$. Because both $\hat{R}$ and N are of rank K, the matrix $\hat{R}-N$ is of rank at most $2K$, and therefore

$$\|\hat{R}^0 - N^0\|_{\mathrm{F}}^2 = 2\|\hat{R} - N\|_{\mathrm{F}}^2 \le 4K\|\hat{R} - N\|^2. \tag{147}$$

By the triangle inequality it then follows that

$$\|\hat{R}^0 - N^0\|_{\mathrm{F}} \le 2\sqrt{K}\big(\|\hat{R} - \hat{N}_\Gamma\| + \|\hat{N}_\Gamma - N\|\big). \tag{148}$$

Since K is independent of n, all that remains is to bound $\|\hat{R} - \hat{N}_\Gamma\|$ using $\|\hat{N}_\Gamma - N\|$.

From the definition of $\hat{R}$,

$$\|\hat{N}_\Gamma - \hat{R}\| = \sigma_{K+1}(\hat{N}_\Gamma). \tag{149}$$

Since the rank of N is at most K, from the Weyl's theorem

$$\sigma_{K+1}(\hat{N}_\Gamma) \le \|\hat{N}_\Gamma - N\|. \tag{150}$$

The proof is completed after bounding (148) by (149) and (150). □

SM4.4. *Proof of Lemma 7.*

PROOF. Define $\bar{N}_k^0 \triangleq \langle N_{z,\cdot}^0\rangle_{z\in\mathcal{V}_k}$ for $k = 1,\ldots,K$. Let $0 < a < 1/2$, $1 + a < b < \infty$ be two constants. Define the set of *cores*:

$$\mathcal{C}_k \triangleq \{x \in \mathcal{V}_k \,|\, \|\hat{R}_{x,\cdot}^0 - \bar{N}_k^0\|_2 \le a h(n,T)\} \quad \text{for} \quad k = 1,\ldots,K, \tag{151}$$

i.e., states from cluster k for which $\hat{R}_{x,\cdot}^0$ is correctly close to cluster k's center. Define also the set of *outliers*:

$$\mathcal{O} \triangleq \{x \in \mathcal{V} \,|\, \|\hat{R}_{x,\cdot}^0 - \bar{N}_k^0\|_2 \ge b h(n,T) \text{ for all } k = 1,\ldots,K\}, \tag{152}$$

so states for which $\hat{R}_{x,\cdot}^0$ is far from any cluster's center.

Let $x \in \mathcal{O}$, and then choose any cluster $k \in \{1,\ldots,K\}$ and any of its core states $y \in \mathcal{C}_k$. By (i) first centering and then applying the reverse triangle inequality, we find

$$\|\hat{R}_{x,\cdot}^0 - \hat{R}_{y,\cdot}^0\|_2 \overset{\text{(i)}}{\ge} \big|\|\hat{R}_{x,\cdot}^0 - \bar{N}_k^0\|_2 - \|\hat{R}_{y,\cdot}^0 - \bar{N}_k^0\|_2\big| \tag{153}$$

Since $x \in \mathcal{O}$ and $y \in \mathcal{C}_k$, it follows that $\|\hat{R}^0_{x,\cdot} - \hat{R}^0_{y,\cdot}\|_2 \geq (b-a)h(n,T)$. Furthermore $b - a > 1$, implying that $y \notin \mathcal{N}_x$. We have shown that $\mathcal{N}_x \cap \big(\cup_{k=1}^K \mathcal{C}_k\big) = \emptyset$ for all $x \in \mathcal{O}$.

By (ii) Lemma 6

$$
\begin{aligned}
&16K\|\hat{N}_\Gamma - N\|^2 \overset{\text{(ii)}}{\geq} \|\hat{R}^0 - N^0\|_{\mathrm{F}}^2 = \sum_{x\in\mathcal{V}} \|\hat{R}^0_{x,\cdot} - \bar{N}^0_{\sigma(x)}\|_2^2 \\
&\geq \big|\big(\cup_{k=1}^K \mathcal{C}_k\big)^{\mathrm{c}}\big| \min_{x\in\left(\cup_{k=1}^K \mathcal{C}_k\right)^{\mathrm{c}}} \{\|\hat{R}^0_{x,\cdot} - \bar{N}^0_{\sigma(x)}\|_2^2\} \geq \big|\big(\cup_{k=1}^K \mathcal{C}_k\big)^{\mathrm{c}}\big| (ah(n,T))^2.
\end{aligned} \tag{154}
$$

Rearrange to conclude that $\big|\big(\cup_{k=1}^K \mathcal{C}_k\big)^{\mathrm{c}}\big| = O_{\mathbb{P}}((f(n,T)/h(n,T))^2) = o_{\mathbb{P}}(n)$ by our assumptions on $h(n,T)$. Similarly for any $k \in \{1,\ldots,K\}$, $16K\|\hat{N}_\Gamma - N\|^2 \geq |\mathcal{C}_k^{\mathrm{c}} \cap \mathcal{V}_k|(ah(n,T))^2$ such that $|\mathcal{C}_k| = |\mathcal{V}_k| - |\mathcal{C}_k^{\mathrm{c}} \cap \mathcal{V}_k| \geq n\alpha_k - O_{\mathbb{P}}((f(n,T)/h(n,T))^2) = n\alpha_k(1 - o_{\mathbb{P}}(1))$ by the assumptions on $h(n,T)$.

For any $x \in \mathcal{O}$, $|\mathcal{N}_x| \leq \big|\big(\cup_{k=1}^K \mathcal{C}_k\big)^{\mathrm{c}}\big| = O_{\mathbb{P}}((f(n,T)/h(n,T))^2)$, since $\mathcal{N}_x \cap \big(\cup_{k=1}^K \mathcal{C}_k\big) = \emptyset$ and therefore $\mathcal{N}_x \subseteq \big(\cup_{k=1}^K \mathcal{C}_k\big)^{\mathrm{c}}$. For any $y \in \cup_{k=1}^K \mathcal{C}_k$, $\mathcal{C}_{\sigma(y)} \subseteq \mathcal{N}_y$ since $a < 1/2$ and therefore $|\mathcal{N}_y| \geq |\mathcal{C}_{\sigma(y)}| = n\alpha_{\sigma(y)} - O_{\mathbb{P}}((f(n,T)/h(n,T))^2)$. Note furthermore that because $h(n,T) = o(\sqrt{T^2 D_N(\alpha,p)/n^3})$, $\mathcal{C}_k \cap \mathcal{C}_l = \emptyset$ for $k \neq l$ and sufficiently large n,T. By (14), it is then impossible that the centers $z_1^*, \ldots, z_K^*$ are outliers if n,T are sufficiently large (we have shown the existence of at least K disjoint sets that would be selected through maximization before any outlier would be considered for promotion to center). Specifically we have that for $k = 1,\ldots,K$

$$
\exists z \in \big(\cup_{l=1}^K \mathcal{C}_l\big) \setminus \cup_{l=0}^{k-1} S_l : |\mathcal{N}_z| \geq |\mathcal{C}^{(k)}| \geq n\alpha_k(1 - o_{\mathbb{P}}(1)), \tag{155}
$$

where the $|\mathcal{C}^{(1)}| \geq \ldots \geq |\mathcal{C}^{(K)}|$ denote the order statistic for the core cardinalities and $\alpha^{(1)} \geq \ldots \geq \alpha^{(K)}$ denote the order statistic for the cluster concentrations. Thus for sufficiently large n,T there exists a permutation γ such that

$$
\|\hat{R}^0_{z_k^*,\cdot} - \bar{N}^0_{\gamma(k)}\|_2 < ah(n,T) \quad \text{for} \quad k = 1,\ldots,K. \tag{156}
$$

Finally, let $x \in \mathcal{E}$ be any misclassified state. Necessarily $x \notin \mathcal{N}_{z^*_{\sigma(x)}}$, for otherwise x would not be misclassified. If $x \in \mathcal{N}_{z_c^*}$ for some $c \neq \sigma(x)$, we have $\|\hat{R}_{x,\cdot} - \bar{P}_c\|_2 \leq (1+a)h(n,T)$ by (156) and thus

$$
\begin{aligned}
\|\hat{R}^0_{x,\cdot} - \bar{N}^0_{\sigma(x)}\|_2 &\overset{\text{(i)}}{\geq} \big|\|\hat{R}^0_{x,\cdot} - \bar{N}^0_c\|_2 - \|\bar{N}^0_c - \bar{N}^0_{\sigma(x)}\|_2\big| \\
&\geq \sqrt{\frac{T^2 D_N(\alpha,p)}{n^3}} - (1+a)h(n,T).
\end{aligned} \tag{157}
$$

Since $h(n,T) = o(\sqrt{T^2 D_N(\alpha,p)/n^3})$, the result in Lemma 7 follows. If $x \in (\cup_{k=1}^K \mathcal{N}_{z_k^*})^{\mathrm{c}}$, the algorithm has associated x to the closest (but incorrect) center via (15), i.e., to some cluster $c \neq \sigma(x)$ satisfying $\|\hat{R}^0_{z_c^*,\cdot} - \hat{R}^0_{x,\cdot}\|_2 \leq \|\hat{R}^0_{z^*_{\sigma(x)},\cdot} - \hat{R}^0_{x,\cdot}\|_2$. Since each center z_k^* is $ah(n,T)$ close to its truth $\bar{N}_k^0$, which themselves are at least $\Omega(\sqrt{T^2 D_N(\alpha,p)/n^3})$ apart, it must be that $\|\hat{R}^0_{x,\cdot} - \bar{N}^0_{\sigma(x)}\|_2 = \Omega(\sqrt{T^2 D_N(\alpha,p)/n^3})$. This completes the proof. □

SM5. Proofs of Chapter 7.

SM5.1. *Bounding the size of $\mathcal{H}^{\mathrm{c}} = \mathcal{V}\backslash\mathcal{H}$ (Proof of (46)).*

PROOF. From the definition of $I(\alpha,p)$,

$$\mathbb{E}\Big[\sum_{k=1}^K \Big(\hat{N}_{x,\mathcal{V}_k} \ln \frac{p_{i,k}}{p_{j,k}} + \hat{N}_{\mathcal{V}_k,x} \ln \frac{p_{k,i}\alpha_j}{p_{k,j}\alpha_i}\Big) + \frac{T}{n}\Big(\frac{\pi_j}{\alpha_j} - \frac{\pi_i}{\alpha_i}\Big)\Big] \geq \frac{T}{n} I(\alpha,p). \tag{158}$$

It follows from (58) that $x \in \mathcal{V}$ does not satisfy (H1) with probability at most $\exp\big(-c_4(T/n)I(\alpha,p)\big)$. Markov's inequality implies that with probability $1 - \exp\big(-\frac{c_4}{2}(T/n)I(\alpha,p)\big)$, the number of states that do not satisfy (H1) is less than $n\exp\big(-\frac{c_4}{2}(T/n)I(\alpha,p)\big)$. Thus, the total number of removed states after the trimming process and the condition (H1) is less than $n\exp\big(-\frac{c_4}{2}(T/n)I(\alpha,p)\big) + n\exp\big(-(T/n)\ln(T/n)\big)$.

We will now prove the following intermediate claim: with high probability, there does not exist a subset $\mathcal{S} \subset \mathcal{V}$ of size $|\mathcal{S}| = s$ such that $\hat{N}_{\mathcal{S},\mathcal{S}} \geq 2s\ln(T/n)^2$, when

$$s = \Big\lfloor 2n\exp\Big(-\frac{c_4}{2}\frac{T}{n}I(\alpha,p)\Big) + 2n\exp\Big(-\frac{T}{n}\ln\frac{T}{n}\Big)\Big\rfloor. \tag{159}$$

For any subset $\mathcal{S} \subset \mathcal{V}$ such that $|\mathcal{S}| = s$ with s as above, it follows using Markov's inequality that

$$\begin{aligned}
\mathbb{P}[\hat{N}^{(1)}_{\mathcal{S},\mathcal{S}} \geq s\ln\Big(\frac{T}{n}\Big)^2] &\leq \inf_{\lambda\geq 0} \frac{\mathbb{E}[\mathrm{e}^{\lambda \hat{N}^{(1)}_{\mathcal{S},\mathcal{S}}}]}{\mathrm{e}^{s\lambda\ln(T/n)^2}} \leq \inf_{\lambda\geq 0} \prod_{i=1}^{\lceil T/2\rceil - 1} \frac{1 + (s/n)^2 p_{\max}\mathrm{e}^\lambda}{\mathrm{e}^{s\lambda\ln(T/n)^2}} \\
&\leq \inf_{\lambda\geq 0} \exp\Big(\frac{s^2 p_{\max} T}{n^2}\mathrm{e}^\lambda - s\lambda\ln\Big(\frac{T}{n}\Big)^2\Big) \\
&\overset{\text{(i)}}{\leq} \exp\Big(-\frac{T}{n}s\Big(\ln\frac{T}{n} - \frac{sp_{\max}}{n}\mathrm{e}^{\frac{T/n}{\ln(T/n)}}\Big)\Big) \overset{\text{(ii)}}{\leq} \mathrm{e}^{-\frac{Ts\ln(T/n)}{2n}},
\end{aligned} \tag{160}$$

where (i) we specify $\lambda = (T/n)/(\ln(T/n))$ and (ii) use the fact that $n/s \geq \exp((T/n)/(\ln(T/n))$. Analogously, one can prove that

$$\mathbb{P}\Big[\hat{N}^{(2)}_{\mathcal{S},\mathcal{S}} \geq s\ln\Big(\frac{T}{n}\Big)^2\Big] \leq \exp\Big(-\frac{Ts\ln(T/n)}{2n}\Big). \tag{161}$$

Because the number of subsets $\mathcal{S} \subset \mathcal{V}$ of size s satisfies $\binom{n}{s} \leq (\mathrm{e}n/s)^s$ we deduce using (160) and (161) that

$$\begin{aligned}
&\mathbb{E}\Big[\Big|\Big\{\mathcal{S}\Big|\hat{N}_{\mathcal{S},\mathcal{S}} \geq 2s\ln\Big(\frac{T}{n}\Big)^2, |\mathcal{S}| = s\Big\}\Big|\Big] \\
&\leq \mathbb{E}\Big[\Big|\Big\{\mathcal{S}\Big|\hat{N}^{(1)}_{\mathcal{S},\mathcal{S}} \geq s\ln\Big(\frac{T}{n}\Big)^2, |\mathcal{S}| = s\Big\}\Big|\Big] + \mathbb{E}\Big[\Big|\Big\{\mathcal{S}\Big|\hat{N}^{(2)}_{\mathcal{S},\mathcal{S}} \geq s\ln\Big(\frac{T}{n}\Big)^2, |\mathcal{S}| = s\Big\}\Big|\Big] \\
&\leq 2\Big(\frac{\mathrm{e}n}{s}\Big)^s \exp\Big(-\frac{Ts\ln(T/n)}{2n}\Big) = 2\exp\Big(-s\Big(\frac{T\ln(T/n)}{2n} - \ln\frac{\mathrm{e}n}{s}\Big)\Big) \\
&\leq 2\exp\Big(-\frac{Ts\ln(T/n)}{4n}\Big).
\end{aligned} \tag{162}$$

Using Markov's inequality we can thus now conclude that with high probability there does not exist a subset $\mathcal{S} \subset \mathcal{V}$ of size $|\mathcal{S}| = s$ such that $\hat{N}_{\mathcal{S},\mathcal{S}} \geq s\ln(T/n)^2$.

To conclude the proof of the lemma, we build the following sequence of sets. Let $Z_1 \subset \mathcal{V} \setminus \Gamma$ denote the set of states that do not satisfy (H1). Then, from the definition of s, $|Z_1| \leq s/2$. Let $\{Z(t) \subset \mathcal{V}\}_{1\leq t\leq t^*}$ be generated as follows:

- $Z(0) = Z_1$.
- For $t \geq 1$, $Z(t) = Z(t-1) \cup \{v_t\}$ if there exists $v_t \in \mathcal{V}$ such that $\hat{N}_{v_t,Z(t-1)} + \hat{N}_{Z(t-1),v_t} > 2\ln(T/n)^2$ and $v_t \notin Z(t-1)$. If such an item does not exist, the sequence ends.

The sequence ends after the construction of $Z(t^*)$. We show that if we assume that the cardinality of items that do not satisfy (H2) is strictly larger than $s/2$, then one the set of the sequence $\{Z(t) \subset \mathcal{V}\}_{1\leq t\leq t^*}$ contradicts the claim we just proved. □

SM5.2. *Proof of Lemma 8.*

SM5.2.1. *Leading order behavior of E_1.*

PROOF. The statement $-E_1 = \Omega_{\mathbb{P}}(I(\alpha,p)(T/n)e_n^{[t+1]})$ is a direct consequence of condition (H1). Specifically, note that $x \in \mathcal{E}_{\mathcal{H}}^{[t+1]}$ implies that $x \in \mathcal{H}$, and therefore condition (H1) is satisfied for each element over which is summed. This completes the proof. □

SM5.2.2. *Leading order behavior of E_2.*

PROOF. By assumption there exists a constant $\eta > 0$ so that $p_{b,a}/p_{c,a} \leq \eta$ for all $a, b, c = 1, \ldots, K$. With this constant it holds moreover that for all $a, b, c = 1, \ldots, K$, $p_{c,a}/p_{b,a} \geq 1/\eta$. By the triangle inequality $|E_2| \leq |E_2^{\mathrm{out}}| + |E_2^{\mathrm{in}}|$, and

$$
\begin{aligned}
|E_2^{\mathrm{out}}| &\leq \sum_{x \in \mathcal{E}_{\mathcal{H}}^{[t+1]}} \sum_{k=1}^{K} \bigl| \hat{N}_{x, \hat{\mathcal{V}}_k^{[t]}} - \hat{N}_{x, \mathcal{V}_k} \bigr| \Bigl| \ln \frac{p_{\sigma^{[t+1]}(x), k}}{p_{\sigma(x), k}} \Bigr| \\
&\leq |\ln \eta| \sum_{x \in \mathcal{E}_{\mathcal{H}}^{[t+1]}} \sum_{k=1}^{K} \bigl| \hat{N}_{x, \hat{\mathcal{V}}_k^{[t]}} - \hat{N}_{x, \mathcal{V}_k} \bigr|. \qquad (163)
\end{aligned}
$$

Similarly $|E_2^{\mathrm{in}}| \leq |\ln(1/\eta)| \sum_{x \in \mathcal{E}_{\mathcal{H}}^{[t+1]}} \sum_{k=1}^{K} |\hat{N}_{\hat{\mathcal{V}}_k^{[t]}, x} - \hat{N}_{\mathcal{V}_k, x}|$. Note that $|\ln \eta| = |\ln(1/\eta)|$. Thus

$$
|E_2| \leq |\ln \eta| \Bigl(\sum_{x \in \mathcal{E}_{\mathcal{H}}^{[t+1]}} \sum_{k=1}^{K} \bigl| \hat{N}_{x, \hat{\mathcal{V}}_k^{[t]}} - \hat{N}_{x, \mathcal{V}_k} \bigr| + \sum_{x \in \mathcal{E}_{\mathcal{H}}^{[t+1]}} \sum_{k=1}^{K} \bigl| \hat{N}_{\hat{\mathcal{V}}_k^{[t]}, x} - \hat{N}_{\mathcal{V}_k, x} \bigr| \Bigr). \qquad (164)
$$

Next we deal with the summations within the brackets. By (i) the triangle inequality and nonnegativity of entries of $\hat{N}_{x,y}$,

$$
\begin{aligned}
\sum_{x \in \mathcal{E}_{\mathcal{H}}^{[t+1]}} \sum_{k=1}^{K} \bigl| \hat{N}_{x, \hat{\mathcal{V}}_k^{[t]}} - \hat{N}_{x, \mathcal{V}_k} \bigr| &\overset{\text{(i)}}{\leq} \sum_{x \in \mathcal{E}_{\mathcal{H}}^{[t+1]}} \sum_{k=1}^{K} \Bigl| \hat{N}_{x, \hat{\mathcal{V}}_k^{[t]} \cap \mathcal{H}} - \hat{N}_{x, \mathcal{V}_k \cap \mathcal{H}} \Bigr| \\
&\quad + \sum_{x \in \mathcal{E}_{\mathcal{H}}^{[t+1]}} \sum_{k=1}^{K} \Bigl(\hat{N}_{x, \hat{\mathcal{V}}_k^{[t]} \cap \mathcal{H}^{\mathrm{c}}} + \hat{N}_{x, \mathcal{V}_k \cap \mathcal{H}^{\mathrm{c}}} \Bigr) \\
&= \sum_{x \in \mathcal{E}_{\mathcal{H}}^{[t+1]}} \sum_{k=1}^{K} \Bigl| \hat{N}_{x, \hat{\mathcal{V}}_k^{[t]} \cap \mathcal{H}} - \hat{N}_{x, \mathcal{V}_k \cap \mathcal{H}} \Bigr| + 2 \sum_{x \in \mathcal{E}_{\mathcal{H}}^{[t+1]}} \hat{N}_{x, \mathcal{V} \backslash \mathcal{H}}. \qquad (165)
\end{aligned}
$$

Since $x \in \mathcal{E}_{\mathcal{H}}^{[t+1]}$ implies that $x \in \mathcal{H}$, it follows from condition (H2) that $\sum_{x \in \mathcal{E}_{\mathcal{H}}^{[t+1]}} \hat{N}_{x, \mathcal{V} \backslash \mathcal{H}} \leq 2 |\mathcal{E}_{\mathcal{H}}^{[t+1]}| \ln((T/n))^2$. We next deal with the remaining sum. By (ii) the definition of $\hat{N}_{\mathcal{A}, \mathcal{B}}$,

$$
\sum_{x \in \mathcal{E}_{\mathcal{H}}^{[t+1]}} \sum_{k=1}^{K} \bigl| \hat{N}_{x, \hat{\mathcal{V}}_k^{[t]} \cap \mathcal{H}} - \hat{N}_{x, \mathcal{V}_k \cap \mathcal{H}} \bigr| \overset{\text{(ii)}}{=} \sum_{x \in \mathcal{E}_{\mathcal{H}}^{[t+1]}} \sum_{k=1}^{K} \Bigl| \sum_{y \in \hat{\mathcal{V}}_k^{[t]} \cap \mathcal{H}} \hat{N}_{x,y} - \sum_{y \in \mathcal{V}_k \cap \mathcal{H}} \hat{N}_{x,y} \Bigr| \qquad (166)
$$

$$= \sum_{x\in\mathcal{E}_{\mathcal{H}}^{[t+1]}} \sum_{k=1}^{K} \Big| \sum_{y\in(\hat{\mathcal{V}}_k^{[t]}\cap\mathcal{H})\setminus(\mathcal{V}_k\cap\mathcal{H})} \hat{N}_{x,y} - \sum_{y\in(\mathcal{V}_k\cap\mathcal{H})\setminus(\hat{\mathcal{V}}_k^{[t]}\cap\mathcal{H})} \hat{N}_{x,y} \Big|$$

$$\overset{\text{(i)}}{\leq} \sum_{x\in\mathcal{E}_{\mathcal{H}}^{[t+1]}} \sum_{k=1}^{K} \sum_{y\in(\hat{\mathcal{V}}_k^{[t]}\cap\mathcal{H})\Delta(\mathcal{V}_k\cap\mathcal{H})} \hat{N}_{x,y} = 2 \sum_{x\in\mathcal{E}_{\mathcal{H}}^{[t+1]}} \sum_{y\in\mathcal{E}_{\mathcal{H}}^{[t]}} \hat{N}_{x,y}.$$

Aside from swapping the indices, the conclusion holds similarly for the second summation in (164). We thus conclude that

$$|E_2| \leq 4|\ln\eta| \Big(\hat{N}_{\mathcal{E}_{\mathcal{H}}^{[t+1]},\mathcal{E}_{\mathcal{H}}^{[t]}} + \hat{N}_{\mathcal{E}_{\mathcal{H}}^{[t]},\mathcal{E}_{\mathcal{H}}^{[t+1]}} + 2|\mathcal{E}_{\mathcal{H}}^{[t+1]}| \ln\frac{T}{n} \Big). \tag{167}$$

We next center both terms around their means. Since the Markov chain is in equilibrium by assumption, it holds for the first term that

$$\begin{aligned} \hat{N}_{\mathcal{E}_{\mathcal{H}}^{[t+1]},\mathcal{E}_{\mathcal{H}}^{[t]}} &= N_{\mathcal{E}_{\mathcal{H}}^{[t+1]},\mathcal{E}_{\mathcal{H}}^{[t]}} + \hat{N}_{\mathcal{E}_{\mathcal{H}}^{[t+1]},\mathcal{E}_{\mathcal{H}}^{[t]}} - N_{\mathcal{E}_{\mathcal{H}}^{[t+1]},\mathcal{E}_{\mathcal{H}}^{[t]}} \\ &\leq \max_{x,y}\{T\Pi_x P_{x,y}\} |\mathcal{E}_{\mathcal{H}}^{[t]}||\mathcal{E}_{\mathcal{H}}^{[t+1]}| + \hat{N}_{\mathcal{E}_{\mathcal{H}}^{[t+1]},\mathcal{E}_{\mathcal{H}}^{[t]}} - N_{\mathcal{E}_{\mathcal{H}}^{[t+1]},\mathcal{E}_{\mathcal{H}}^{[t]}}. \end{aligned} \tag{168}$$

Then after applying Lemma 14 (iii), see §SM6.4, we find that
(169)

$$\hat{N}_{\mathcal{E}_{\mathcal{H}}^{[t+1]},\mathcal{E}_{\mathcal{H}}^{[t]}} - N_{\mathcal{E}_{\mathcal{H}}^{[t+1]},\mathcal{E}_{\mathcal{H}}^{[t]}} = 1_{\mathcal{E}_{\mathcal{H}}^{[t+1]}}{}^{\mathrm{T}} (\hat{N} - N) 1_{\mathcal{E}_{\mathcal{H}}^{[t]}} \overset{\text{(iii)}}{\leq} \|\hat{N} - N\| \sqrt{|\mathcal{E}_{\mathcal{H}}^{[t]}||\mathcal{E}_{\mathcal{H}}^{[t+1]}|}.$$

The same conclusion holds for $\hat{N}_{\mathcal{E}_{\mathcal{H}}^{[t]},\mathcal{E}_{\mathcal{H}}^{[t+1]}} - N_{\mathcal{E}_{\mathcal{H}}^{[t]},\mathcal{E}_{\mathcal{H}}^{[t+1]}}$.

Summarizing, we have so far shown that

$$\begin{aligned} |E_2| \leq 4|\ln\eta| \Big(&\max_{x,y}\{T\Pi_x P_{x,y}\} |\mathcal{E}_{\mathcal{H}}^{[t]}||\mathcal{E}_{\mathcal{H}}^{[t+1]}| \\ &+ \|\hat{N} - N\| \sqrt{|\mathcal{E}_{\mathcal{H}}^{[t]}||\mathcal{E}_{\mathcal{H}}^{[t+1]}|} + 2|\mathcal{E}_{\mathcal{H}}^{[t+1]}| \ln\frac{T}{n} \Big). \end{aligned} \tag{170}$$

By recalling that $\Pi_x P_{x,y} = O(1/n^2)$ and applying Lemma 15, see §SM6.5, the result is finally proven. □

SM5.2.3. *Leading order behavior of U.* We write $U = E_3 + E_4$ where $E_3 = E_3^{\mathrm{out}} + E_3^{\mathrm{in}}$,

$$\begin{aligned} E_3^{\mathrm{out}} &= \sum_{x\in\mathcal{E}_{\mathcal{H}}^{[t+1]}} \sum_{k=1}^{K} \hat{N}_{x,\hat{\mathcal{V}}_k^{[t]}} \Big(\ln\frac{\hat{p}_{\sigma^{[t+1]}(x),k}}{\hat{p}_{\sigma(x),k}} - \ln\frac{p_{\sigma^{[t+1]}(x),k}}{p_{\sigma(x),k}} \Big), \\ E_3^{\mathrm{in}} &= \sum_{x\in\mathcal{E}_{\mathcal{H}}^{[t+1]}} \sum_{k=1}^{K} \hat{N}_{\hat{\mathcal{V}}_k^{[t]},x} \Big(\ln\frac{\hat{p}_{k,\sigma^{[t+1]}(x)}}{\hat{p}_{k,\sigma(x)}} - \ln\frac{p_{k,\sigma^{[t+1]}(x)}}{p_{k,\sigma(x)}} \Big). \end{aligned} \tag{171}$$

and

(172)
$$E_4 = \sum_{x\in\mathcal{E}_{\mathcal{H}}^{[t+1]}} \Big(\frac{\hat{N}_{\hat{\mathcal{V}}^{[t]}_{\sigma(x)},\mathcal{V}}}{|\hat{\mathcal{V}}^{[t]}_{\sigma(x)}|} - \frac{\hat{N}_{\mathcal{V}_{\sigma(x)},\mathcal{V}}}{|\mathcal{V}_{\sigma(x)}|} \Big) - \sum_{x\in\mathcal{E}_{\mathcal{H}}^{[t+1]}} \Big(\frac{\hat{N}_{\hat{\mathcal{V}}^{[t]}_{\sigma^{[t+1]}(x)},\mathcal{V}}}{|\hat{\mathcal{V}}^{[t]}_{\sigma^{[t+1]}(x)}|} - \frac{\hat{N}_{\mathcal{V}_{\sigma^{[t+1]}(x)},\mathcal{V}}}{|\mathcal{V}_{\sigma^{[t+1]}(x)}|} \Big).$$

LEMMA 9. *It holds that* $|E_3| = O_{\mathbb{P}}\Big(\sqrt{\frac{T}{n}}\Big(\ln\frac{T}{n}\Big)e_n^{[t+1]}\Big)$.

PROOF. By the triangle inequality, we have $E_3 \le |E_3| \le |E_3^{\mathrm{in}}| + |E_3^{\mathrm{out}}|$ with

$$|E_3^{\mathrm{in}}| \le \sum_{x\in\mathcal{E}_{\mathcal{H}}^{[t+1]}} \sum_{k=1}^{K} \hat{N}_{x,\hat{\mathcal{V}}^{[t]}_k} \Big(\Big| \ln \frac{\hat{p}_{\sigma^{[t+1]}(x),k}}{p_{\sigma^{[t+1]}(x),k}} \Big| + \Big| \ln \frac{\hat{p}_{\sigma(x),k}}{p_{\sigma(x),k}} \Big| \Big),$$

$$|E_3^{\mathrm{out}}| \le \sum_{x\in\mathcal{E}_{\mathcal{H}}^{[t+1]}} \sum_{k=1}^{K} \hat{N}_{\hat{\mathcal{V}}^{[t]}_k,x} \Big(\Big| \ln \frac{\hat{p}_{k,\sigma^{[t+1]}(x)}}{p_{k,\sigma^{[t+1]}(x)}} \Big| + \Big| \ln \frac{\hat{p}_{k,\sigma(x)}}{p_{k,\sigma(x)}} \Big| \Big). \tag{173}$$

We first bound the summands. From the inequalities $x/(1+x) \le \ln(1+x) \le x$ for $x > -1$, it follows that for $a, b = 1, \dots, K$,

$$\begin{aligned} \Big| \ln \frac{\hat{p}_{a,b}}{p_{a,b}} \Big| =& \Big| \ln \Big(1 + \frac{\hat{p}_{a,b} - p_{a,b}}{p_{a,b}} \Big) \Big| \le \Big| \frac{\hat{p}_{a,b} - p_{a,b}}{p_{a,b}} \Big| \\ \le& \Big| \frac{1}{p_{a,b}} \frac{\hat{N}_{\hat{\mathcal{V}}_a,\hat{\mathcal{V}}_b}}{\hat{N}_{\hat{\mathcal{V}}_a,\mathcal{V}}} - 1 \Big| = \Big| \frac{1}{p_{a,b}} \frac{N_{\hat{\mathcal{V}}_a,\hat{\mathcal{V}}_b}}{N_{\hat{\mathcal{V}}_a,\mathcal{V}}} \frac{\hat{N}_{\hat{\mathcal{V}}_a,\hat{\mathcal{V}}_b}}{N_{\hat{\mathcal{V}}_a,\hat{\mathcal{V}}_b}} \frac{N_{\hat{\mathcal{V}}_a,\mathcal{V}}}{\hat{N}_{\hat{\mathcal{V}}_a,\mathcal{V}}} - 1 \Big| \\ =& O\Big(\sqrt{\frac{n}{T}}\Big), \end{aligned} \tag{174}$$

where the last equation is obtained from (67).

Next, since $x \in \mathcal{E}_{\mathcal{H}}^{[t+1]}$ implies that $x \in \Gamma$,

$$\hat{N}_{x,\mathcal{V}} + \hat{N}_{\mathcal{V},x} = O\Big(\frac{T}{n}\ln\frac{T}{n}\Big). \tag{175}$$

Then from (174) and (175)

$$|E_3| = O\Big(|\mathcal{E}_{\mathcal{H}}^{[t+1]}| \sqrt{\frac{T}{n}} \ln\frac{T}{n} \Big). \tag{176}$$

This completes the proof. □

LEMMA 10. *It holds that* $|E_4| = O_{\mathbb{P}}\Big(\sqrt{\frac{T}{n}}e_n^{[t+1]}\Big)$.

PROOF. Let $k \in \{1, \dots, K\}$ to examine any one of the summands in E_4. We (i) center and use the triangle inequality to bound all summands as

$$\Big|\frac{\hat{N}_{\hat{\mathcal{V}}_k^{[t]},\mathcal{V}}}{|\hat{\mathcal{V}}_k^{[t]}|} - \frac{\hat{N}_{\mathcal{V}_k,\mathcal{V}}}{|\mathcal{V}_k|}\Big| \overset{\text{(i)}}{\leq} \Big|\frac{\hat{N}_{\hat{\mathcal{V}}_k^{[t]},\mathcal{V}} - N_{\hat{\mathcal{V}}_k^{[t]},\mathcal{V}}}{|\hat{\mathcal{V}}_k^{[t]}|}\Big| + \Big|\frac{\hat{N}_{\mathcal{V}_k,\mathcal{V}} - N_{\mathcal{V}_k,\mathcal{V}}}{|\mathcal{V}_k|}\Big|$$

$$+ \Big|\frac{N_{\hat{\mathcal{V}}_k^{[t]},\mathcal{V}}}{|\hat{\mathcal{V}}_k^{[t]}|} - \frac{N_{\mathcal{V}_k,\mathcal{V}}}{|\mathcal{V}_k|}\Big| = O\Big(\sqrt{\frac{T}{n}}\Big), \tag{177}$$

where the last equation is obtained from (67). Thus, $|E_4| = O(\sqrt{(T/n)}|\mathcal{E}_{\mathcal{H}}^{[t+1]}|)$. Using Lemma 15 then completes the proof. □

SM6. Supporting propositions.

SM6.1. *Properties of uniform vertex selection.*

LEMMA 11. *If a state V^* is selected uniformly at random from two specific clusters $a, b \in \{1, \dots, K\}$, $a \neq b$, and a state V is selected uniformly at random from all states,*

$$\mathbb{P}_\Phi[V^* \in \mathcal{E}] = \mathbb{P}_\Phi[V \in \mathcal{E} | V \in \mathcal{V}_a \cup \mathcal{V}_b]. \tag{178}$$

PROOF. We have:

$$\mathbb{P}_\Phi[V^* \in \mathcal{E}] = \sum_{v \in \mathcal{V}_a \cup \mathcal{V}_b} \mathbb{P}_\Phi[V^* \in \mathcal{E} | V^* = v]\mathbb{P}_\Phi[V^* = v]$$

$$= \frac{1}{|\mathcal{V}_a| + |\mathcal{V}_b|} \sum_{v \in \mathcal{V}_a \cup \mathcal{V}_b} \mathbb{P}_\Phi[v \in \mathcal{E}], \tag{179}$$

and

$$\mathbb{P}_\Phi[V \in \mathcal{E} | V \in \mathcal{V}_a \cup \mathcal{V}_b] = \frac{\sum_{v \in \mathcal{V}} \mathbb{P}_\Phi[V \in \mathcal{E}, V \in \mathcal{V}_a \cup \mathcal{V}_b | V = v]\mathbb{P}_\Phi[V = v]}{\mathbb{P}_\Phi[V \in \mathcal{V}_a \cup \mathcal{V}_b]}$$

$$= \frac{\sum_{v \in \mathcal{V}_a \cup \mathcal{V}_b} \mathbb{P}_\Phi[v \in \mathcal{E}]/|\mathcal{V}|}{(|\mathcal{V}_a| + |\mathcal{V}_b|)/|\mathcal{V}|} = \frac{1}{|\mathcal{V}_a| + |\mathcal{V}_b|} \sum_{v \in \mathcal{V}_a \cup \mathcal{V}_b} \mathbb{P}_\Phi[v \in \mathcal{E}]. \tag{180}$$

The lemma follows. □

LEMMA 12. *If a state V is selected uniformly at random from all states,*

$$\mathbb{E}_\Phi[|\mathcal{E}|] = n\mathbb{P}_\Phi[V \in \mathcal{E}]. \tag{181}$$

PROOF. We have:

$$\mathbb{E}_\Phi[|\mathcal{E}|] = \mathbb{E}_\Phi[\sum_{v\in\mathcal{V}} \mathbb{1}[v \in \mathcal{E}]] = \sum_{v\in\mathcal{V}} \mathbb{E}_\Phi[\mathbb{1}[v \in \mathcal{E}]] = \sum_{v\in\mathcal{V}} \mathbb{P}_\Phi[v \in \mathcal{E}], \tag{182}$$

and

$$\begin{aligned} n\mathbb{P}_\Phi[V \in \mathcal{E}] &= n \sum_{v\in\mathcal{V}} \mathbb{P}_\Phi[V \in \mathcal{E}|V = v]\mathbb{P}_\Phi[V = v] \\ &= n \sum_{v\in\mathcal{V}} \mathbb{P}_\Phi[v \in \mathcal{E}] \frac{1}{|\mathcal{V}|} = \sum_{v\in\mathcal{V}} \mathbb{P}_\Phi[v \in \mathcal{E}], \end{aligned} \tag{183}$$

which completes the proof. □

SM6.2. *Asymptotic comparisons between P and Q's entries.* Recall that $R_{x,y} = Q_{x,y}/P_{x,y}$ for $x, y \in \mathcal{V}$.

LEMMA 13. *The following properties hold:*

(i) $R_{x,y} = 1+n^{-1}(\mathbb{1}[\sigma(y) = \sigma(V^*)]/\alpha_{\sigma(y)} - q_{\sigma(x),0}/(p_{\sigma(x),\sigma(y)}K))+O(n^{-2})$ *for* $x, y \neq V^*$,
(ii) $R_{x,V^*} = q_{\omega(x),0}\alpha_{\sigma(V^*)}/p_{\omega(x),\sigma(V^*)} + O(n^{-1})$ *for* $x \in \mathcal{V}\backslash\{V^*\}$,
(iii) $R_{V^*,y} = q_{0,\omega(x)}/p_{\sigma(V^*),\omega(x)} + O(n^{-1})$ *for* $y \in \mathcal{V}\backslash\{V^*\}$.

PROOF. Let $x, y \in \mathcal{V}\backslash\{V^*\}$. Using a Taylor expansion (i), we find that:

$$\begin{aligned} R_{x,y} &\overset{(4,31)}{=} \frac{p_{\sigma(x),\sigma(y)} - \frac{q_{\sigma(x),0}}{Kn}}{p_{\sigma(x),\sigma(y)}} \cdot \frac{|\mathcal{V}_{\sigma(y)}| - \mathbb{1}[\sigma(x) = \sigma(y)]}{|\mathcal{V}_{\sigma(y)}| - \mathbb{1}[\sigma(y) = \sigma(V^*)] - \mathbb{1}[\sigma(x) = \sigma(y)]} \\ &\overset{\text{(i)}}{=} 1 + \frac{1}{n}\Big(\frac{\mathbb{1}[\sigma(y) = \sigma(V^*)]}{\alpha_{\sigma(y)}} - \frac{q_{\sigma(x),0}}{p_{\sigma(x),\sigma(y)}K}\Big) + O\Big(\frac{1}{n^2}\Big). \end{aligned} \tag{184}$$

Similarly for $x \in \mathcal{V}\backslash\{V^*\}$

$$R_{x,V^*} \overset{(4,31)}{=} \frac{q_{\omega(x),0}}{p_{\sigma(x),\sigma(V^*)}} \cdot \frac{|\mathcal{V}_{\sigma(V^*)}| - \mathbb{1}[\sigma(x) = \sigma(V^*)]}{n} \overset{\text{(i)}}{=} \frac{q_{\omega(x),0}\alpha_{\sigma(V^*)}}{p_{\sigma(x),\sigma(V^*)}} + O\Big(\frac{1}{n}\Big), \tag{185}$$

and for $y \in \mathcal{V}\backslash\{V^*\}$

$$R_{V^*,y} \overset{(4,31)}{=} \frac{q_{0,\omega(y)}}{p_{\sigma(V^*),\sigma(y)}} \cdot \frac{|\mathcal{V}_{\sigma(y)}| - \mathbb{1}[\sigma(V^*) = \sigma(y)]}{|\mathcal{W}_{\omega(y)}|} \overset{\text{(i)}}{=} \frac{q_{0,\omega(y)}}{p_{\sigma(V^*),\sigma(y)}} + O\Big(\frac{1}{n}\Big). \tag{186}$$

This completes the proof. □

Recall that $S_{x,y,u,v} = \ln R_{x,y} \cdot \ln R_{u,v}$ for $x, y, u, v \in \mathcal{V}$.

COROLLARY 1. *The following properties hold:*

(i) $S_{x,y,u,v} = O(n^{-2})$ *if all* $x, y, u, v \neq V^*$,
(ii) $S_{x,y,u,v} = O(n^{-1})$ *if one of* x, y, u, v *is* V^*,
(iii) $S_{x,y,u,v} = O(1)$ *if two of* $x \neq y, u \neq v$ *are* V^*.

PROOF. These properties are all direct consequences of Lemma 13, which can be seen by using the Taylor expansion $\ln(1+x) = x + O(x^2)$ for $x \approx 0$ and expanding the product. Consider for example the case $x, y, u, v \in \mathcal{V}\backslash\{V^*\}$:
(187)

$$S_{x,y,u,v} = \ln R_{x,y} \cdot \ln R_{u,v} = \ln\Big(1 + O\Big(\frac{1}{n}\Big)\Big) \cdot \ln\Big(1 + O\Big(\frac{1}{n}\Big)\Big) = O\Big(\frac{1}{n^2}\Big).$$

The remaining cases follow similarly. □

SM6.3. *The objective is a log-likelihood function.* In this section, we show that as for the leading terms are concerned, for any vertex $x \in \mathcal{V}$ and $c \in \{1, \dots, K\}$, maximizing (18) is equivalent to maximizing

$$u_x(c) = \ln \frac{\mathbb{P}_M[X_0 = x_0, \dots, X_T = x_T]}{\mathbb{P}_L[X_0 = x_0, \dots, X_T = x_T]} = \sum_{s=1}^{T} \ln \frac{M_{x_{s-1},x_s}}{L_{x_{s-1},x_s}}. \tag{188}$$

Here, L denotes the transition matrix of a BMC constructed from the cluster assignment $\{\hat{\mathcal{V}}_k^{[t]}\}_{k=1,\dots,K}$, and M denotes the transition matrix of a modified BMC. Specifically, it is the transition matrix of a BMC in which the state x is moved into cluster c. Note that the conclusions in the paper do not require a formal proof of this statement, which is why we have opted to include only a rough justification here.

By construction of L and M, we have that $M_{x_{s-1},x_s} \neq L_{x_{s-1},x_s}$ only if $\{x_{s-1} = x, x_s \neq x\}$, $\{x_{s-1} \neq x, x_s \in \hat{\mathcal{V}}^{[t]}_{\sigma^{[L]}(x)}\}$ or $\{x_{s-1} \neq x, x_s \in \hat{\mathcal{V}}^{[t]}_c\}$. Let $\sigma^{[L]}(x)$ denote the cluster of state x w.r.t. the cluster structure used to construct L. Hence only the ratios

$$\begin{aligned}\frac{M_{x,y}}{L_{x,y}} =& \frac{\hat{p}_{c,\sigma^{[L]}(y)}}{\hat{p}_{\sigma^{[L]}(x),\sigma^{[L]}(y)}} \times \cdots \\ &\times \frac{|\hat{\mathcal{V}}^{[t]}_{\sigma^{[L]}(y)}| - \mathbb{1}[\sigma^{[L]}(x) = \sigma^{[L]}(y)]}{(|\hat{\mathcal{V}}^{[t]}_{\sigma^{[L]}(y)}| - \mathbb{1}[\sigma^{[L]}(y) = \sigma^{[L]}(x)] + \mathbb{1}[\sigma^{[L]}(y) = c]) - \mathbb{1}[c = \sigma^{[L]}(y)]}\end{aligned}$$

(189)

$$=\frac{\hat{p}_{c,\sigma^{[L]}(y)}}{\hat{p}_{\sigma^{[L]}(x),\sigma^{[L]}(y)}} \cdot \frac{|\hat{\mathcal{V}}^{[t]}_{\sigma^{[L]}(y)}| - \mathbb{1}[\sigma^{[L]}(x) = \sigma^{[L]}(y)]}{|\hat{\mathcal{V}}^{[t]}_{\sigma^{[L]}(y)}| - \mathbb{1}[\sigma^{[L]}(y) = \sigma^{[L]}(x)]} = \frac{\hat{p}_{c,\sigma^{[L]}(y)}}{\hat{p}_{\sigma^{[L]}(x),\sigma^{[L]}(y)}}$$

for $y \in \mathcal{V}\backslash\{x\}$,

$$\begin{aligned}
\frac{M_{y,x}}{L_{y,x}} =& \frac{\hat{p}_{\sigma^{[L]}(y),c}}{\hat{p}_{\sigma^{[L]}(y),\sigma^{[L]}(x)}} \cdot \frac{|\hat{\mathcal{V}}^{[t]}_{\sigma^{[L]}(x)}| - \mathbb{1}[\sigma^{[L]}(y) = \sigma^{[L]}(x)]}{(|\hat{\mathcal{V}}^{[t]}_{c}| + 1) - \mathbb{1}[\sigma^{[L]}(y) = \sigma^{[L]}(x)]} \\
=& \frac{\hat{p}_{\sigma^{[L]}(y),c}}{\hat{p}_{\sigma^{[L]}(y),\sigma^{[L]}(x)}} \cdot \frac{|\hat{\mathcal{V}}^{[t]}_{\sigma^{[L]}(x)}| - \mathbb{1}[\sigma^{[L]}(y) = \sigma^{[L]}(x)]}{|\hat{\mathcal{V}}^{[t]}_{c}| - \mathbb{1}[\sigma^{[L]}(y) = \sigma^{[L]}(x)]} \times \\
& \cdots \times \frac{1}{1 + 1/(|\hat{\mathcal{V}}^{[t]}_{c}| - \mathbb{1}[\sigma^{[L]}(y) = \sigma^{[L]}(x)])} \\
\sim& \frac{\hat{p}_{\sigma^{[L]}(y),c}}{\hat{p}_{\sigma^{[L]}(y),\sigma^{[L]}(x)}} \cdot \frac{\hat{\alpha}_{\sigma^{[L]}(x)}}{\hat{\alpha}_c} + O\Big(\frac{1}{n}\Big)
\end{aligned} \tag{190}$$

for $y \in \mathcal{V}\backslash\{x\}$,

$$\frac{M_{y,z}}{L_{y,z}} = \frac{\hat{p}_{\sigma^{[L]}(y),\sigma^{[L]}(x)}}{\hat{p}_{\sigma^{[L]}(y),\sigma^{[L]}(x)}} \cdot \frac{|\hat{\mathcal{V}}^{[t]}_{\sigma^{[L]}(x)}| - \mathbb{1}[\sigma^{[L]}(y) = \sigma^{[L]}(x)]}{(|\hat{\mathcal{V}}^{[t]}_{\sigma^{[L]}(x)}| - 1) - \mathbb{1}[\sigma^{[L]}(y) = \sigma^{[L]}(x)]}$$

(191)

$$= \frac{1}{1 - 1/(|\hat{\mathcal{V}}^{[t]}_{\sigma^{[L]}(x)}| - \mathbb{1}[\sigma^{[L]}(y) = \sigma^{[L]}(x)])} \sim 1 + \frac{1}{n\hat{\alpha}_{\sigma^{[L]}(x)}} + O\Big(\frac{1}{n^2}\Big).$$

for $y \in \mathcal{V}\backslash\{x\}$, $z \in \hat{\mathcal{V}}^{[t]}_{\sigma^{[L]}(x)}\backslash\{x\}$, and

$$\begin{aligned}
\frac{M_{y,z}}{L_{y,z}} &= \frac{\hat{p}_{\sigma^{[L]}(y),c}}{\hat{p}_{\sigma^{[L]}(y),c}} \cdot \frac{|\hat{\mathcal{V}}^{[t]}_{c}| - \mathbb{1}[\sigma^{[L]}(y) = c]}{(|\hat{\mathcal{V}}^{[t]}_{c}| + 1) - \mathbb{1}[\sigma^{[L]}(y) = c]} \\
&= \frac{1}{1 + 1/(|\hat{\mathcal{V}}^{[t]}_{c}| - \mathbb{1}[\sigma^{[L]}(y) = c])} \sim 1 - \frac{1}{n\hat{\alpha}_c} + O\Big(\frac{1}{n^2}\Big).
\end{aligned} \tag{192}$$

for $y \in \mathcal{V}\backslash\{x\}$, $z \in \hat{\mathcal{V}}^{[t]}_{c}\backslash\{x\}$ differ from unity.

We now rewrite $u_x(c)$ to identify $\hat{N}$. Specifically, we have

(193)

$$u_x(c) = \sum_{s=1}^{T} (\mathbb{1}[x_{s-1} = x, x_s \neq x] + \mathbb{1}[x_{s-1} \neq x, x_s \in \hat{\mathcal{V}}^{[t]}_{\sigma^{[L]}(x)} \cup \hat{\mathcal{V}}^{[t]}_{c}]) \ln \frac{M_{x_{s-1},x_s}}{L_{x_{s-1},x_s}}$$

and write

$$
\begin{aligned}
u_x(c) &= \sum_{s=1}^{T} \mathbb{1}[x_{s-1}=x] \underbrace{\mathbb{1}[x_s \neq x] \ln \frac{M_{x,x_s}}{L_{x,x_s}}}_{f(x_s)} \\
&\quad + \sum_{s=1}^{T} \sum_{z \in \hat{\mathcal{V}}^{[t]}_{\sigma^{[L]}(x)} \cup \hat{\mathcal{V}}^{[t]}_c} \mathbb{1}[x_s = z] \underbrace{\mathbb{1}[x_{s-1} \neq x] \ln \frac{M_{x_{s-1},z}}{L_{x_{s-1},z}}}_{g_z(x_{s-1})}. \qquad (194)
\end{aligned}
$$

Then, since the summands of both terms above depend on only one variable (x_s and x_{s-1}, respectively),

$$
\begin{aligned}
u_x(c) &= \sum_{s=1}^{T} \sum_{y \in \mathcal{V} \backslash \{x\}} \Big(\mathbb{1}[x_{s-1}=x] \mathbb{1}[x_s = y] f(y) \\
&\qquad + \sum_{z \in \hat{\mathcal{V}}^{[t]}_{\sigma^{[L]}(x)} \cup \hat{\mathcal{V}}^{[t]}_c} \mathbb{1}[x_{s-1}=y] \mathbb{1}[x_s = z] g_z(y) \Big) \\
&= \sum_{y \in \mathcal{V} \backslash \{x\}} \hat{N}_{x,y} f(y) + \sum_{y \in \mathcal{V} \backslash \{x\}} \sum_{z \in \hat{\mathcal{V}}^{[t]}_{\sigma^{[L]}(x)} \cup \hat{\mathcal{V}}^{[t]}_c} \hat{N}_{y,z} g_z(y). \qquad (195)
\end{aligned}
$$

Substituting f and g_z's definitions, we obtain

$$
\begin{aligned}
u_x(c) &= \sum_{y \in \mathcal{V} \backslash \{x\}} \Big(\hat{N}_{x,y} \ln \frac{M_{x,y}}{L_{x,y}} + \hat{N}_{y,x} \ln \frac{M_{y,x}}{L_{y,x}} \Big) \\
&\quad + \sum_{y \in \mathcal{V} \backslash \{x\}} \sum_{z \in (\hat{\mathcal{V}}^{[t]}_{\sigma^{[L]}(x)} \cup \hat{\mathcal{V}}^{[t]}_c) \backslash \{x\}} \hat{N}_{y,z} \ln \frac{M_{y,z}}{L_{y,z}}. \qquad (196)
\end{aligned}
$$

By now substituting (189)–(192), we find that by restricting our attention to the leading terms

$$
\begin{aligned}
u_x(c) &\sim \sum_{y \in \mathcal{V} \backslash \{x\}} \Big(\hat{N}_{x,y} \ln \frac{\hat{p}_{c,\sigma^{[L]}(y)}}{\hat{p}_{\sigma^{[L]}(x),\sigma^{[L]}(y)}} + \hat{N}_{y,x} \ln \Big(\frac{\hat{p}_{\sigma^{[L]}(y),c}}{\hat{p}_{\sigma^{[L]}(y),\sigma^{[L]}(x)}} \cdot \frac{\hat{\alpha}_{\sigma^{[L]}(x)}}{\hat{\alpha}_c} \Big) \Big) \\
&\quad + \frac{T}{n} \cdot \frac{\frac{1}{T} \sum_{y \in \mathcal{V} \backslash \{x\}} \sum_{z \in \hat{\mathcal{V}}^{[t]}_{\sigma^{[L]}(x)} \backslash \{x\}} \hat{N}_{y,z}}{\hat{\alpha}_{\sigma^{[L]}(x)}} - \frac{T}{n} \cdot \frac{\frac{1}{T} \sum_{y \in \mathcal{V} \backslash \{x\}} \sum_{z \in \hat{\mathcal{V}}^{[t]}_c \backslash \{x\}} \hat{N}_{y,z}}{\hat{\alpha}_c}. \qquad (197)
\end{aligned}
$$

In particular, recognize that for any $k = 1, \ldots, K$, asymptotically

$$\frac{1}{T} \sum_{y \in \mathcal{V} \backslash \{x\}} \sum_{z \in \hat{\mathcal{V}}_k^{[t]} \backslash \{x\}} \hat{N}_{y,z} \sim \frac{1}{T} \sum_{y \in \mathcal{V}} \sum_{z \in \hat{\mathcal{V}}_k^{[t]}} \hat{N}_{y,z} \overset{\text{(i)}}{\sim} \hat{\pi}_k \tag{198}$$

where for (i) we have used global balance. Finally expand the logarithms and separate out all terms that do not depend on c. Then conclude that when maximizing over c, this is equivalent to maximizing the reduced objective function

$$\begin{aligned} u_x^{\mathrm{red}}(c) &= \sum_{y \in \mathcal{V} \backslash \{x\}} \big(\hat{N}_{x,y} \ln \hat{p}_{c,\sigma^{[t]}(y)} + \hat{N}_{y,x} \ln \hat{p}_{\sigma^{[t]}(y),c} \big) - \frac{T}{n} \cdot \frac{\hat{\pi}_c}{\hat{\alpha}_c} \\ &= \sum_{k=1}^{K} \big(\hat{N}_{x,\hat{\mathcal{V}}_k^{[t]}} \ln \hat{p}_{c,k} + \hat{N}_{\hat{\mathcal{V}}_k^{[t]},x} \ln \frac{\hat{p}_{k,c}}{\hat{\alpha}_c} \big) - \frac{T}{n} \cdot \frac{\hat{\pi}_c}{\hat{\alpha}_c} \end{aligned} \tag{199}$$

over c. This concludes the proof.

SM6.4. *Spectral norm bound for sums of elements of matrices.*

LEMMA 14. *For any matrix $B \in \mathbb{R}^{n \times n}$ and subsets $\mathcal{A}, \mathcal{C} \subseteq \{1, \ldots, n\}$, we have*

$$\sum_{r \in \mathcal{A}} \sum_{c \in \mathcal{C}} B_{rc} = 1_{\mathcal{A}}{}^{\mathrm{T}} B 1_{\mathcal{C}}. \tag{200}$$

Furthermore, $1_{\mathcal{A}}{}^{\mathrm{T}} B 1_{\mathcal{C}} \leq \|B\| \sqrt{|\mathcal{A}||\mathcal{C}|}$.

PROOF. We have:

$$\begin{aligned} 1_{\mathcal{A}}{}^{\mathrm{T}} B 1_{\mathcal{C}} &= 1_{\mathcal{A}}{}^{\mathrm{T}} \Big(\sum_{r=1}^{n} \Big(\sum_{c=1}^{n} B_{rc} \mathbb{1}[c \in \mathcal{C}] e_{n,r} \Big) \Big) \\ &= \sum_{c'=1}^{n} \mathbb{1}[c' \in \mathcal{A}] e_{n,c'}{}^{\mathrm{T}} \Big(\sum_{r=1}^{n} \Big(\sum_{c \in \mathcal{C}} B_{rc} e_{n,r} \Big) \Big) = \sum_{c' \in \mathcal{A}} \sum_{r=1}^{n} \sum_{c \in \mathcal{C}} B_{rc} e_{n,c'}{}^{\mathrm{T}} e_{n,r} \\ &= \sum_{c' \in \mathcal{A}} \sum_{r=1}^{n} \sum_{c \in \mathcal{C}} B_{rc} \mathbb{1}[c' = r] = \sum_{r \in \mathcal{A}} \sum_{c \in \mathcal{C}} B_{rc}, \end{aligned}$$

which proves the first statement.

For the second statement, first note that (i) $1_{\mathcal{A}}{}^{\mathrm{T}} B 1_{\mathcal{C}} \in \mathbb{R}$ and therefore $1_{\mathcal{A}}{}^{\mathrm{T}} B 1_{\mathcal{C}} \leq |1_{\mathcal{A}}{}^{\mathrm{T}} B 1_{\mathcal{C}}|$. By (ii) applying the Cauchy–Schwarz inequality twice, and (iii) the consistency of subordinate norms, we obtain

$$1_{\mathcal{A}}{}^{\mathrm{T}} B 1_{\mathcal{C}} \overset{\text{(i)}}{\leq} |1_{\mathcal{A}}{}^{\mathrm{T}} B 1_{\mathcal{C}}| \overset{\text{(ii)}}{\leq} \|1_{\mathcal{A}}\|_2 \|B 1_{\mathcal{C}}\|_2 \overset{\text{(iii)}}{\leq} \|1_{\mathcal{A}}\|_2 \|B\| \|1_{\mathcal{C}}\|_2. \tag{201}$$

Lastly for any set $\mathcal{A} \subseteq \{1, \dots, n\}$, we have that $1_{\mathcal{A}} \in \{0,1\}^n$, and therefore $\|1_{\mathcal{A}}\|_2 = \sqrt{\|1_{\mathcal{A}}\|_1} = \sqrt{|\mathcal{A}|}$. Applying this bound for the sets $\mathcal{A}, \mathcal{C}$ concludes the proof. □

SM6.5. *Stochastic boundedness properties.* Recall that when we write $X_n = O_{\mathbb{P}}(a_n)$ for a sequence of random variables $\{X_n\}_{n=1}^{\infty}$ and some deterministic sequence $\{a_n\}_{n=1}^{\infty}$, this is equivalent to saying

$$\forall_{\varepsilon>0} \exists_{\delta_\varepsilon, N_\varepsilon} : \mathbb{P}\Big[\Big|\frac{X_n}{a_n}\Big| \geq \delta_\varepsilon\Big] \leq \varepsilon \, \forall_{n > N_\varepsilon}. \tag{202}$$

LEMMA 15. *Let* $\cup_{n=1}^{\infty} \{X_n\}_{n\geq 0}$, $\cup_{n=1}^{\infty}\{Y_n\}$ *denote two families of random variables with the properties that* $X_n, Y_n \geq 0$, $X_n = O_{\mathbb{P}}(x_n)$, *and* $Y_n = O_{\mathbb{P}}(y_n)$, *where* $\{x_n\}_{n=1}^{\infty}$, $\{y_n\}_{n=1}^{\infty}$ *denote two deterministic sequences with* $x_n, y_n \in [0,\infty)$. *Then* $X_n Y_n = O_{\mathbb{P}}(x_n y_n)$. *Similarly if* $X_n = \Omega_{\mathbb{P}}(x_n)$, $Y_n = \Omega_{\mathbb{P}}(y_n)$, *then* $X_n Y_n = \Omega_{\mathbb{P}}(x_n y_n)$.

PROOF. Let $\varepsilon > 0$. Choose $\delta_\varepsilon^X, N_\varepsilon^X$ and $\delta_\varepsilon^Y, N_\varepsilon^Y$ such that $\mathbb{P}[X_n \geq \delta_\varepsilon^X x_n] \leq \varepsilon/3$ and $\mathbb{P}[Y_n \geq \delta_\varepsilon^Y y_n] \leq \varepsilon/3$. Pick any $\delta_\varepsilon > \delta_\varepsilon^X \delta_\varepsilon^Y$. With these choices,

$$\begin{aligned}
\mathbb{P}\Big[\Big|\frac{X_n Y_n}{x_n y_n}\Big| \geq \delta_\varepsilon\Big] =& \mathbb{P}\Big[\Big|\frac{X_n Y_n}{x_n y_n}\Big| \geq \delta_\varepsilon, X_n \geq \delta_\varepsilon^X x_n, Y_n \geq \delta_\varepsilon^Y y_n\Big] \\
&+ \mathbb{P}\Big[\Big|\frac{X_n Y_n}{x_n y_n}\Big| \geq \delta_\varepsilon, X_n \geq \delta_\varepsilon^X x_n, Y_n < \delta_\varepsilon^Y y_n\Big] \\
&+ \mathbb{P}\Big[\Big|\frac{X_n Y_n}{x_n y_n}\Big| \geq \delta_\varepsilon, X_n < \delta_\varepsilon^X x_n, Y_n \geq \delta_\varepsilon^Y y_n\Big] \\
&+ \mathbb{P}\Big[\Big|\frac{X_n Y_n}{x_n y_n}\Big| \geq \delta_\varepsilon, X_n < \delta_\varepsilon^X x_n, Y_n < \delta_\varepsilon^Y y_n\Big] \leq \varepsilon.
\end{aligned} \tag{203}$$

We have shown that

$$\forall_{\varepsilon>0} \exists_{\delta_\varepsilon = \delta_\varepsilon^X \delta_\varepsilon^Y, N_\varepsilon = \max\{N_\varepsilon^X, N_\varepsilon^Y\}} : \mathbb{P}\Big[\Big|\frac{X_n Y_n}{x_n y_n}\Big| \geq \delta_\varepsilon\Big] \leq \varepsilon \, \forall_{n > N_\varepsilon}. \tag{204}$$

This completes the proof. □

LEMMA 16. *Let* $\{s_n\}_{n=1}^{\infty}$ *denote a deterministic sequence with* $s_n \in \mathbb{N}_+$. *Let* $\cup_{n=1}^{\infty} \cup_{m=1}^{s_n} \{X_{m,n}\}$ *denote a family of random variables with the properties that* $X_{m,n} \geq 0$, *and* $\exists_{\delta,N} : \mathbb{E}[X_{m,n}] \leq \delta x_n \, \forall_{m=1,\dots,s_n} \forall_{n>N}$. *Then* $S_n = \sum_{m=1}^{s_n} X_{m,n} = O_{\mathbb{P}}(s_n x_n)$.

PROOF. Let $\varepsilon > 0, \delta_\varepsilon^\Sigma > 0$. Since (i) $X_{m,n} > 0$ for all m, n, by (ii) Markov's inequality

$$\mathbb{P}\Big[\Big|\frac{S_n}{s_n x_n}\Big| \geq \delta_\varepsilon^\Sigma\Big] \overset{\text{(i)}}{=} \mathbb{P}\Big[\frac{1}{s_n x_n} \sum_{m=1}^{s_n} X_{m,n} \geq \delta_\varepsilon^\Sigma\Big] \overset{\text{(ii)}}{\leq} \frac{\sum_{m=1}^{s_n} \mathbb{E}[X_{m,n}]}{\delta_\varepsilon^\Sigma s_n x_n}. \tag{205}$$

By assumption $\exists_{\delta,N} : \mathbb{E}[X_{m,n}] \leq \delta x_n \, \forall_{m=1,\ldots,s_n} \forall_{n>N}$. Choose δ, N as such. Specify $\delta_\varepsilon^\Sigma = \delta/\varepsilon$. By (205), we have thus shown that

$$\forall_{\varepsilon>0} \exists_{\delta_\varepsilon^\Sigma = \delta/\varepsilon, N_\varepsilon = N} : \mathbb{P}\Big[\Big| \frac{S_n}{s_n x_n} \Big| \geq \delta_\varepsilon^\Sigma \Big] \leq \varepsilon \, \forall_{n>N_\varepsilon}. \tag{206}$$

Equivalently, $S_n = O_{\mathbb{P}}(s_n x_n)$. This completes the proof. $\square$

LEMMA 17. *Let $\cup_{n=1}^\infty \cup_{m=1}^n \{X_{m,n}\}$ denote a family of random variables with the properties that $X_{m,n} \geq 0$, and $\exists_{\delta,N} : \mathbb{E}[X_{m,n}] \leq \delta x_n \, \forall_{m=1,\ldots,n} \forall_{n>N}$. If $\{Y_n\}_{n=1}^\infty$ is a sequence of random variables with the properties that $Y_n \in \{1, \ldots, n\}$, and $Y_n = O_{\mathbb{P}}(y_n)$ for some deterministic sequence $\{y_n\}_{n=1}^\infty$ with $y_n \in \mathbb{N}_+$, then $Z_n = \sum_{m=1}^{Y_n \wedge n} X_{m,n} = O_{\mathbb{P}}((y_n \wedge n) x_n)$.*

PROOF. Let $\varepsilon > 0, \delta_\varepsilon^Z > 0$. Then

$$\begin{aligned} \mathbb{P}\Big[\Big| \frac{Z_n}{y_n x_n} \Big| \geq \delta_\varepsilon^Z \Big] &= \mathbb{P}\Big[\Big| \frac{Z_n}{y_n x_n} \Big| \geq \delta_\varepsilon^Z, \Big| \frac{Y_n}{y_n} \Big| \geq \delta_\varepsilon^Y \Big] + \mathbb{P}\Big[\Big| \frac{Z_n}{y_n x_n} \Big| \geq \delta_\varepsilon^Z, \Big| \frac{Y_n}{y_n} \Big| < \delta_\varepsilon^Y \Big] \\ &\leq \mathbb{P}\Big[\Big| \frac{Y_n}{y_n} \Big| \geq \delta_\varepsilon^Y \Big] + \mathbb{P}\Big[\Big| \frac{1}{y_n x_n} \sum_{m=1}^{(\delta_\varepsilon^Y y_n) \wedge n} X_{m,n} \Big| \geq \delta_\varepsilon^Z \Big]. \end{aligned} \tag{207}$$

By assumption $Y_n = O_{\mathbb{P}}(y_n)$, so we can choose $\delta_\varepsilon^Y \in \mathbb{N}_+, N_\varepsilon^Y > 0$ such that $\mathbb{P}[|Y_n/y_n| \geq \delta_\varepsilon^Y] \leq \varepsilon/2$ for all $n > N_\varepsilon^Y$. Write $\delta_\varepsilon^Z = \delta_\varepsilon^Y \delta_\varepsilon^\Sigma$, and we will specify $\delta_\varepsilon^\Sigma$ in a moment. Presently, we are at

$$\begin{aligned} \mathbb{P}\Big[\Big| \frac{Z_n}{y_n x_n} \Big| \geq \delta_\varepsilon^Z \Big] &\leq \frac{\varepsilon}{2} + \mathbb{P}\Big[\Big| \frac{1}{(\delta_\varepsilon^Y y_n) x_n} \sum_{m=1}^{(\delta_\varepsilon^Y y_n) \wedge n} X_{m,n} \Big| \geq \delta_\varepsilon^\Sigma \Big] \\ &\leq \frac{\varepsilon}{2} + \mathbb{P}\Big[\Big| \frac{1}{(\delta_\varepsilon^Y y_n \wedge n) x_n} \sum_{m=1}^{\delta_\varepsilon^Y y_n \wedge n} X_{m,n} \Big| \geq \delta_\varepsilon^\Sigma \Big]. \end{aligned} \tag{208}$$

The assumptions on the family $\{X_{m,n}\}_{m,n=1}^\infty$ now allow us to apply Lemma 16: specifically, there exist $\delta_\varepsilon^\Sigma, N_\varepsilon^\Sigma$ such that the final term is bounded by $\varepsilon/2$ for all $n > N_\varepsilon^\Sigma$. Summarizing, we have shown that

$$\forall_{\varepsilon>0} \exists_{\delta_\varepsilon^Z = \delta_\varepsilon^Y \delta_\varepsilon^\Sigma, N_\varepsilon^Z = \max\{N_\varepsilon^Y, N_\varepsilon^\Sigma,\}} : \mathbb{P}\Big[\Big| \frac{Z_n}{y_n x_n} \Big| \geq \delta_\varepsilon^\Sigma \Big] \leq \varepsilon \, \forall_{n>N_\varepsilon^Z}. \tag{209}$$

Equivalently, $Z_n = O_{\mathbb{P}}(y_n x_n)$. $\square$

LEMMA 18. *Let $\cup_{n=1}^\infty \{X_n\}_{n\geq 0}$, $\cup_{n=1}^\infty \{Y_n\}$ denote two families of random variables with the properties that $\mathbb{P}[X_n \leq Y_n] = 1$, $X_n = \Omega_{\mathbb{P}}(x_n)$, and $Y_n = O_{\mathbb{P}}(y_n)$, where $\{x_n\}_{n=1}^\infty$, $\{y_n\}_{n=1}^\infty$ denote two deterministic sequences with $x_n, y_n \in \mathbb{R}$. Then, $x_n = O(y_n)$.*

PROOF. We prove the result by contradiction. Recall first that the assumptions imply that for every $\varepsilon^X, \varepsilon^Y > 0$, there exist $\delta_\varepsilon^X, \delta_\varepsilon^Y > 0$ such that

$$\lim_{n\to\infty} \mathbb{P}[X_n \le \delta_\varepsilon^X x_n] \le \varepsilon^X, \quad \lim_{n\to\infty} \mathbb{P}[Y_n \ge \delta_\varepsilon^Y y_n] \le \varepsilon^Y. \tag{210}$$

Also note that by (i) definition of conditional probability, (ii) the De Morgan laws, and (iii) $\mathbb{P}[\{X_n \le \delta^X x_n\} \cap \{Y_n \ge \delta^Y y_n\}] \ge 0$, it follows that

$$\begin{aligned}
0 =& \mathbb{P}[X_n > Y_n] \ge \mathbb{P}[\{X_n > Y_n\} \cap \{X_n > \delta^X x_n\} \cap \{Y_n < \delta^Y y_n\}] \\
\overset{\text{(i)}}{=}& \mathbb{P}[X_n > Y_n | \{X_n > \delta^X x_n\} \cap \{Y_n < \delta^Y y_n\}] \times \cdots \\
& \times \big(1 - \mathbb{P}[(\{X_n > \delta^X x_n\} \cap \{Y_n < \delta^Y y_n\})^{\mathrm{c}}]\big) \\
\overset{\text{(ii)}}{=}& \mathbb{P}[X_n > Y_n | \{X_n > \delta^X x_n\} \cap \{Y_n < \delta^Y y_n\}] \times \cdots \\
& \times \big(1 - \mathbb{P}[\{X_n \le \delta^X x_n\} \cup \{Y_n \ge \delta^Y y_n\}]\big) \\
\overset{\text{(iii)}}{\ge}& \mathbb{P}[X_n > Y_n | \{X_n > \delta^X x_n\} \cap \{Y_n < \delta^Y y_n\}] \times \cdots \\
& \times \big(1 - \mathbb{P}[\{X_n \le \delta^X x_n\}] - \mathbb{P}[\{Y_n \ge \delta^Y y_n\}]\big). \qquad (211)
\end{aligned}$$

Now suppose that $x_n = \omega(y_n)$. By then taking the limit $n \to \infty$ both left and right, we obtain the inequality $0 \ge 1 - \varepsilon^X - \varepsilon^Y$, which is a contradiction. Hence it must be that $x_n = O(y_n)$. □

(This concludes the supplementary material).

KTH ROYAL INSTITUTE OF TECHNOLOGY
SCHOOL OF ELECTRICAL ENGINEERING
DEPT. OF AUTOMATIC CONTROL
OSQULDASVÄG 10, STOCKHOLM 10044, SWEDEN
E-MAIL: alepro@kth.se

DELFT UNIVERSITY OF TECHNOLOGY
FACULTY OF ELECTRICAL ENGINEERING, MATHEMATICS & COMPUTER SCIENCE
DEPT. OF QUANTUM & COMPUTER ENGINEERING
MEKELWEG 4, 2628CD DELFT, THE NETHERLANDS
E-MAIL: j.sanders@tudelft.nl

KOREA ADVANCED INSTITUTE OF SCIENCE AND TECHNOLOGY
DEPT. OF INDUSTRIAL & SYSTEMS ENGINEERING
291 DAEHAK-RO, EOEUN-DONG, YUSEONG-GU, SOUTH KOREA
E-MAIL: yunseyoung@kaist.ac.kr