Learning Fast-Mixing Models for Structured Prediction

Jacob Steinhardt JSTEINHARDT@CS.STANFORD.EDU
Percy Liang PLIANG@CS.STANFORD.EDU
Stanford University, 353 Serra Street, Stanford, CA 94305 USA

Abstract

Markov Chain Monte Carlo (MCMC) algorithms are often used for approximate inference inside learning, but their slow mixing can be difficult to diagnose and the approximations can seriously degrade learning. To alleviate these issues, we define a new model family using strong Doeblin Markov chains, whose mixing times can be precisely controlled by a parameter. We also develop an algorithm to learn such models, which involves maximizing the data likelihood under the induced stationary distribution of these chains. We show empirical improvements on two challenging inference tasks.

1. Introduction

Conventional wisdom suggests that rich features and highly-dependent variables necessitate intractable inference. Indeed, the dominant paradigm is to first define a joint model, and then use approximate inference (e.g., MCMC) to learn that model. While this recipe can generate good results in practice, it has two notable drawbacks: (i) diagnosing convergence of Markov chains is extremely difficult (Gelman and Rubin, 1992; Cowles and Carlin, 1996); and (ii) approximate inference can be highly suboptimal in the context of learning (Wainwright, 2006; Kulesza and Pereira, 2007).

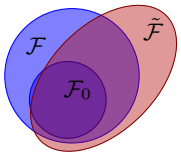
In this paper, we instead use MCMC to *define* the model family itself: For a given T, we construct a family of Markov chains using arbitrary rich features, but whose mixing time is *guaranteed* to be at most $O(T)$. The corresponding stationary distributions make up the model family. We can think of our Markov chains as parameterizing a family of "computationally accessible" distributions, where the amount of computation is controlled by T.

For concreteness, suppose we are performing a structured prediction task from input x to a complex output y. We construct Markov chains of the following form, called *strong Doeblin chains* (Doeblin, 1940):

$$\tilde{A}_\theta(y_t \mid y_{t-1}, x) = (1-\epsilon)A_\theta(y_t \mid y_{t-1}, x) + \epsilon\, u_\theta(y_t \mid x), \tag{1}$$

where ϵ is a mixture coefficient and θ parameterizes A_θ and u_θ. Importantly, u_θ does not depend on the previous state y_{t-1}. For intuition, think of u_θ as a simple tractable model and A_θ as Gibbs sampling in a complex intractable model. With probability $1-\epsilon$, we progress according to A_θ, and with probability ϵ we draw a fresh sample from u_θ, which performs an informed random restart. When $\epsilon = 1$, we are drawing i.i.d. samples from u_θ; we therefore mix in a single step, but our stationary distribution must necessarily be very simple. When $\epsilon = 0$, the stationary distribution can be much richer, but we have no guarantees on the mixing time. For intermediate values of ϵ, we trade off between representational power and mixing time.

A classic result is that a given strong Doeblin chain mixes in time at most $\frac{1}{\epsilon}$ (Doeblin, 1940), and that we can draw an exact sample from the stationary distribution in expected time $O(\frac{1}{\epsilon})$ (Corcoran and Tweedie, 1998). In this work, we prove new results that help us understand the strong Doeblin model families. Let $\mathcal{F}$ and $\tilde{\mathcal{F}}$ be the family of stationary distributions corresponding to A_θ and $\tilde{A}_\theta$ as defined in (1), respectively. Our first result is that as ϵ decreases, the stationary distribution of any $\tilde{A}_\theta$ monotonically approaches the stationary distribution of the corresponding A_θ (as measured by either direction of the KL divergence). Our second result is that if $\frac{1}{\epsilon}$ is much larger than the mixing time of A_θ, then the stationary distributions of A_θ and $\tilde{A}_\theta$ are close under a certain Mahalanobis distance. This shows that any member of $\mathcal{F}$ that is computationally accessible via the Markov chain is well-approximated by its counterpart in $\tilde{\mathcal{F}}$.



The figure above shows $\mathcal{F}$ and $\tilde{\mathcal{F}}$, together with the subset

$\mathcal{F}_0$ of $\mathcal{F}$ whose Markov chains mix quickly. $\tilde{\mathcal{F}}$ (approximately) covers $\mathcal{F}_0$, and contains some distributions outside of $\mathcal{F}$ entirely.

In order to learn over $\tilde{\mathcal{F}}$, we show how to maximize the likelihood of the data under the stationary distribution of $\tilde{A}_\theta$. Specifically, we show that we can compute a stochastic gradient of the log-likelihood in expected time $O(\frac{1}{\epsilon})$. Thus, in a strong sense, our objective function explicitly accounts for computational constraints.

We also generalize strong Doeblin chains, which are a mixture of two base chains, u_θ and A_θ, to *staged* strong Doeblin chains, which allow us to combine more than two base chains. We introduce an auxiliary variable z representing the "stage" that the chain is in. We then transition between stages, using the base chain corresponding to the current stage z to advance the concrete state y. A common application of this generalization is defining a sequence of increasingly more complex chains, similar in spirit to annealing. This allows sampling to become gradually more sensitive to the structure of the problem.

We evaluated our methods on two tasks: (i) inferring words from finger gestures on a touch screen and (ii) inferring DNF formulas for program verification. Unlike many structured prediction problems where local potentials provide a large fraction of the signal, in the two tasks above, local potentials offer a very weak signal; reasoning carefully about the higher-order potentials is necessary to perform well. On word inference, we showed that learning strong Doeblin chains obtained a 3.6% absolute improvement in character accuracy over Gibbs sampling while requiring 5x fewer samples. On DNF formula inference, our staged strong Doeblin chain obtains an order of magnitude speed improvement over plain Metropolis-Hastings.

To summarize, the contributions of this paper are: We formally define a family of MCMC algorithms based on strong Doeblin chains with guaranteed fast mixing times (Section 2). We provide an extensive analysis of the theoretical properties of this family (Section 3), together with a generalization to a staged version (Section 3.1). We provide an algorithm for learning the parameters of a strong Doeblin chain (Section 4). We demonstrate superior experimental results relative to baseline MCMC samplers on two tasks, word inference and DNF formula synthesis (Section 5).

2. A Fast-Mixing Family of Markov Chains

Given a Markov chain with transition matrix $A(y_t \mid y_{t-1})$ and a distribution $u(y_t)$, define a new Markov chain with transitions given by $\tilde{A}(y_t \mid y_{t-1}) \stackrel{\text{def}}{=} (1-\epsilon)A(y_t \mid y_{t-1}) + \epsilon u(y_t)$. (We suppress the dependence on θ and x for now.)

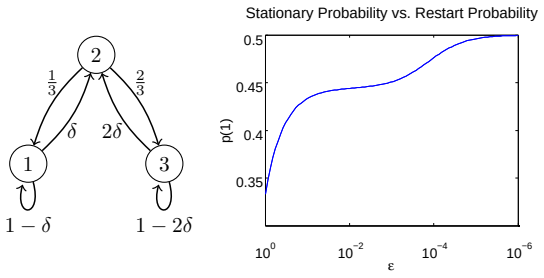


Figure 1. Left: A simple 3-state Markov chain. Arcs denote transition probabilities. Right: plot of the stationary probability of state 1 as a function of restart probability ϵ, for $\delta = 10^{-4}$. Note the two regimes for $\epsilon \ll \delta$ and $\epsilon \gg \delta$.

In matrix notation, we can write $\tilde{A}$ as

$$\tilde{A} \stackrel{\text{def}}{=} (1-\epsilon)A + \epsilon u \mathbb{1}^\top. \tag{2}$$

In other words, with probability ϵ we restart from u; otherwise, we transition according to A. Intuitively, $\tilde{A}$ should mix quickly because a restart from u renders the past independent of the future (we formalize this in Section 3). We think of u as a simple tractable model that provides *coverage*, and A as a complex model that provides *precision*.

Simple example. To gain some intuition, we work through a simple example with the Markov chain A depicted in Figure 1. The stationary distribution of this chain is $\left[\begin{array}{ccc} \frac{1}{2+3\delta} & \frac{3\delta}{2+3\delta} & \frac{1}{2+3\delta} \end{array}\right]$, splitting most of the probability mass evenly between states 1 and 3. The mixing time of this chain is approximately $\frac{1}{\delta}$, since once the chain falls into either state 1 or state 3, it will take about $\frac{1}{\delta}$ steps for it to escape back out. If we run this Markov chain for T steps with $T \ll \frac{1}{\delta}$, then our samples will be either almost all in state 1 or almost all in state 3, and thus will provide a poor summary of the distribution. If instead we perform random restarts with probability ϵ from a uniform distribution u over $\{1,2,3\}$, then the restarts give us the opportunity to explore both modes of the distribution. After a restart, however, the chain will more likely fall into state 3 than state 1 ($\frac{5}{9}$ probability vs. $\frac{4}{9}$), so for $\epsilon \gg \delta$ the stationary distribution will be noticeably perturbed by the restarts. If $\epsilon \ll \delta$, then there will be enough time for the chain to mix between restarts, so this bias will vanish. See Figure 1 for an illustration of this phenomenon.

3. Theoretical Properties

Markov chains that can be expressed according to (2) are said to have *strong Doeblin parameter* ϵ (Doeblin, 1940). In this section, we characterize the stationary distribution and mixing time of $\tilde{A}$, and also relate the stationary distribution of $\tilde{A}$ to that of A as a function of ϵ. Often the easiest way to study the mixing time of $\tilde{A}$ is via its spectral gap,

which is defined as $1 - \lambda_2(\tilde{A})$, where $\lambda_2(\tilde{A})$ is the second-largest eigenvalue (in complex norm). A standard result for Markov chains is that, under mild assumptions, the mixing time of $\tilde{A}$ is $O\left(\frac{1}{1-\lambda_2(\tilde{A})}\right)$. We assume throughout this section that A is ergodic but not necessarily that it is reversible. See Section 12.4 of Levin et al. (2009) for more details.

Our first result relates the spectral gap (and hence the mixing time) to ϵ. This result (as well as the next) are well-known but we include them for completeness. For most results in this section, we sketch the proof here and provide the full details in the appendix.

Proposition 3.1. *The spectral gap of $\tilde{A}$ is at least ϵ; that is, $1 - \lambda_2(\tilde{A}) \geq \epsilon$. In particular, $\tilde{A}$ mixes in time $O(\frac{1}{\epsilon})$.*

The key idea is that all eigenvectors of $\tilde{A}$ and A (except for the stationary distribution) are equal, and that $\lambda_k(\tilde{A}) = (1-\epsilon)\lambda_k(A)$ for $k > 1$.

Having established that $\tilde{A}$ mixes quickly, the next step is to determine its stationary distribution:

Proposition 3.2. *Let $\tilde{\pi}$ be the stationary distribution of $\tilde{A}$. Then*

$$\tilde{\pi} = \epsilon \sum_{j=0}^{\infty} (1-\epsilon)^j A^j u = \epsilon (I - (1-\epsilon)A)^{-1} u. \qquad (3)$$

This can be directly verified algebraically. The summation over j shows that we can in fact draw an exact sample from $\tilde{\pi}$ by drawing $T \sim \text{Geometric}(\epsilon)$,[1] initializing from u, and transitioning T times according to A. This is intuitive, since at a generic point in time we expect the most recent sample from u to have occurred $\text{Geometric}(\epsilon)$ steps ago. Note that $\mathbb{E}[T+1] = \frac{1}{\epsilon}$, which is consistent with the fact that the mixing time is $O(\frac{1}{\epsilon})$ (Proposition 3.1).

We would like to relate the stationary distributions $\tilde{\pi}$ and π of $\tilde{A}$ and A. The next two results (which are new) do so.

Let $\tilde{\pi}_\epsilon$ denote the stationary distribution of $\tilde{A}$ at a particular value of ϵ; note that $\tilde{\pi}_1 = u$ and $\tilde{\pi}_0 = \pi$. We will show that $\tilde{\pi}_\epsilon$ approaches π *monotonically*, for both directions of the KL divergence. In particular, for any $\epsilon < 1$, $\tilde{\pi}_\epsilon$ is at least as good as u at approximating π.

To show this, we make use of the following lemma from Murray and Salakhutdinov (2008):

Lemma 3.3. *If B is a transition matrix with stationary distribution π, then $\text{KL}(\pi \parallel B\pi') \leq \text{KL}(\pi \parallel \pi')$ and $\text{KL}(B\pi' \parallel \pi) \leq \text{KL}(\pi' \parallel \pi)$.*

Using this lemma, we can prove the following monotonicity result:

[1] If $T \sim \text{Geometric}(\epsilon)$, we have $\mathbb{P}[T = j] = \epsilon(1-\epsilon)^j$ for $j \geq 0$.

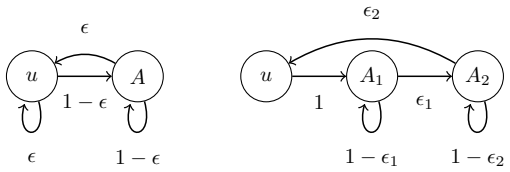


Figure 2. Markov chains over (a) two stages (strong Doeblin chains); and (b) three stages (restart from u followed by transitions from A_1 and then from A_2).

Proposition 3.4. *Both $\text{KL}(\tilde{\pi}_\epsilon \parallel \pi)$ and $\text{KL}(\pi \parallel \tilde{\pi}_\epsilon)$ are monotonic functions of ϵ.*

The idea is to construct a transition matrix B that maps $\tilde{\pi}_{\epsilon_1}$ to $\tilde{\pi}_{\epsilon_2}$ for given $\epsilon_2 < \epsilon_1$, then show that its stationary distribution is π and apply Lemma 3.3.

With Proposition 3.4 in hand, a natural next question is how small ϵ must be before $\tilde{\pi}$ is reasonably close to π. Proposition 3.5 provides one such bound: $\tilde{\pi}$ is close to π if ϵ is small compared to the spectral gap $1 - \lambda_2(A)$.

Proposition 3.5. *Suppose that A satisfies detailed balance with respect to π. Let $\tilde{\pi}$ be the stationary distribution of $\tilde{A}$. Define $d_\pi(\pi') \stackrel{\text{def}}{=} \|\pi - \pi'\|_{\text{diag}(\pi)^{-1}} = \sqrt{-1 + \sum_y \frac{\pi'(y)^2}{\pi(y)}}$, where $\|v\|_M$ is the Mahalonobis distance $\sqrt{v^\top M v}$. Then $d_\pi(\tilde{\pi}) \leq \frac{\epsilon}{1-\lambda_2(A)} \cdot d_\pi(u)$. (In particular, $d_\pi(\tilde{\pi}) \ll 1$ if $\epsilon \ll (1 - \lambda_2(A))/d_\pi(u)$.)*

The proof is somewhat involved, but the key step is to establish that $d_\pi(\pi')$ is convex in π' and contractive with respect to A (more precisely, that $d_\pi(A\pi') \leq \lambda_2(A) d_\pi(\pi')$).

Proposition 3.5 says that if A mixes quickly, then $\tilde{A}$ and A will have similar stationary distributions. This serves as a sanity check: if A already mixes quickly, then $\tilde{\pi}$ is a good approximation to π; otherwise, the Doeblin construction ensures that we are at least converging to *some* distribution, which by Proposition 3.4 approximates π at least as well as u does.

3.1. Staged strong Doeblin chains

Recall that to run a strong Doeblin chain $\tilde{A}$, we first sample from u, and then transition according to A for approximately $\frac{1}{\epsilon}$ steps. The intuition is that sampling from the crude distribution u faciliates global exploration of the state space, while the refined transition A hones in on a mode. However, for complex problems, there might be a considerable gap between what is possible with exact inference (u) and what is needed for accurate modeling (A). This motivates using multiple stages of MCMC to bridge the gap.

To do this, we introduce an auxiliary variable $z \in \mathcal{Z}$ denoting which stage of MCMC we are currently in. For each

stage z, we have a Markov chain $A_z(y_t \mid y_{t-1})$ over the original state space. We also define a Markov chain $C(z_t \mid z_{t-1})$ over the stages. To transition from (y_{t-1}, z_{t-1}) to (y_t, z_t), we first sample z_t from $C(z_t \mid z_{t-1})$ and then y_t from $A_{z_t}(y_t \mid y_{t-1})$. If there is a special state z^* for which $A_{z^*}(y_t \mid y_{t-1}) = u(y_t)$ (i.e., A_{z^*} does not depend on y_{t-1}), then we call the resulting chain a *staged strong Doeblin chain*.

For example, if $z \in \{0, 1\}$ and we transition from 0 to 1 with probability $1 - \epsilon$ and from 1 to 0 with probability ϵ, then we recover strong Doeblin chains assuming $z^* = 0$ (Figure 2(a)). As another example (Figure 2(b)), let $z \in \{0, 1, 2\}$. When $z = z^* = 0$, transition according to a restart distribution $u\mathbb{1}^\top$; when $z = 1$, transition according to a simple chain A_1; and when $z = 2$ transition according to a more complex chain A_2. If we transition from $z = 0$ to $z = 1$ with probability 1, from $z = 1$ to $z = 2$ with probability ϵ_1, and from $z = 2$ to $z = 0$ with probability ϵ_2, then we will on average draw 1 sample from u, $\frac{1}{\epsilon_1}$ samples from A_1, and $\frac{1}{\epsilon_2}$ samples from A_2.

We now show that staged strong Doeblin chains mix quickly as long as we visit z^* reasonably often. In particular, the following theorem provides guarantees on the mixing time that depend only on z^* and on the structure of $C(z_t \mid z_{t-1})$, analogous to the previous dependence only on ϵ. The condition of the theorem asks for times a and b such that the first time after a that we hit z^* is almost independent of the starting state z_0, and is less than b with high probability.

Theorem 3.6. *Let M be a staged strong Doeblin chain on $\mathcal{Z} \times \mathcal{Y}$. Let τ_a be the earliest time $s \geq a$ for which $z_s = z^*$. Let $\beta_{a,s} = \min_{z \in \mathcal{Z}} \mathbb{P}[\tau_a = s \mid z_0 = z]$ and $\gamma_{a,b} \stackrel{\text{def}}{=} \sum_{s=a}^{b} \beta_{a,s}$. Then M^b has strong Doeblin parameter $\gamma_{a,b}$. In particular, the spectral gap of M is at least $\frac{\gamma_{a,b}}{b}$. (Setting $a = b = 1$ recovers Proposition 3.1.)*

The key idea is that, conditioned on τ_a, (y_b, z_b) is independent of (y_0, z_0) for all $b \geq \tau_a$. For the special case that the stages form a cycle as in Figure 2, we have the following corollary:

Corollary 3.7. *Let C be a transition matrix on $\{0, \ldots, k-1\}$ such that $C(z_t = i \mid z_{t-1} = i) = 1 - \delta_i$ and $C(z_t = (i+1) \bmod k \mid z_{t-1} = i) = \delta_i$. Suppose that $\delta_{k-1} \leq \frac{1}{\max(2,k-1)} \min\{\delta_0, \ldots, \delta_{k-2}\}$. Then the spectral gap of the joint Markov chain is at least $\frac{\delta_{k-1}}{78}$.*

The key idea is that, when restricting to the time interval $[2/\delta_{k-1}, 3/\delta_{k-1}]$, the time of first transition from $k-1$ to 0 is approximately $\text{Geometric}(\delta_{k-1})$-distributed (independent of the initial state), which allows us to invoke Theorem 3.6. We expect the optimal constant to be much smaller than 78.

4. Learning strong Doeblin chains

Section 3 covered properties of strong Doeblin chains $(1-\epsilon)A_\theta + \epsilon u_\theta \mathbb{1}^\top$ for a fixed parameter vector θ. Now we turn to the problem of learning θ from data. We will focus on the discriminative learning setting where we are given a dataset $\{(x^{(i)}, y^{(i)})\}_{i=1}^n$ and want to maximize the conditional log-likelihood:

$$\mathcal{O}(\theta) = \frac{1}{n} \sum_{i=1}^{n} \log p_\theta(y^{(i)} \mid x^{(i)}), \tag{4}$$

where now p_θ is the stationary distribution of $\tilde{A}_\theta = (1-\epsilon)A_\theta + \epsilon u_\theta \mathbb{1}^\top$. We assume for simplicity that the chains A_θ and u_θ are given by conditional exponential families:

$$\begin{aligned} A_\theta(y \mid y', x) &\stackrel{\text{def}}{=} \exp\left(\theta^\top \phi(x, y', y) - \log Z(\theta; x, y)\right), \\ u_\theta(y \mid x) &\stackrel{\text{def}}{=} \exp\left(\theta^\top \phi(x, y) - \log Z(\theta; x)\right), \end{aligned} \tag{5}$$

where each ϕ outputs a feature vector and the Z are partition functions. By Proposition 3.1, $\tilde{A}_\theta$ mixes quickly for all θ. On the other hand, the parameterization of A_θ captures a rich family of transition kernels, including Gibbs sampling.

At a high level, our learning algorithm performs stochastic gradient descent on the negative log-likelihood. However, the negative log-likelihood is only defined implicitly in terms of the stationary distribution of a Markov chain, so the main challenge is to show that it can be computed efficiently. To start, we assume that we can operate on the base chains u_θ and A_θ for one step efficiently:

Assumption 4.1. *We can efficiently sample y from $u_\theta(\cdot \mid x)$ and $A_\theta(\cdot \mid y', x)$, as well as compute $\frac{\partial \log u_\theta(y|x)}{\partial \theta}$ and $\frac{\partial \log A_\theta(y|y',x)}{\partial \theta}$.*

Under Asssumption 4.1, we will show how to efficiently compute the gradient of $\log p_\theta(y^{(i)} \mid x^{(i)})$ with respect to θ. The impatient reader may skip ahead to the final pseudocode, which is given in Algorithm 1.

For convenience, we will suppress the dependence on x and i and just refer to $p_\theta(y)$ instead of $p_\theta(y^{(i)} \mid x^{(i)})$. Computing the gradient of $\log p_\theta(y)$ is non-trivial, since the formula for p_θ is somewhat involved:

$$p_\theta(y) = \epsilon \sum_{j=0}^{\infty} (1-\epsilon)^j [A_\theta^j u_\theta](y). \tag{6}$$

We are helped by the following generic identity on gradients of conditional log-probabilities, proved in the appendix.

Lemma 4.2. *Let z have distribution $p_\theta(z)$ parameterized by a vector θ. Let S be any measurable set. Then*

$$\frac{\partial \log p_\theta(z \in S)}{\partial \theta} = \mathbb{E}_z \left[\frac{\partial \log p_\theta(z)}{\partial \theta} \middle| z \in S \right]. \tag{7}$$

We can utilize Lemma 4.2 by interpreting $y \mid \theta$ as the output of the following generative process, which by Proposition 3.2 yields the stationary distribution of $\tilde{A}_\theta$:

- Sample y_0 from u_θ and $y_{t+1} \mid y_t$ from A_θ for $t = 0, 1, \ldots$.
- Sample $T \sim \text{Geometric}(\epsilon)$ and let $y = y_T$.

We then invoke Lemma 4.2 with $z = (T, y_{0:T})$ and S encoding the event that $y_T = y$. As long as we can sample from the posterior distribution of $(T, y_{0:T})$ conditioned on $y_T = y$, we can compute an estimate of $\frac{\partial}{\partial\theta} \log p_\theta(y)$ as follows:

- Sample $(T, y_{0:T}) \mid y_T = y$.
- Return $\frac{\partial \log p_\theta(T, y_{0:T})}{\partial\theta} = \frac{\partial \log u_\theta(y_0)}{\partial\theta} + \sum_{t=1}^{T} \frac{\partial \log A_\theta(y_t \mid y_{t-1})}{\partial\theta}$.

4.1. Sampling schemes for $(T, y_{0:T})$

By the preceding comments, it suffices to construct a sampler for $(T, y_{0:T}) \mid y_T = y$. A natural approach is to use importance sampling: sample $(T, y_{0:T-1})$, then weight by $p(y_T = y \mid y_{T-1})$. However, this throws away a lot of work — we make T MCMC transitions but obtain only one sample $(T, y_{0:T})$ with which to estimate the gradient.

We would like to ideally make use of all the MCMC transitions when constructing our estimate of $(T, y_{0:T}) \mid y_T = y$. For any $t \le T$, the pair $(t, y_{0:t})$ would itself have been a valid sample under different randomness, and we would like to exploit this. Suppose that we sample T from some distribution F and let $q(t)$ be the probability that $T \ge t$ under F. Then we can use the following scheme:

- Sample T from F, then sample $y_{0:T-1}$.
- For $t = 0, \ldots, T$, weight $(t, y_{0:t-1})$ by $\frac{\epsilon(1-\epsilon)^t}{q(t)} \times p(y_t = y \mid y_{t-1})$.

For any q, this yields unbiased (although unnormalized) weights (see Section B in the appendix). Typically we will choose $q(t) = (1-\epsilon)^t$, e.g. F is a geometric distribution. If the y_t are perfectly correlated, this will not be any more effective than vanilla importance sampling, but in practice this method should perform substantially better. Even though we obtain weights on all of $y_{0:T}$, these weights will typically be highly correlated, so we should still repeat the sampling procedure multiple times to minimize the bias from estimating the normalization constant. The full procedure is given as pseudocode in Algorithm 1.

4.2. Implementation

With the theory above in place, we now describe some important implementation details of our learning algorithm.

Algorithm 1 Algorithm for computing an estimate of $\frac{\partial}{\partial\theta} \log p_\theta(y \mid x)$. This estimate is unbiased in the limit of infinitely many samples k, but will be biased for a finite number of samples due to variance in the estimate of the partition function.

SampleGradient$(x, y, \theta, \epsilon, k)$
$\triangleright$ k is the number of samples to take
$Z \leftarrow 0; g \leftarrow 0$ $\quad \triangleright$ Z is the total importance mass of all samples, $\frac{g}{Z}$ is the gradient
for $i = 1$ **to** k **do**
  Sample $T \sim \text{Geometric}(\epsilon)$
  Sample y_0 from $u_\theta(\cdot \mid x)$
  For $1 \le t \le T-1$: sample y_t from $A_\theta(\cdot \mid y_{t-1}, x)$
  $w_0 \leftarrow \epsilon \cdot u_\theta(y)$
  For $1 \le t \le T$: $w_t \leftarrow \epsilon \cdot A_\theta(y \mid y_{t-1}, x)$
  $Z \leftarrow Z + \sum_{t=0}^{T} w_t$
  $g \leftarrow g + w_0 \frac{\partial \log u_\theta(y|x)}{\partial\theta} + \sum_{t=1}^{T} w_t \left(\frac{\partial \log u_\theta(y_0|x)}{\partial\theta} + \sum_{s=1}^{t-1} \frac{\partial \log A_\theta(y_s|y_{s-1},x)}{\partial\theta} + \frac{\partial \log A_\theta(y|y_{t-1},x)}{\partial\theta} \right)$.
end for
Output $\frac{g}{Z}$

At a high level, we can just use Algorithm 1 to compute estimates of the gradient and then apply an online learning algorithm such as AdaGrad (Duchi et al., 2011) to identify a good choice of θ. Since the log-likelihood is a non-convex function of θ, the initialization is important. We make the following (weak) assumption:

Assumption 4.3. *The chains u_θ and A_θ are controlled by disjoint coordinates of θ, and for any setting of u_θ there is a corresponding choice of A_θ that leaves u_θ invariant (i.e., $A_\theta u_\theta = u_\theta$).*

In practice, Assumption 4.3 is easy to satisfy. For instance, suppose that $\phi : \mathcal{Y} \to \mathbb{R}^d$ is a feature function, $\theta = [\theta_0 \ \theta_1] \in \mathbb{R}^{d_0+d}$ are the features controlling u and A, and u_{θ_0} is made tractable by zeroing some features out: $u_{\theta_0}(y) \propto \exp([\theta_0 \ \vec{0}_{d-d_0}]^\top \phi(y))$. Also suppose that A_{θ_1} is a Gibbs sampler that uses all the features: $A_{\theta_1}(y \mid y') \propto \exp(\theta_1^\top \phi(y_i, y'_{\neg i}))$, where i is a randomly chosen coordinate of y. Then, we can satisfy Assumption 4.3 by setting $\theta_1 = [\theta_0 \ \vec{0}_{d-d_0}]$.

Under Assumption 4.3, we can initialize θ by first training u in isolation (which is a convex problem if u_θ parameterizes an exponential family), then initializing A to leave u invariant; this guarantees that the initial log-likelihood is what we would have obtained by just using u by itself. We found this to work well empirically.

As another note, Algorithm 1 naïvely looks like it takes $O(T^2)$ time to compute the gradient for each sample, due

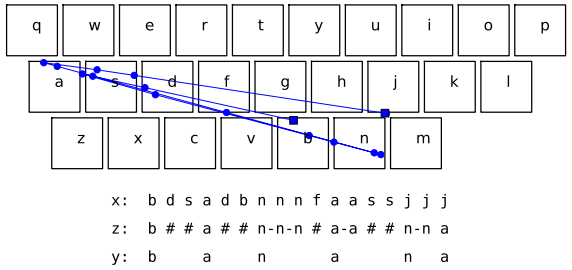


Figure 3. Generated sequence of keyboard gestures for the word *banana*. The input x is a sequence of characters (the recorded key presses), and the output y is the intended word. Most characters in x are incidental and do not correspond to any character in y; this is reflected by the (unobserved) alignment z.

to the nested sum. However, most terms are of the form $w_t \frac{\partial \log A_\theta(y_s|y_{s-1},x)}{\partial \theta}$; by grouping them for a fixed s we can compute the sum in $O(T)$ time, leading to expected runtime $O\left(\frac{k}{\epsilon}\right)$ for Algorithm 1 (since $\mathbb{E}[T+1] = \frac{1}{\epsilon}$).

5. Experiments

We validated our method on two challenging inference tasks. These tasks are difficult due to the importance of high-arity factors; local information is insufficient to even identify high-probability regions of the space.

Inferring Words from Keyboard Gestures We first considered the task of inferring words from keyboard gestures. We generated the data by sampling words from the New York Times corpus (Sandhaus, 2008). For each word, we used a time series model to synthetically generate finger gestures for the word. A typical instantiation of this process is given in Figure 3. The learning task is to discriminatively infer the intended word y given the sequence of keys x that the finger was over (for instance, predicting `banana` from `bdsadbnnnfaassjjj`). In our model, we posit a latent alignment z between key presses and intended letter. Given an input x of length l, the alignment z also has length l; each z_i is either 'c' (x_i starts an output letter c), '$-c$' (x_i continues an output letter c), or '#' (x_i is unaligned); see Figure 3 for an example. Note that y is a deterministic function of z.

The base model u_θ consists of indicator features on (x_i, z_i), (x_i, z_{i-1}, z_i), and (x_i, x_{i-1}, z_i). The full A_θ is a Gibbs sampler in a model where we include the following features in addition to those above:

- indicator features on (x_i, y_i, y_{i-1})
- indicator of y being in the dictionary, as well as log of word frequency (conditioned on being in the dictionary)
- for each i, indicator of $y_{1:i}$ matching a prefix of a word in the dictionary

We compared three approaches:

- Our approach (*Doeblin sampling*)
- Regular Gibbs sampling, initialized by setting $z_i = x_i$ for all i (*basic-Gibbs*)
- Gibbs sampling initialized from u_θ (u_θ-*Gibbs*)

At test time, all three of these methods are almost identical: they all initialize from some distribution, then make a certain number of Gibbs samples. For basic-Gibbs and u_θ-Gibbs, this is always a fixed number of steps T, while for Doeblin sampling the number of steps is a geometric distribution with mean T.

The main difference is in how the methods are trained. Our method is trained using the ideas in Section 4; for the other two methods, we train by approximating the gradient:

$$\nabla \log p_\theta(y \mid x) = \mathbb{E}_{\hat{z} \sim p_\theta(z|x,y)}[\phi(y, \hat{z}, x)] - \mathbb{E}_{\hat{y},\hat{z} \sim p_\theta(y,z|x)}[\phi(\hat{y}, \hat{z}, x)],$$

where $\phi(y, z, x)$ is the feature function and p_θ is the stationary distribution of A_θ. For the second term, we use MCMC samples from A_θ to approximate $p_\theta(y, z \mid x)$. For the first term, we could take the subset of samples where $\hat{y} = y$, but this is problematic if no such samples exist. Instead, we reweight all samples with $\hat{y} \neq y$ by $\exp(-(D+1))$, where D is the edit distance between y and $\hat{y}$. We use the same reweighting approach for the Doeblin sampler, using this as the importance weight rather than using $A_\theta(y \mid y_{t-1})$ as in Algorithm 1.

To provide a fair comparison of the methods, we set ϵ in the Doeblin sampler to the inverse of the number of transitions T, so that the expected number of transitions of all algorithms is the same. We also devoted the first half of each chain to burn-in.

All algorithms are trained with AdaGrad (Duchi et al., 2011) with 16 independent chains run for each example. We measure word-level accuracy by computing the fraction of (non-burn-in) samples whose output y is correct.

The results are reported in Figure 4. Overall, our Doeblin sampler outperforms u_θ-Gibbs by a significant margin, which in turn outperforms basic-Gibbs. Interestingly, while the accuracy of our method continues to improve with more training time, u_θ-Gibbs quickly asymptotes and then slightly decreases, even for training accuracy.

What is happening to u_θ-Gibbs? Since the inference problem in this task is hard, the samples provide a poor gradient approximation. As a result, optimization methods that take the approximation at face value may not converge to even a local optimum. This phenomenon has already been studied in other contexts, for instance by Kulesza and Pereira

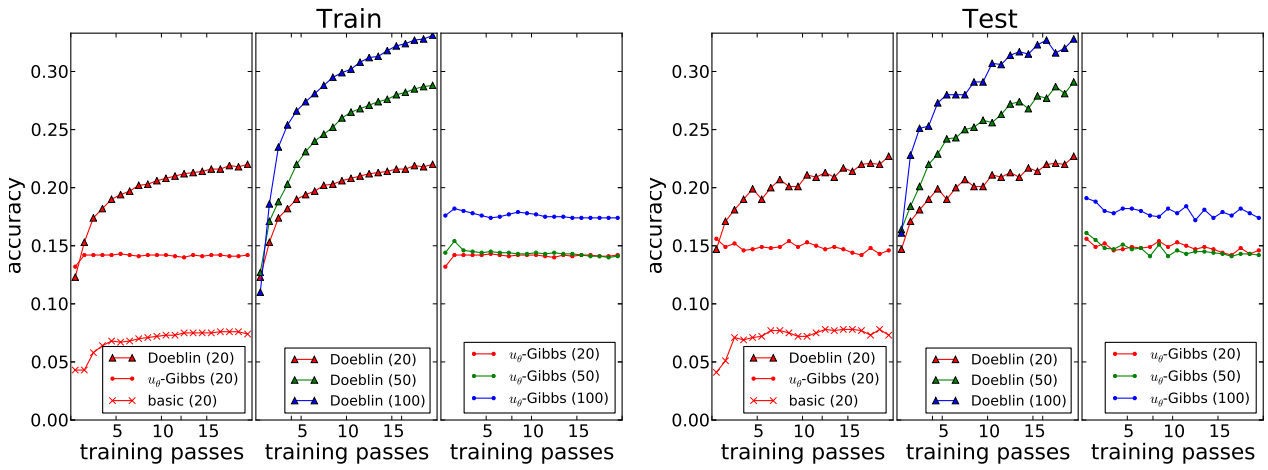


Figure 4. Plots of word-level (left) and character-level (right) accuracy. The first panel gives the performance of all 3 methods (Doeblin chains, smart restarts, and simple Gibbs) for a computational budget of 20 transitions per example. The second and third panels give the performance of Doeblin chains and smart restarts, respectively, for increasing computational budgets (20, 50, and 100 transitions).

(2007) and Huang et al. (2012).

In contrast, our method directly optimizes the log-likelihood of the data under the distribution $\tilde{\pi}_\theta$, so that accuracy continues to increase with more passes through the training data. This demonstrates that the MCMC samples do provide enough signal to train from, but that naïvely plugging them into a method designed for exact inference will fail to exploit that signal.

Inferring DNF Formulas We next study the use of our staged Doeblin chain construction as a tool for hierarchical initialization. We ignore learning for now, instead treating MCMC as a stochastic search algorithm. Our task of interest is to infer a DNF formula f from its input-output behavior. This is an important subroutine in loop invariant synthesis, where MCMC methods have recently shown great promise (Gulwani and Jojic, 2007; Sharma and Aiken, 2014).

Concretely, the input x might look like this:

$$f(1,2,3) = \texttt{True}$$
$$f(1,4,4) = \texttt{True}$$
$$f(0,1,0) = \texttt{False}$$
$$f(0,2,2) = \texttt{True}$$

Our task is to reconstruct f; in this case, $f(x_1, x_2, x_3) = [x_1 \neq 0] \vee [x_2 = x_3]$.

More formally, we consider DNF formulae with linear inequality predicates: $f(x) = \bigvee_{i=1}^{n} \bigwedge_{j=1}^{m} [a_{ij}^\top x \leq b_{ij}]$, where $a_{ij}, x \in \mathbb{Z}^d$ and $b_{ij} \in \mathbb{Z}$. The formula f maps input vectors to $\{\texttt{True}, \texttt{False}\}$. Given a collection of example inputs and outputs, our goal is to find an f consistent with all examples. Our evaluation metric is the time to find such a formula.

The search space for this problem is extremely large. Even if we set $n = m = 3$ and restrict our search to $a_{ij} \in \{-1, 0, 1\}^5$, $b \in \{-1, 0, 1\}$, the total number of candidate formulae is still $\left(3^6\right)^{3\times 3} \approx 5.8 \times 10^{25}$.

We consider three MCMC methods: no restarts (0-stage), uniformly random restarts (1-stage), and a staged method (2-stage) as in Section 3.1. All base chains perform Metropolis-Hastings using proposals that edit individual atoms (e.g., $[a_{ij}^\top x \leq b_{ij}]$), either by changing a single entry of $[a_{ij}\ b_{ij}]$ or by changing all entries of $[a_{ij}\ b_{ij}]$ at once. For the staged method, we initialize uniformly at random, then take $\text{Geometric}(0.04)$ transitions based on a simplified cost function, then take $\text{Geometric}(0.0002)$ steps with the full cost (this is the staged Doeblin chain in Figure 2).

The full cost function is $I(f)$, the number of examples f errs on. We stop the Markov chain when it finds a formula with $I(f) = 0$. The simplified cost function decomposes over the disjuncts: for each disjunct $d(x)$, if $f(x) = \texttt{False}$ while $d(x) = \texttt{True}$, we incur a large cost (since in order for $f(x)$ to be false, all disjuncts comprising $f(x)$ must also be false). If $f(x) = \texttt{True}$ while $d(x) = \texttt{False}$, then we incur a smaller cost. If $f(x) = d(x)$ then we incur no cost.

We used all three methods as a subroutine in verifying properties of C programs; each such verification requires solving many instances of DNF formula inference. Using the staged method we are able to obtain a 30% speedup over uniformly random restarts and a 50x improvement over no restarts, as shown in Table 1.

Table 1. Comparison of 3 different MCMC algorithms. 0-stage uses no restarts, 1-stage uses random restarts, and 2-stage uses random restarts followed by a short period of MH with a simplified cost function. The table gives mean time and standard error (in seconds) taken to verify 5 different C programs, for 1000 trials. Each verification requires inferring many DNF formulae as a sub-routine.

Task	fig1	cegar2	nested	tacas06	hard
0-stage	2.6 ± 1.0	320 ± 9.3	120 ± 7.0	≥ 600	≥ 600
1-stage	0.074 ± 0.001	0.41 ± 0.01	2.4 ± 0.10	6.8 ± 0.15	52 ± 1.5
2-stage	0.055 ± 0.005	0.33 ± 0.007	2.3 ± 0.12	4.6 ± 0.12	31 ± 0.90

6. Discussion

We have proposed a model family based on strong Doeblin Markov chains, which guarantee fast mixing. Our construction allows us to simultaneously leverage a simple, tractable model (u_θ) that provides coverage together with a complex, accurate model (A_θ) that provides precision. As such, we sidestep a typical dilemma—whether to use a simple model with exact inference, or to deal with the consequences of approximate inference in a more complex model.

While our approach works well in practice, there are still some outstanding issues. One is the non-convexity of the learning objective, which makes the procedure dependent on initialization. Another issue is that the gradients returned by Algorithm 1 can be large, heterogeneous, and high-variance. The adaptive nature of AdaGrad alleviates this somewhat, but it would still be ideal to have a sampling procedure that had lower variance than Algorithm 1.

Though Gibbs sampling is the de facto method for many practitioners, there are also many more sophisticated approaches to MCMC (Green, 1995; Earl and Deem, 2005). Since our framework is orthogonal to the particular choice of transition kernel, it would be interesting to apply our method in these contexts.

Finally, we would like to further explore the staged construction from Section 3.1. As the initial results on DNF formula synthesis are promising, it would be interesting to apply the construction to high-dimensional feature spaces as well as rich, multi-level hierarchies. We believe this might be a promising approach for extremely rich models in which a single level of re-initialization is insufficient to capture the complexity of the cost landscape.

Related work. Our learning algorithm is reminiscent of policy gradient algorithms in reinforcement learning (Sutton et al., 2000), as well as Searn, which tries to learn an optimal search policy for structured prediction (Daumé III et al., 2009); see also Shi et al. (2015), who apply reinforcement learning in the context of MCMC. Our staged construction is also similar in spirit to path sampling (Gelman and Meng, 1998), as it uses a multi-stage approach to smoothly transition from a very simple to a very complex distribution.

Our staged Doeblin construction belongs to the family of coarse-to-fine inference methods, which operate on progressively more complex models (Viola and Jones, 2004; Shen et al., 2004; Collins and Koo, 2005; Charniak et al., 2006; Carreras et al., 2008; Gu et al., 2009; Weiss et al., 2010; Sapp et al., 2010; Petrov, 2011; Yadollahpour et al., 2013).

On the theoretical front, we make use of the well-developed theory of *strong Doeblin chains*, often also referred to with the terms *minorization* or *regeneration time* (Doeblin, 1940; Roberts and Tweedie, 1999; Meyn and Tweedie, 1994; Athreya and Ney, 1978). The strong Doeblin property is typically used to study convergence of continuous-space Markov chains, but Rosenthal (1995) has used it to analyze Gibbs sampling, and several authors have provided algorithms for sampling exactly from arbitrary strong Doeblin chains (Propp and Wilson, 1996; Corcoran and Tweedie, 1998; Murdoch and Green, 1998). We are the first to use strong Doeblin properties to construct model families and learn them from data.

At a high level, our idea is to identify a family of models for which an approximate inference algorithm is known to work well, thereby constructing a computationally tractable model family that is nevertheless more expressive than typical tractable families such as low-tree-width graphical models. We think this general program is very interesting, and could be applied to other inference algorithms as well, thus solidfying the link between statistical theory and practical reality.

References

KB Athreya and P Ney. A new approach to the limit theory of recurrent Markov chains. *Transactions of the AMS*, 1978.

Xavier Carreras, Michael Collins, and Terry Koo. Tag, dynamic programming, and the perceptron for efficient, feature-rich parsing. In *CoNLL*, 2008.

E Charniak, M Johnson, M Elsner, J Austerweil, D Ellis,

I Haxton, C Hill, R Shrivaths, J Moore, M Pozar, et al. Multilevel coarse-to-fine PCFG parsing. In *NAACL*, 2006.

Michael Collins and Terry Koo. Discriminative reranking for natural language parsing. *Computational Linguistics*, 31(1):25–70, 2005.

JN Corcoran and RL Tweedie. Perfect sampling of Harris recurrent Markov chains. *preprint*, 1998.

MK Cowles and BP Carlin. Markov chain Monte Carlo convergence diagnostics: a comparative review. *Journal of the American Statistical Association*, 1996.

H Daumé III, J Langford, and D Marcu. Search-based structured prediction. *Machine learning*, 2009.

W Doeblin. Elements d'une theorie generale des chaines simples constantes de markoff. In *Annales scientifiques de l'École Normale Supérieure*, volume 57, pages 61–111. Société mathématique de France, 1940.

J Duchi, E Hazan, and Y Singer. Adaptive subgradient methods for online learning and stochastic optimization. *Journal of Machine Learning Research*, pages 2121–2159, 2011.

David J Earl and Michael W Deem. Parallel tempering: Theory, applications, and new perspectives. *Physical Chemistry Chemical Physics*, 7(23):3910–3916, 2005.

A Gelman and XL Meng. Simulating normalizing constants: From importance sampling to bridge sampling to path sampling. *Statistical science*, 1998.

A Gelman and DB Rubin. A single series from the Gibbs sampler provides a false sense of security. *Bayesian statistics*, 1992.

PJ Green. Reversible jump Markov chain Monte Carlo computation and Bayesian model determination. *Biometrika*, 1995.

Chunhui Gu, Joseph J Lim, Pablo Arbeláez, and Jitendra Malik. Recognition using regions. In *CVPR*, pages 1030–1037. IEEE, 2009.

S Gulwani and N Jojic. Program verification as probabilistic inference. In *ACM SIGPLAN Notices*, 2007.

Liang Huang, Suphan Fayong, and Yang Guo. Structured perceptron with inexact search. In *Proceedings of the 2012 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies*, pages 142–151. Association for Computational Linguistics, 2012.

Alex Kulesza and Fernando Pereira. Structured learning with approximate inference. In *Advances in neural information processing systems*, pages 785–792, 2007.

DA Levin, Y Peres, and EL Wilmer. *Markov chains and mixing times*. 2009.

SP Meyn and RL Tweedie. Computable bounds for geometric convergence rates of Markov chains. *The Annals of Applied Probability*, 1994.

DJ Murdoch and PJ Green. Exact sampling from a continuous state space. *Scandinavian Journal of Stat.*, 1998.

I Murray and R Salakhutdinov. Notes on the KL-divergence between a Markov chain and its equilibrium distribution. 2008.

S Petrov. *Coarse-to-fine natural language processing*. 2011.

JG Propp and DB Wilson. Exact sampling with coupled Markov chains and applications to statistical mechanics. *Random structures and Algorithms*, 9(1-2):223–252, 1996.

GO Roberts and RL Tweedie. Bounds on regeneration times and convergence rates for Markov chains. *Stochastic Processes and their applications*, 80(2):211–229, 1999.

JS Rosenthal. Minorization conditions and convergence rates for markov chain monte carlo. *JASA*, 1995.

Evan Sandhaus. The new york times annotated corpus. *Linguistic Data Consortium, Philadelphia*, 6(12):e26752, 2008.

B Sapp, A Toshev, and B Taskar. Cascaded models for articulated pose estimation. In *ECCV*, 2010.

R Sharma and A Aiken. From invariant checking to invariant inference using randomized search. In *CAV*, 2014.

Libin Shen, Anoop Sarkar, and Franz Josef Och. Discriminative reranking for machine translation. In *NAACL*, pages 177–184, 2004.

Tianlin Shi, Jacob Steinhardt, and Percy Liang. Learning where to sample in structured prediction. 2015.

RS Sutton, D Mcallester, S Singh, and Y Mansour. Policy gradient methods for reinforcement learning with function approximation. In *NIPS*, 2000.

Paul Viola and Michael J Jones. Robust real-time face detection. *International journal of computer vision*, 57(2): 137–154, 2004.

Martin J Wainwright. Estimating the wrong graphical model: Benefits in the computation-limited setting. *The Journal of Machine Learning Research*, 7:1829–1859, 2006.

David Weiss, Benjamin Sapp, and Ben Taskar. Sidestepping intractable inference with structured ensemble cascades. In *NIPS*, volume 1281, pages 1282–1284, 2010.

Payman Yadollahpour, Dhruv Batra, and Gregory Shakhnarovich. Discriminative re-ranking of diverse segmentations. In *CVPR*, pages 1923–1930. IEEE, 2013.

A. Proofs

Proof of Proposition 3.1. We will in fact show that, for all $k > 1$, $\lambda_k(\tilde{A}) = (1-\epsilon)\lambda_k(A)$, with the same eigenvector for both matrices. In other words, while the stationary distribution of $\tilde{A}$ is different from A, all other eigenvectors are unchanged.

Let w_k be the eigenvector of A corresponding to λ_k. First note that $1^\top w_k = 0$. This is because

$$1^\top A w_k = 1^\top w_k \tag{8}$$

since A is stochastic, and

$$1^\top A w_k = \lambda_k 1^\top w_k \tag{9}$$

since w_k is an eigenvector of A. Since $\lambda_k \neq 1$, this implies that $1^\top w_k = 0$.

Now we have

$$\begin{aligned}\tilde{A} w_k &= (1-\epsilon) A w_k + \epsilon u 1^\top w_k \\ &= (1-\epsilon)\lambda_k w_k,\end{aligned}$$

which proves that $\lambda_k(\tilde{A}) = (1-\epsilon)\lambda_k(A)$. In particular, $\lambda_2(\tilde{A}) = (1-\epsilon)\lambda_2(A) \leq 1-\epsilon$. The mixing time of $\tilde{A}$ is $\frac{1}{1-\lambda_2(\tilde{A})}$, and is therefore upper bounded by $\frac{1}{\epsilon}$, which completes the proof. □

Proof of Proposition 3.2. We can verify algebraically that $\tilde{A}\tilde{\pi} = \tilde{\pi}$, as follows:

$$\begin{aligned}\tilde{A}\tilde{\pi} &= (1-\epsilon)A\tilde{\pi} + \epsilon u 1^\top \tilde{\pi} \\ &= \epsilon(1-\epsilon)A(I-(1-\epsilon)A)^{-1}u + \epsilon u \\ &= \epsilon\left[(1-\epsilon)A(I-(1-\epsilon)A)^{-1} + I\right]u \\ &= \epsilon\left[(1-\epsilon)A + (I-(1-\epsilon)A)\right](I-(1-\epsilon)A)^{-1}u \\ &= \epsilon(I-(1-\epsilon)A)^{-1}u \\ &= \tilde{\pi},\end{aligned}$$

so that $\tilde{\pi}$ is indeed the stationary distribution of $\tilde{A}$. □

Proof of Proposition 3.5. From the characterization of $\tilde{\pi}$ in Proposition 3.2, we know that $\tilde{\pi}$ is equal to

$$\epsilon \sum_{j=0}^{\infty} (1-\epsilon)^j A^j u. \tag{10}$$

The rest of the proof consists of determining some useful properties of $d_\pi(\pi')$. The most important (and the motivation for defining d_π in the first place) is given in the following lemma, which we prove separately:

Lemma A.1. *If π is the stationary distribution of A and A satisfies detailed balance, then $d_\pi(A\pi') \leq \lambda_2(A) d_\pi(\pi')$.*

The other important property of $d_\pi(\pi')$ is convexity: $d_\pi(w\pi' + (1-w)\pi'') \leq w d_\pi(\pi') + (1-w) d_\pi(\pi'')$, which follows directly from the characterization of $d_\pi(\pi')$ as a Mahalanobis distance.

Putting these two properties together, we have

$$\begin{aligned}d_\pi(\tilde{\pi}) &\leq \epsilon \sum_{j=0}^{\infty} (1-\epsilon)^j d_\pi(A^j u) \\ &\leq \epsilon \sum_{j=0}^{\infty} (1-\epsilon)^j \lambda_2(A)^j d_\pi(u) \\ &\leq \frac{\epsilon}{1-(1-\epsilon)\lambda_2(A)} d_\pi(u) \\ &\leq \frac{\epsilon}{1-\lambda_2(A)} d_\pi(u),\end{aligned}$$

which completes the proof. □

Proof of Lemma A.1. Recall we want to show that $d_\pi(A\pi') \leq \lambda_2(A) d_\pi(\pi')$. To see this, first define $S = \operatorname{diag}(\pi)^{-1/2} A \operatorname{diag}(\pi)^{1/2}$, which is symmetric by the detailed balance condition, and satisfies $\lambda_k(S) = \lambda_k(A)$ by similarity. Furthermore, the top eigenvector of S is $\mathbb{1}^\top \operatorname{diag}(\pi)^{1/2}$. Putting these together, we have

$$\begin{aligned} d_\pi(A\pi') &= \|\operatorname{diag}(\pi)^{-1/2}(\pi - A\pi')\|_2 \\ &= \|\operatorname{diag}(\pi)^{-1/2} A(\pi - \pi')\|_2 \\ &= \|S \operatorname{diag}(\pi)^{-1/2}(\pi - \pi')\|_2 \\ &\leq \lambda_2(S) \|\operatorname{diag}(\pi)^{-1/2}(\pi - \pi')\|_2 \\ &= \lambda_2(S) d_\pi(\pi') \\ &= \lambda_2(A) d_\pi(\pi'). \end{aligned}$$

The inequality step $\|S \operatorname{diag}(\pi)^{-1/2}(\pi - \pi')\|_2 \leq \lambda_2(S) \|\operatorname{diag}(\pi)^{-1/2}(\pi - \pi')\|_2$ follows because $\operatorname{diag}(\pi)^{-1/2}(\pi - \pi')$ is orthogonal to the top eigenvector $\mathbb{1}^\top \operatorname{diag}(\pi)^{1/2}$ of S. □

Proof of Proposition 3.4. For any value of ϵ, the stationary distribution $\tilde{\pi}_\epsilon$ of $(1-\epsilon)A + \epsilon u \mathbb{1}^\top$ can be obtained by applying A a $\text{Geometric}(\epsilon)$-distributed number of times to u (by Proposition 3.2). For $\epsilon_2 < \epsilon_1$, it therefore suffices to construct a random variable $F \geq 0$ such that if $s \sim F$ and $t \sim \text{Geometric}(\epsilon_1)$ then $s + t \sim \text{Geometric}(\epsilon_2)$; if we can do this, then we can let B be the matrix that applies A an F-distributed number of times, and we would have $B\tilde{\pi}_{\epsilon_1} = \tilde{\pi}_{\epsilon_2}$; but B would clearly have stationary distribution π, and so Lemma 3.3 would give $\mathrm{KL}(\pi \parallel \tilde{\pi}_{\epsilon_2}) \leq \mathrm{KL}(\pi \parallel \tilde{\pi}_{\epsilon_1})$ and $\mathrm{KL}(\tilde{\pi}_{\epsilon_2} \parallel \pi) \leq \mathrm{KL}(\tilde{\pi}_{\epsilon_1} \parallel \pi)$, which is the desired result.

To construct the desired F, we use the fact that addition of random variables corresponds to convolution of the probability mass functions, and furthermore represent the probability mass functions as formal power series; in particular, we let

$$f(x) = \sum_{n=0}^{\infty} \mathbb{P}[t = n \mid t \sim F] x^n, \tag{11}$$

and similarly

$$\begin{aligned} g_\epsilon(x) &= \sum_{n=0}^{\infty} \mathbb{P}[t = n \mid t \sim \text{Geometric}(\epsilon)] x^n \\ &= \sum_{n=0}^{\infty} \epsilon(1-\epsilon)^n x^n \\ &= \frac{\epsilon}{1 - (1-\epsilon)x}. \end{aligned}$$

We want $f(x) g_{\epsilon_1}(x)$ to equal $g_{\epsilon_2}(x)$, so we take

$$\begin{aligned} f(x) &= \frac{g_{\epsilon_2}(x)}{g_{\epsilon_1}(x)} \\ &= \frac{\epsilon_2}{\epsilon_1} \frac{1 - (1-\epsilon_1)x}{1 - (1-\epsilon_2)x} \\ &= \frac{\epsilon_2}{\epsilon_1} \left(1 + \sum_{n=1}^{\infty} \left[(1-\epsilon_2)^n - (1-\epsilon_2)^{n-1}(1-\epsilon_1) \right] x^n \right) \\ &= \frac{\epsilon_2}{\epsilon_1} \left(1 + \sum_{n=1}^{\infty} (1-\epsilon_2)^{n-1}(\epsilon_1 - \epsilon_2) x^n \right). \end{aligned}$$

From this we see that the random variable F with probability function

$$\mathbb{P}[t = n \mid t \sim F] = \begin{cases} \frac{\epsilon_2}{\epsilon_1} & : \quad n = 0 \\ \frac{\epsilon_2}{\epsilon_1}(1-\epsilon_2)^{n-1}(\epsilon_1 - \epsilon_2) & : \quad n > 0 \end{cases} \tag{12}$$

satisfies the required property that $F + \text{Geometric}(\epsilon_1) = \text{Geometric}(\epsilon_2)$. Note that the condition $\epsilon_2 < \epsilon_1$ is necessary here so that all of the probability masses are positive in the above expression.

We can also prove the result purely algebraically. Motivated by the above construction, we define

$$\begin{aligned} B &= \epsilon_2 (I - (1-\epsilon_2)A)^{-1} \left[\epsilon_1 (I - (1-\epsilon_1)A)^{-1}\right]^{-1} \\ &= \frac{\epsilon_2}{\epsilon_1} \left[I + (\epsilon_1 - \epsilon_2) A (I - (1-\epsilon_2)A)^{-1}\right]. \end{aligned}$$

By construction we have $B\tilde{\pi}_{\epsilon_1} = \tilde{\pi}_{\epsilon_2}$, but Taylor expanding the second expression for B shows that we can write it as a (infinite) convex combination of non-negative powers of A, and hence that B has stationary distribution π. This again yields the desired result by Lemma 3.3. □

Proof of Theorem 3.6. We use an equivalent characterization of the strong Doeblin parameter as the quantity $\Gamma(A) = \sum_y \inf_{y'} A(y \mid y')$. In the context of the Markov chain M, this yields

$$\begin{aligned} \Gamma(M^b) &= \sum_{(z_b, y_b)} \inf_{(z_0, y_0)} \mathbb{P}[z_b, y_b \mid z_0, y_0] \\ &= \sum_{(z_b, y_b)} \inf_{(z_0, y_0)} \sum_{\tau=a}^{b} \mathbb{P}[\tau_a = \tau \mid y_0] \times \mathbb{P}[z_b, y_b \mid \tau_a = \tau] \\ &\geq \sum_{(z_b, y_b)} \sum_{\tau=a}^{b} \inf_{y_0} \mathbb{P}[\tau_a = \tau \mid y_0] \times \mathbb{P}[z_b, y_b \mid \tau_a = \tau] \\ &= \sum_{\tau=a}^{b} \inf_{y_0} \mathbb{P}[\tau_a = \tau \mid y_0] \sum_{(z_b, y_b)} \mathbb{P}[z_b, y_b \mid \tau_a = \tau] \\ &= \sum_{\tau=a}^{b} \inf_{y_0} \mathbb{P}[\tau_a = \tau \mid y_0] \\ &= \gamma_{a,b}. \end{aligned}$$

Finally, by Proposition 3.1, the spectral gap of M^b is at least $\gamma_{a,b}$, hence the spectral gap of M is at least $\frac{1}{b}\gamma_{a,b}$, which proves the theorem. □

Proof of Corollary 3.7. Note that the time to transition from i to $i+1$ is $\text{Geometric}(\delta_i)$-distributed. Suppose we start from an arbitrary $j \in \{0, \ldots, k-1\}$. Then the time t' to get to $k-1$ is distributed as $\sum_{i=j}^{k-2} \text{Geometric}(\delta_i)$. t' has mean $\sum_{i=j}^{k-2} \frac{1}{\delta_i} \leq \frac{1}{\delta_{k-1}}$, and variance $\sum_{i=j}^{k-2} \frac{1-\delta_i}{\delta_i^2} \leq \frac{1}{2\delta_{k-1}^2}$. In particular, with probability $\frac{1}{2}$, t' lies between 0 and $\left\lfloor \frac{2}{\delta_{k-1}} \right\rfloor$. Now, consider the time t'' to get from $k-1$ to 0; this is $\text{Geometric}(\delta_{k-1})$-distributed, and conditioned on t'' being at least $\frac{2}{\delta_{k-1}}$, $t'' + t' - \frac{2}{\delta_{k-1}}$ is also $\text{Geometric}(\delta_{k-1})$-distributed. But t'' is at least $\lfloor \frac{2}{\delta_{k-1}} \rfloor$ with probability at least $(1-\delta_{k-1})^{2/\delta k-1} \geq \frac{1}{16}$ (since $\delta_{k-1} \leq \frac{1}{2}$). Hence independently of j, $t'' + t'$ is, with probability at least $\frac{1}{16}$, distributed according to $\lfloor \frac{2}{\delta_{k-1}} \rfloor + \text{Geometric}(\delta_{k-1})$. But $t'' + t' = \tau$ by construction, and so we need only compute the probability that $\tau \leq \lceil \frac{3}{\delta_{k-1}} \rfloor$; but this is just the probability that the geometric distribution is less than $\frac{1}{\delta_{k-1}}$, which is $1 - (1-\delta_{k-1})^{1/\delta_{k-1}} \geq 1 - e^{-1}$. Therefore, $\gamma(t_0, t) \geq \frac{1-e^{-1}}{16} \geq \frac{1}{26}$; expanding the definitions of t_0 and t, we have that $\gamma_{\lfloor 2/\delta_{k-1} \rfloor, \lceil 3/\delta_{k-1} \rceil} \geq \frac{1}{26}$. Applying Theorem 3.6 then implies that the spectral gap of M is at least $\frac{\delta_{k-1}}{78}$, as was to be shown. □

Proof of Lemma 4.2. The key idea is to use the identity $\frac{\partial f}{\partial x} = f(x)\frac{\partial \log f(x)}{\partial x}$ in two places. We have

$$\begin{aligned} p_\theta(z \in S)\frac{\partial \log p_\theta(z \in S)}{\partial \theta} &= \frac{\partial}{\partial \theta} p_\theta(z \in S) \\ &= \int_S \frac{\partial p_\theta(z)}{\partial \theta} dz \\ &= \int_S p_\theta(z)\frac{\partial \log p_\theta(z)}{\partial \theta} dz \\ &= p_\theta(z \in S)\mathbb{E}_z\left[\frac{\partial \log p_\theta(z)}{\partial \theta}\middle| z \in S\right], \end{aligned}$$

which completes the lemma. □

B. Correctness of Importance Sampling Algorithm

In Section 4.1 of the main text, we had a distribution u over $\mathcal{Y}$ and a Markov chain $A(y_t \mid y_{t-1})$ on the same space. We then built a distribution over $\mathcal{Y}^* \stackrel{\text{def}}{=} \bigcup_{T \geq 0}\{T\} \times \mathcal{Y}^T$ by sampling $T \sim \text{Geometric}(\epsilon)$, $y_0 \sim u$, and $y_t \mid y_{t-1} \sim A$ for $y = 1, \ldots, T$ (we use $p_T(y_{0:T})$ to represent the distribution over $y_{0:T}$ given T).

For a given y, we were interested in constructing an importance sampler for $(T, y_{0:T}) \mid y_T = y$. The following Lemma establishes the correctness of the importance sampler that was presented. We assume we are interested in computing the expectation of some function $g : \mathcal{Y}^* \to \mathbb{R}$ and show that the given importance weights correctly estimate $\mathbb{E}[g]$.

Lemma B.1. *For a distribution F, suppose that we sample $T \sim F$ and then sample $y_{0:T-1} \sim p_{T-1}$. Let $w_t = \frac{\epsilon(1-\epsilon)^t}{\mathbb{P}[T \geq t | T \sim F]} A(y \mid y_{t-1})$. Consider the random variable*

$$\hat{g} \stackrel{\text{def}}{=} \sum_{t=0}^{T} w_t g(t, y_{0:t-1}, y). \tag{13}$$

Then

$$\mathbb{E}_{T \sim F, y_{0:T-1} \sim p_{T-1}}[\hat{g}] = \mathbb{E}_{T \sim \text{Geometric}(\epsilon), y_{0:T} \sim p_T}\left[g(T, y_{0:T})\mathbb{I}[y_T = y]\right]. \tag{14}$$

Proof. We have

$$\begin{aligned} \mathbb{E}_{T \sim F, y_{0:T-1} \sim p}[\hat{g}] &= \mathbb{E}_{T \sim F, y_{0:T-1} \sim p_{T-1}}\left[\sum_{t=0}^{T} w_t g(t, y_{0:t-1}, y)\right] \\ &= \sum_{t=0}^{\infty} \mathbb{P}[T \geq t \mid T \sim F]\mathbb{E}_{y_{0:t-1} \sim p_{t-1}}\left[w_t g(t, y_{0:t-1}, y)\right] \\ &= \sum_{t=0}^{\infty} \epsilon(1-\epsilon)^t \mathbb{E}_{y_{0:t-1} \sim p_{t-1}}\left[A(y \mid y_{t-1}) g(t, y_{0:t-1}, y)\right] \\ &= \sum_{t=0}^{\infty} \epsilon(1-\epsilon)^t \mathbb{E}_{y_{0:t} \sim p_t}\left[g(t, y_{0:t})\mathbb{I}[y_t = y]\right] \\ &= \mathbb{E}_{T \sim \text{Geometric}(\epsilon), y_{0:T} \sim p_T}\left[g(T, y_{0:T})\mathbb{I}[y_T = y]\right], \end{aligned}$$

as was to be shown. □