Abstract

State space models (SSMs) are a flexible approach to modeling complex time series. However, inference in SSMs is often computationally prohibitive for long time series. Stochastic gradient MCMC (SGMCMC) is a popular method for scalable Bayesian inference for large independent data. Unfortunately when applied to dependent data, such as in SSMs, SGMCMC’s stochastic gradient estimates are biased as they break crucial temporal dependencies. To alleviate this, we propose stochastic gradient estimators that control this bias by performing additional computation in a ‘buffer’ to reduce breaking dependencies. Furthermore, we derive error bounds for this bias and show a geometric decay under mild conditions. Using these estimators, we develop novel SGMCMC samplers for discrete, continuous and mixed-type SSMs. Our experiments on real and synthetic data demonstrate the effectiveness of our SGMCMC algorithms compared to batch MCMC, allowing us to scale inference to long time series with millions of time points.

1 Introduction

State space models (SSMs) are ubiquitous in the analysis of time series in fields as diverse as biology [69], finance and economics [40, 74], and systems and control [26]. As a defining feature, SSMs augment the observed time series with a latent state sequence to model complex time series dynamics with a latent Markov chain dependence structure. Given a time series, inference of model parameters involves sampling or marginalizing this latent state sequence. Unfortunately, both the runtime and memory required scale with the length of the time series, which is prohibitive for long time series (e.g. high frequency stock prices [33], genome sequences [25], or neural impulse recordings [16]). In practice, given a long time series, one could ‘segment’ or ‘downsample’ to reduce length; however, this preprocessing can destroy or change important signals and computational considerations should ideally not limit scientific modeling.

To help scale inference in SSMs, we consider stochastic gradient Markov chain Monte Carlo (SGMCMC), a popular method for scaling Bayesian inference to large data sets [12, 47, 68]. The key idea of SGMCMC is to employ stochastic gradient estimates based on subsets or ‘minibatches’ of data, avoiding costly computation of gradients on the full dataset, such that the resulting dynamics produce samples from the posterior distribution over SSM parameters. This approach has found much success in independent data models, where the stochastic gradients are unbiased estimates of the true gradients. However, when applying SGMCMC to SSMs, naive stochastic gradients are biased, as subsampling the data breaks dependencies.

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in the SSM’s latent state sequence. This bias can destroy the dynamics of SGMCMC causing it to fail when applied to SSMs. The challenge is to correct these stochastic gradients for SSMs while maintaining the computational benefits of SGMCMC.

In this work, we develop computationally efficient stochastic gradient estimators for inference in general discrete-time SSMs. To control the bias of stochastic gradients, we marginalize the latent state sequence in a buffer around each subsequence, propagating critical information from outside each subsequence to its local gradient estimate while avoiding costly full-chain computations. Similar buffering ideas have been previously considered for belief propagation [32], variational inference [27], and in our earlier work on SGMCMC for hidden Markov models (HMMs) [48], but all are limited to discrete latent states. Here, we present buffering as an approximation to Fisher’s identity [9], allowing us to naturally extend buffering trick to continuous and mixed-type latent states.

We further develop analytic bounds on the bias of our proposed gradient estimator that, under mild conditions, decay geometrically in the buffer size. To obtain these bounds we prove that the latent state sequence posterior distribution has an exponential forgetting property [9, 17]. However unlike classic results which prove a geometric decay between the approximate and exact marginal posterior distributions in total variation distance, we use Wasserstein distance [66] to allow analysis of continuous and mixed-type latent state SSMs. Our approach is similar to proofs of Wasserstein ergodicity in homogeneous Markov chains [24, 49, 57]; however we extend these ideas to the nonhomogeneous Markov chains defined by the latent state sequence posterior distribution. These geometrically decaying bounds guarantee that we only need a small buffer size in practice, allowing scalable inference in SSMs.

Although our proposed gradient estimator can be generally applied to any stochastic gradient method, here, we develop SGMCMC samplers for Bayesian inference in a variety of SSMs such as HMMs, linear Gaussian SSMs (LGSSM), and switching linear dynamical systems (SLDS) [9, 29]. We also derive preconditioning matrices to take advantage of information geometry, which allows for more rapid mixing and convergence of our samplers [31, 52]. Finally, we validate our algorithms and theory on a variety of synthetic and real data experiments, finding that our gradient estimator can provide orders of magnitude run-time speed ups compared to batch sampling.

This paper significantly expands upon our initial work [48], by (i) connecting buffering to Fisher’s identity, simplifying its presentation and analysis, (ii) non-trivially generalizing the approach to SSMs beyond the HMM, including continuous and mixed-type latent states, (iii) developing a general framework for bounding the error of buffered gradient estimators using Wasserstein distance, and (iv) providing extensive validation on a number of real and synthetic datasets.

The paper is organized as follows. First, we review background on SSMs and SGMCMC methods in Section 2. We then present our framework of constructing buffered gradient estimators to extend SGMCMC to SSMs in Section 3. We prove the geometrically decaying bounds for our proposed buffered gradient estimate in Section 4. We apply our framework and error bounds to discrete, continuous and mixed-type latent state SSMs in Section 5. Finally, we investigate our algorithms on both synthetic and real data in Section 6.
2 Background

2.1 State Space Models for Time Series

State space models (SSMs) for time series are a class of discrete-time bivariate stochastic process \( \{u_t, y_t\}_{t \in T}, \ T = \{-T, \ldots, T\} \), consisting of a latent state sequence \( u := u_{-T:T} \) generated by a homogeneous Markov chain and an observation sequence \( y := y_{-T:T} \) generated independently conditioned on \( u \) [9]. Examples of state space models include: HMMs, LGSSMs, and SLDSs (see Section 5 for details). For a generic SSM, the joint distribution of \( y \) and \( u \) factorizes as

\[
\Pr(y, u | \theta) = \prod_{t=1}^{T} \Pr(y_t | u_t, \theta) \Pr(u_t | u_{t-1}, \theta),
\]

(1)

where \( \theta \) are model-specific parameters. As the latent state sequence \( u \) is unobserved, the likelihood of \( \theta \) given only the observations \( y \) (marginalizing \( u \)) is

\[
\Pr(y | \theta) = \int \prod_{t=1}^{T} \Pr(y_t | u_t, \theta) \Pr(u_t | u_{t-1}, \theta) \, du,
\]

(2)

Unconditionally, the observations \( y \) are not independent and the graphical model of this marginal likelihood, Eq. (2), has many long term dependencies, Figure 1 (right). In contrast, when conditioned on \( u \) the observations \( y \) are independent and the complete-data likelihood, Eq. (1), has a simpler chain structure, Figure 1 (left).

To infer \( \theta \) given \( y \), we can maximize the marginal likelihood \( \Pr(y | \theta) \) or, given a prior \( \Pr(\theta) \), sample from the posterior \( \Pr(\theta | y) \propto \Pr(y | \theta) \Pr(\theta) \). However, traditional inference methods for \( \theta \), such as expectation maximization (EM), variational inference, or Markov chain Monte Carlo (MCMC), take advantage of the conditional independence structure in \( \Pr(y, u | \theta) \), Eq. (1), rather than working directly with \( \Pr(y | \theta) \), Eq. (2) [5, 58]. To use \( \Pr(y, u | \theta) \) with unobserved \( u \), these methods rely on sampling or taking expectations of \( u \) from the posterior \( \gamma(u) := \Pr(u | y, \theta) \). As an example, gradient-based methods take advantage of Fisher’s identity [9]

\[
\nabla \log \Pr(y | \theta) = \mathbb{E}_{u,y,\theta}[\nabla \log \Pr(y, u | \theta)] = \mathbb{E}_{u \sim \gamma}[\nabla \log \Pr(y, u | \theta)],
\]

(3)

which allows gradients of Eq. (2) to be computed in terms of Eq. (1). To compute the posterior \( \gamma(u) \), these methods use the well-known forward-backward algorithm [9, 58]. The algorithm works by recursively computing a sequence of forward messages \( \alpha_t(u_t) \) and backward messages
\( \beta_t(u_t) \) which are used to compute the pairwise marginals of \( \gamma \). More specifically,

\[
\alpha_t(u_t) := \Pr(u_t, y \leq t | \theta) = \int \Pr(y, u_t, u_{t-1} | \theta) \alpha_{t-1}(u_{t-1}) \, du_{t-1} \tag{4}
\]

\[
\beta_t(u_t) := \Pr(y > t | u_t, \theta) = \int \Pr(y_{t+1}, u_{t+1} | u_t, \theta) \beta_{t+1}(u_{t+1}) \, du_{t+1} \tag{5}
\]

\[
\gamma_{t-1:t}(u_{t-1}, u_t) := \Pr(u_{t-1}, u_t | y, \theta) \propto \alpha_{t-1}(u_{t-1}) \Pr(y, u_t | u_{t-1}, \theta) \beta_t(u_t). \tag{6}
\]

When message passing is tractable (i.e., when Eqs. (4)-(5) involve discrete or conjugate likelihoods), the forward-backward algorithm can be calculated in closed form. When message passing is intractable, the messages can be approximated using Monte-Carlo sampling methods (e.g., blocked Gibbs sampling \([10, 28]\), particle methods \([2, 21, 60]\)). In both cases, when the length of the time series \(|T|\) is much larger than the dimension of \( \theta \), the forward-backward algorithm (running over the entire sequence) requires \( O(|T|) \) time and memory at each iteration.

The SSM challenge is to scale inference of model parameters \( \theta \) to long time series when the computation and storage per iteration \( O(|T|) \) is prohibitive.

### 2.2 Stochastic Gradient MCMC

One popular method for scalable Bayesian inference is stochastic gradient Markov chain Monte Carlo (SGMCMC) \([12, 47, 68]\). The idea behind gradient-based MCMC is to simulate continuous dynamics of a potential energy function \( U(\theta) \propto -\log \Pr(y, \theta) \) such that the dynamics generate samples from the posterior distribution \( \Pr(\theta | y) \). For example, the Langevin diffusion over \( U(\theta) \) is given by the stochastic differential equation (SDE)

\[
d\theta_s = -\nabla U(\theta) \, ds + \sqrt{2} \, dW_s, \tag{7}
\]

where \( dW_s \) is Brownian motion, \( \nabla U(\theta) = -\nabla \theta \log \Pr(y, \theta) \), and \( s \) indexes continuous time. As \( s \to \infty \), the distribution of \( \theta_s \) converges to the SDE’s stationary distribution, which by the Fokker-Planck equation is the posterior \( \Pr(\theta | y) \) \([47, 55]\). Because we cannot perfectly simulate Eq. (7), in practice we use a discretized numerical approximation. One straightforward approximation is the Euler-Mayuruma discretization

\[
\theta^{(s+1)} \leftarrow \theta^{(s)} - h \nabla U(\theta^{(s)}) + \mathcal{N}(0, 2h), \tag{8}
\]

where \( h \) is the stepsize and \( s \) indexes discrete time steps. This recursive update defines the Langevin Monte-Carlo (LMC) algorithm. Typically, a Metropolis-Hastings correction step is added to account for the discretization error \([55]\).

For large datasets, computing \( \nabla U(\theta) \) at every step in Eq. (8) is computationally prohibitive. To alleviate this, the key ideas of stochastic gradient Langevin dynamics (SGLD) are to replace \( \nabla U(\theta) \) with a quick-to-compute unbiased estimator \( \nabla \hat{U}(\theta) \) and to use a decreasing stepsize \( h^{(s)} \) to avoid costly Metropolis-Hastings correction steps \([68]\)

\[
\theta^{(s+1)} \leftarrow \theta^{(s)} - h^{(s)} \nabla \hat{U}(\theta^{(s)}) + \mathcal{N}(0, 2h^{(s)}). \tag{9}
\]

For i.i.d. data, an example of \( \nabla \hat{U}(\theta) \) is to use a random minibatch \( S \subset T \), \(|S| \ll |T|\)

\[
\nabla \hat{U}(\theta) = -\frac{1}{\Pr(S)} \sum_{t \in S} \nabla \log \Pr(y_t | \theta) - \nabla \log \Pr(\theta), \tag{10}
\]
which only requires \(O(|S|)\) time to compute. When \(\nabla \tilde{U}(\theta)\) is unbiased and with an appropriate decreasing stepsize schedule \(h^{(s)}\), SGLD converges to the posterior distribution [12, 61]. However, in practice one uses a small, finite step-size for greater efficiency, which introduces a small bias [15].

A Riemannian extension of SGLD (SGRLD) simulates the Langevin diffusion over a Riemannian manifold with metric \(G(\theta)\) by preconditioning the gradient and noise of Eq. (9) by \(D(\theta) = G(\theta)^{-1}\). By incorporating geometric information about structure of \(\theta\), SGRLD aims for a diffusion which mixes more rapidly. Suggested examples of the metric \(G(\theta)\) are the Fisher information matrix \(I(\theta) = \mathbb{E}_y[\nabla^2 \log \Pr(y | \theta)]\) or a noisy Hessian estimate \(\nabla^2 \tilde{U}(\theta)\) [31, 52]. Given \(G(\theta)\), each step of SGRLD is

\[
\theta^{(s+1)} \leftarrow \theta^{(s)} - h \left[ D(\theta^{(s)}) \nabla \tilde{U}(\theta^{(s)}) + \Gamma(\theta^{(s)}) \right] + \mathcal{N}(0, 2hD(\theta^{(s)}))
\]  

(11)

where the vector \(\Gamma(\theta)\) is a correction term \(\Gamma(\theta)_i = \sum_j \frac{\partial D(\theta)_{ij}}{\partial \theta_j}\) to ensure the dynamics converge to the target posterior [47, 70]. Many other SGMCMC have been proposed [4, 12, 13, 19, 43]. Although our ideas extend to these formulations as well, we focus on the popular SGLD and SGRLD algorithms.

To apply SGMCMC to SSMs, we must choose whether to use the complete-data loglikelihood or the marginal data loglikelihood in the potential \(U(\theta)\). If we use the complete-data loglikelihood, then we treat \((u, \theta)\) as the parameters. Although the observations \(y\) conditioned on \((u, \theta)\) are independent, we must calculate gradients for \(u_{-T:T}\) at each iteration, which is prohibitive for long sequences \(|T|\) and intractable for discrete or mixed-type \(u\). On the other hand, if we use the marginal loglikelihood, then we only need to take gradients in \(\theta\). However, the observations \(y\) conditioned on \(\theta\) alone are not independent and therefore the minibatch gradient estimator Eq. (10) breaks crucial dependencies causing it to be biased. Our SGMCMC challenge is correcting the bias in stochastic gradient estimates \(\nabla \tilde{U}(\theta)\) when applied to SSMs.

### 3 General Framework

We now present our framework for scalable Bayesian inference in SSMs with long observation sequences. Our approach is to extend SGMCMC to SSMs by developing a gradient estimator that ameliorates the issue of broken temporal dependencies. In particular, we develop a computationally efficient gradient estimator that uses a \(u\)-buffer to avoid breaking crucial dependencies, only breaking weak dependencies. We first present a (computationally prohibitive) unbiased estimator of \(\nabla U(\theta)\) for SSMs using Fisher’s identity. We then derive a general computationally efficient gradient estimate \(\nabla \tilde{U}(\theta)\) that accounts for the dependence in observations using a buffer. We also propose preconditioning matrices for SGRLD with SSMs. Finally, we present our general SGMCMC pseudocode for SGRLD.

#### 3.1 Unbiased Gradient Estimate

The main challenge in constructing an efficient estimate \(\nabla \tilde{U}(\theta)\) of \(\nabla U(\theta)\) for SSMs is handling the lack of independence (marginally) in \(y\). Because the observations in SSMs are not independent, we cannot produce an unbiased estimate of \(U(\theta)\) with a randomly selected subset of data points as in Eq. (10). For example, a naive estimate for \(\nabla U(\theta)\) is to take the gradient of a random contiguous subsequence \(S = \{t_1, \ldots, t_S\} \subset T\) with \(t_i = t_{i-1} + 1\)

\[
\nabla \tilde{U}(\theta) = -\frac{1}{\Pr(S)} \nabla \log \Pr(y_S | \theta) - \nabla \log \Pr(\theta) .
\]

(12)
This estimate only requires $O(|S|)$ time compared to the $O(|T|)$ for $\nabla U(\theta)$. However because the marginal likelihood does not factorize as in the independent observations case, this estimate is biased $\mathbb{E}_S[\nabla \hat{U}(\theta)] \neq \nabla U(\theta)$.

To obtain an unbiased estimate for $\nabla U(\theta)$, we use Fisher's identity Eq. (3) to rewrite $\nabla U(\theta)$ in terms of the complete-data loglikelihood as a sum over time points

$$\nabla U(\theta) = -\nabla \log \Pr(y | \theta) - \nabla \log \Pr(\theta)$$

$$= -\mathbb{E}_{u|y, \theta}[\nabla \log \Pr(y, u | \theta)] - \nabla \log \Pr(\theta)$$

$$= -\sum_{t \in T} \mathbb{E}_{u|y, \theta}[\nabla \log \Pr(y_t, u_t | u_{t-1}, \theta)] - \nabla \log \Pr(\theta)$$

From this, we straightforwardly identify an unbiased estimator for a subsequence $S$

$$\nabla \hat{U}(\theta) = -\frac{1}{\Pr(S)} \sum_{t \in S} \mathbb{E}_{u|y, \theta}[\nabla \log \Pr(y_t, u_t | u_{t-1}, \theta)] - \nabla \log \Pr(\theta) .$$

Although Eq. (14) reduces the number of gradient terms to compute from $|T|$ to $|S|$, the summation terms require calculating expectations of $u|y, \theta$. More specifically, Eq. (14) requires expectations with respect to the pairwise marginal posteriors $\Pr(u_t, u_{t-1} | y_T)$ for $t \in S$. Recall that computing these marginals take $O(|T|)$ time to pass messages over the entire sequence $T$. This defeats the purpose of using a subsequence. If we instead only pass messages over the subsequence $S$, then the pairwise marginals are $\Pr(u_t, u_{t-1} | y_S)$ and we return to the naive biased gradient estimator

$$\nabla \hat{U}(\theta) = -\frac{1}{\Pr(S)} \sum_{t \in S} \mathbb{E}_{u|y, \theta}[\nabla \log \Pr(y_t, u_t | u_{t-1}, \theta)] - \nabla \log \Pr(\theta) ,$$

3.2 Approximate Gradient Estimate

We instead propose passing messages over a buffered subsequence $S^* := \{t-B, \ldots, t_S-B\}$ for some positive buffer size $B$, with $S \subset S^* \subset T$ (see Figure 2). The idea is that there exists a large enough $B$ such that $\Pr(u_S | y_S, \theta) \approx \Pr(u_S | y_T, \theta)$. Our buffered gradient estimator sums only over $S$, but takes expectations over $u_S | y_S, \theta$ instead of $u_S | y_T, \theta$

$$\nabla \hat{U}(\theta) = -\frac{1}{\Pr(S)} \sum_{t \in S} \mathbb{E}_{u|y_S, \theta}[\nabla \log \Pr(y_t, u_t | u_{t-1}, \theta)] - \nabla \log \Pr(\theta) .$$

When $B = 0$ this is equivalent to the naive biased estimator $\nabla \hat{U}$ of Eq. (15). When $B = T$ this is equivalent to the unbiased estimator $\nabla \hat{U}$ of Eq. (14).

The trade-off between accuracy (bias) and runtime depends on the size of the buffer $B$ and current model parameters $\theta(s)$. Intuitively, when $\theta(s)$ produces pairwise marginals
that are similar to i.i.d. data, we can use a small buffer $B$. When $\theta^{(s)}$ produces strongly
dependent pairwise marginals, we must use a larger buffer $B$. In Section 4, we analyze, for a
fixed value of $\theta$, how quickly the bias between $\nabla U$ and $\tilde{\nabla} U$ decays with increasing $B$. We
show a geometric decay
$$
\mathbb{E}_{S} \| \nabla U - \tilde{\nabla} U \|_2 \leq C_\theta \rho^B_{\theta}, \quad \text{for some } C_\theta > 0,
$$
where $\rho_\theta$ is large for i.i.d. data and small for strongly dependent data. For a gradient accuracy
of $\delta$, we only need a logarithmic buffer size $O(\log \delta^{-1})$. Therefore our buffered gradient estimator reduces
the computation time from $O(|T|)$ to $O(|S| + \log \delta^{-1})$. In our experiments (Section 6), we find that modest buffers are both necessary and sufficient to correct for bias.

### 3.3 Preconditioning and Fisher Information

The desirable properties for the preconditioning matrix $D(\theta)$ for SGRLD are (i) the resulting
dynamics takes advantage of the geometric structure of $\theta$, (ii) both $D(\theta)$ and $\Gamma(\theta)$ can be
efficiently computed, and (iii) neither $D(\theta) \nabla U(\theta)$ nor $\Gamma(\theta)$ are numerically unstable.

The expected Fisher information $I_y$ is the Riemannian metric proposed in [31]
$$
D^{-1}(\theta) = G(\theta) = I_y = \mathbb{E}_{y|\theta} \left[ \nabla^2 \log \Pr(y|\theta) \right].
$$
This corresponds to the Riemannian manifold over $\theta$ with distance measured by the symmetric Kullback-Liebler (KL) divergence between marginal likelihoods. Unfortunately for SSMs, the lack of independence in the marginal likelihood requires a double sum over $T$ to compute $I_y$, which is computationally intractable for long time series. We instead replace $I_y$ with the complete data Fisher information $I_{u,y}$
$$
I_{u,y} = \mathbb{E}_{u,y|\theta} \left[ \nabla^2 \log \Pr(y,u|\theta) \right] = |T| \cdot \mathbb{E}_{u,y|\theta} \left[ \nabla^2 \log \Pr(y,u_t|u_{t-1},\theta) \right].
$$
Similar to $I_y$, using $I_{u,y}$ corresponds to the manifold with distance measured by the symmetric KL divergence between complete-data likelihoods. Because $I_{u,y}$ can be calculated analytically for the SSMs we consider (Section 5), we use $D(\theta) = I_{u,y}^{-1}$ when possible. In our experiments, we find that in practice, using the complete data Fisher information matrix works well and outperforms vanilla SGLD.

### 3.4 Algorithm Pseudocode

Algorithms 1 and 2 summarize our generic SGMCMC method for SSMs.

### 4 Buffered Gradient Estimator Error Bounds

In this section, we establish a bound on the expected error between the full data gradient $\nabla U(\theta)$ and our buffered gradient estimator $\tilde{\nabla} U(\theta)$ Eq. (16). Given such a bound, we can

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1 As $\delta \geq C_\theta \rho^{-B}_\theta \Rightarrow B \geq - \log \delta / \log \rho_\theta + \log C_\theta / \log \rho_\theta$

2 Python code for our method will be available at [https://github.com/aicherc/sgmcmc_ssm_code](https://github.com/aicherc/sgmcmc_ssm_code)

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control the overall error in our SGLD or SGRLD scheme when the SGMCMC dynamics possess a contraction property [36]. Using the triangle inequality, we decompose the error of $\nabla \hat{U}(\theta)$ using the unbiased gradient estimator $\nabla U(\theta)$ Eq. (14)

$$E_S \|\nabla U(\theta) - \nabla \hat{U}(\theta)\|_2 \leq E_S \|\nabla U(\theta) - \nabla \bar{U}(\theta)\|_2 + E_S \|\nabla \bar{U}(\theta) - \nabla \hat{U}(\theta)\|_2 , \tag{20}$$

where the expectation is taken over the random subsequence $S$. The first term is the error from subsampling and is the same error from minibatching in SGMCMC for i.i.d. data, Eq. (10) [68]. The second term is the error from approximating the latent state posterior, which is unique to our buffered gradient estimator. Because error in the first term is studied in depth in the existing stochastic gradient MCMC literature [4, 11, 22, 61], we restrict our focus to bounding the second term. In particular, we will uniformly bound $\|\nabla \bar{U}(\theta) - \nabla \hat{U}(\theta)\|_2$ for any $S$.

Our approach is to bound $\|\nabla U(\theta) - \nabla \hat{U}(\theta)\|_2$ in terms of the Wasserstein distance between the exact posterior $\gamma_t(u_t) = \Pr(u_t \mid y_{S^t}, \theta)$ and our approximate posterior $\tilde{\gamma}_t(u_t) = \Pr(u_t \mid y_{S^t}, \theta)$ and then show this Wasserstein distance decays geometrically. To bound the Wasserstein distance, we follow existing work on bounding Markov processes in Wasserstein distance [24, 49, 57]. However, unlike previous work that focuses on the homogeneous Markov process of the joint model $\{u, y \mid \theta\}$, we instead focus on the induced nonhomogeneous Markov process of the conditional model $\{u \mid y, \theta\}$. To do so, we use the forward ($f_t$) and backward ($b_t$) random maps of $\{u \mid y, \theta\}$ [18]

$$u_t \sim \Pr(u_t \mid y, \theta) \Rightarrow (f_t(u_t), u_t) \sim \Pr(u_{t+1}, u_t \mid y, \theta) \tag{21}$$

$$u_t \sim \Pr(u_t \mid y, \theta) \Rightarrow (b_t(u_t), u_t) \sim \Pr(u_{t-1}, u_t \mid y, \theta) , \tag{22}$$

If $f_t$ and $b_t$ satisfy a contractive property, then we can bound the Wasserstein distance between $\gamma_t, \tilde{\gamma}_t$ in terms of $\gamma_{t-1}, \tilde{\gamma}_{t-1}$ and $\gamma_{t+1}, \tilde{\gamma}_{t+1}$ respectively. Bounding the error of the induced nonhomogeneous Markov process has been previously studied in the SSM literature using total variation (TV) distance [9, 17, 42, 62]. These works bound the error in total variation distance by quantifying how quickly the smoothed posterior forgets the initial condition. However, these bounds typically require stringent regularity conditions, which

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**Algorithm 1 SGRLD**

Input: data $y$, parameters $\theta^{(0)}$, stepsize $h$, subsequence length $S$, error tolerance $\epsilon$

for $s = 0, 1, 2, \ldots, N_{\text{steps}} - 1$ do

$\nabla \hat{U}(\theta^{(s)}) = \text{NoisyGradient}(y, \theta^{(s)}, S, \epsilon)$ // Algorithm 2 or 3

$D^{(s)}(\theta^{(s)}) = \text{GetPreconditioner}(\theta^{(s)})$ // e.g. Eq. (18)

$\theta^{(s+1)} = \theta^{(s)} - h^{(s)} \left[ D^{(s)} \nabla \hat{U}(\theta^{(s)}) + \Gamma^{(s)} \right] + \mathcal{N}(0, 2h^{(s)} D^{(s)})$ // Eq. (11)

end for

Return $\theta^{(N_{\text{steps}})}$

**Algorithm 2 NoisyGradient** for analytic message passing

Input: data $y$, parameters $\theta$, subsequence length $S$, error tolerance $\epsilon$

$B = \text{BufferLength}(\theta, S, \epsilon)$ // From Theory (Section 4)

$S, S^* = \text{GetBufferedSubsequence}(y, S, B)$

$\Pr(u_t \mid y_{S^*}, \theta) = \text{ForwardBackward}(y, S^*, \theta)$ // Message Passing

$\nabla \hat{U}(\theta) = - \frac{1}{|\mathcal{S}|} \sum_{t \in S} \mathbb{E}_{u \mid y_{S^*}, \theta} [\nabla U \log \Pr(y_t, u_t \mid u_{t-1})]$ // Eq. (16)

Return $\nabla \hat{U}(\theta)$

---
are hard to prove outside of finite or compact spaces. In particular, these bounds are not immediately applicable for LGSSMs. In contrast, we bound the error in Wasserstein distance by proving contraction properties of $f_t$ and $b_t$, allowing us to extend results to continuous and mixed-type SSMs such as the LGSSM (Section 5.3.1).

Our main result is that if, for fixed $\theta$, the gradient of $\log \Pr(y, u | \theta)$ satisfies a Lipschitz condition and the random maps $\{f_t, b_t\}_{t \in S}$ all satisfy a contraction property, then the error $\|\nabla U(\theta) - \nabla \tilde{U}(\theta)\|_2$ decays geometrically in the buffer size $B$.

**Theorem 1.** Let $\epsilon_{-\gamma}$ and $\epsilon_{+\gamma}$ be the 1-Wasserstein distances between $\gamma$ and $\tilde{\gamma}$ at the left and right ends of $S^*$ respectively. Let $\epsilon_1 = \max\{\epsilon_{-\gamma}, \epsilon_{+\gamma}\}$. If the gradients of $\log \Pr(y_t, u_t | u_{t-1}, \theta)$ are all Lipschitz in $u_{t-1}$ with constant $L_U$, and random maps $f_t$ and $b_t$ are all Lipschitz in $u_t$ with constant $L < 1$, then we have

$$\|\nabla U(\theta) - \nabla \tilde{U}(\theta)\|_2 \leq |T| \cdot L_U \cdot L^\frac{1}{1 - L} \cdot L^\frac{1 - L}{S} \cdot 2 \epsilon_1 .$$

(23)

As $L \leq 1$, Theorem 1 states that the error of the buffered gradient estimator decays geometrically as $O(L^p)$. Therefore, the required buffer size $B$ for an error tolerance of $\delta$ scales logarithmically as $O(\log \delta^{-1})$. In contrast, the error of the gradient estimator decays only linearly in the subsequence length, $O(S^{-1})$; therefore much longer subsequences, $O(\delta^{-1})$, are required to reduce bias. This agrees with the intuition that the bias is dominated by the error at the endpoints of subsequence. A similar result for when the gradient of the complete data loglikelihood is Lipschitz in $u^T$ instead of $u$ (as needed for LGSSM) will be proved in Section 4.3.

The remainder of this section is as follows. First, in Section 4.1, we show how to bound the error in $\nabla U(\theta)$ in terms of Wasserstein distances between $\gamma, \tilde{\gamma}$. Second, in Section 4.2, we show these Wasserstein distances decay geometrically in $B$. Finally, in Section 4.3, we prove our main results: Theorems 1 and 2. To keep the presentation clean, we leave proofs of Lemmas to the Supplement.

### 4.1 Functional Bound in terms of Wasserstein

We first review the definition of Wasserstein distance. Let $W_p(\gamma, \tilde{\gamma})$ be the $p$-Wasserstein distance

$$W_p(\gamma, \tilde{\gamma}) := \left[ \inf_{\xi} \int \|u - \tilde{u}\|_p^p d\xi(u, \tilde{u}) \right]^{1/p}$$

(24)

where $\xi$ is a joint measure or coupling over $(u, \tilde{u})$ with marginals $\int d\gamma(u) = \int d\tilde{\gamma}(u)$ and $\int d\epsilon(u) = \int d\tilde{\epsilon}(u)$. Wasserstein distance satisfies all the properties of a metric. A useful property of the 1-Wasserstein distance is the following Kantorovich-Rubinstein duality formula for the difference of expectations of Lipschitz functions [66]

$$W_1(\gamma, \tilde{\gamma}) = \sup_{\|\psi\|_{L_{1p}} \leq 1} \left\{ \int \psi d\gamma - \int \psi d\tilde{\gamma} \right\} \Rightarrow \|E_{\gamma}[\psi] - E_{\tilde{\gamma}}[\psi]\| \leq \|\psi\|_{L_{1p}} \cdot W_1(\gamma, \tilde{\gamma}) ,$$

(25)

where $\|\psi\|_{L_{1p}}$ denotes the Lipschitz constant of $\psi$.

We connect the error $\|\nabla U - \nabla \tilde{U}\|_2$ to the Wasserstein distances between $\gamma, \tilde{\gamma}$, by applying this duality formula Eq. (25) to the difference of Eqs. (14) and (16)

$$\nabla U - \nabla \tilde{U} = \frac{|T|}{S} \sum_{t \in S} \left[ E_{\gamma, t-1} \cdot [\nabla \log \Pr(y_t, u_t | u_{t-1}, \theta)] - E_{\tilde{\gamma}, t-1} \cdot [\nabla \log \Pr(y_t, u_t | u_{t-1}, \theta)] \right].$$

(26)

Applying the triangle inequality gives Lemma 1.
Lemma 1. If $\nabla \log \Pr(y_t, u_t | u_{t-1}, \theta)$ are Lipschitz in $u_{t-1}$ with constant $L_U$,

$$
\| \nabla U(\theta) - \nabla \hat{U}(\theta) \|_2 \leq \frac{|T|}{S} \cdot L_U \cdot \sum_{t \in S} W_1(\gamma_{t-1:t}, \hat{\gamma}_{t-1:t}).
$$

(27)

If $\nabla \log \Pr(y_t, u_t | u_{t-1}, \theta)$ is not Lipschitz in $u_{t-1:t}$, but is Lipschitz in $u_{t-1:t} u_T$ (as in LGSSMs), then the following Lemma lets us bound the 1-Wasserstein distance of $uu^T$ in terms of the 2-Wasserstein distance of $u$.

Lemma 2. Let $\gamma'$ be the distribution of $uu^T$. Let $\tilde{\gamma}'$ be the distribution of $\hat{u}\hat{u}^T$. Let $M = \mathbb{E}_{\gamma} [\|u\|_2^2] < \infty$. (Note $W_2(\gamma, \tilde{\gamma}) < \infty$ implies $\mathbb{E}_{\gamma} [\|u\|_2^2] < \infty$.) Then,

$$
W_1(\gamma', \tilde{\gamma}') \leq (2\sqrt{M} + 1) \cdot \max \left\{ W_2(\gamma, \tilde{\gamma})^{1/2}, W_2(\gamma, \tilde{\gamma}) \right\}.
$$

4.2 Geometric Wasserstein Decay

We first review why contractive random maps induce Wasserstein bounds. If two distributions $\gamma_t, \gamma'_t$ have identically distributed random maps $f_t, f'_t$, that is there exists a random function $f_t$ satisfying

$$
u \sim \gamma_t \text{ and } \nu' \sim \gamma'_t \Rightarrow f_t(\nu) \sim \gamma_{t+1} \text{ and } f_t(\nu) \sim \gamma'_{t+1},
$$

then we can bound the Wasserstein distance of $\gamma_{t+1}, \gamma'_{t+1}$ in terms of the Wasserstein distance of $\gamma_t, \gamma'_t$ given a bound on the random map’s Lipschitz constant $\|f_t\|_{Lip} < L$

$$
W_p(\gamma_{t+1}, \gamma'_{t+1})^p = \inf_{\xi_{t+1}} \| u_{t+1} - u'_{t+1} \|_2^p d\xi_{t+1}(u_{t+1}, u'_{t+1})
$$

$$
\leq \inf_{\xi_t} \| f_t(u) - f_t(u') \|_2^p d\xi_t(u, u') df_t
$$

$$
\leq \inf_{\xi_t} L^p \cdot \| u - u' \|_2^p d\xi_t(u, u') = L^p \cdot W_p(\gamma_t, \gamma'_t)^p.
$$

Unfortunately for SSMs, Eq. (29) does not apply as the random maps $f_t, b_t$ of $\gamma$ and $\tilde{f}_t, \tilde{b}_t$ of $\tilde{\gamma}$ are not identically distributed. To see this, we first review the conditional probability distributions used to define $f_t, b_t$. The forward random map $f_t$ draws $u_{t+1} | u_t$ from the forward smoothing kernel

$$
\mathcal{F}_t(u_{t+1} | u_t) := \Pr(u_{t+1} | u_t, y_{t:t}) = \Pr(u_{t+1} | u_t) \Pr(y_{t+1} | u_{t+1}) \beta_{t+1}(u_{t+1}) / \beta_t(u_t)
$$

(30)

and the backward random map $b_t$ draws $u_{t-1} | u_t$ from the backward smoothing kernel

$$
\mathcal{B}_t(u_{t-1} | u_t) := \Pr(u_{t-1} | u_t, y_{t:t}) = \Pr(u_t | u_{t-1}) \Pr(y_t | u_t) \alpha_t(u_{t-1}) / \alpha_t(u_t).
$$

(31)

Because $\gamma$ uses different forward and backward messages $\hat{\alpha}, \hat{\beta}$ in Eqs. (30) and (31), the kernels $\tilde{\mathcal{F}}_t, \tilde{\mathcal{B}}_t$ are not identical to $\mathcal{F}_t, \mathcal{B}_t$ (and the random maps are not identically distributed). This is unlike homogeneous Markov chains, where the kernels are identical at each time $t$ (and the random maps are identical distributed).

Instead of connecting $\gamma$ to $\tilde{\gamma}$ directly, we use the triangle inequality to connect them through an intermediate distribution $\hat{\gamma} := \Pr(u | y_{t-\infty:t}, \theta)$

$$
W_p(\gamma, \tilde{\gamma}) \leq W_p(\gamma, \hat{\gamma}) + W_p(\hat{\gamma}, \tilde{\gamma}).
$$

(32)
Introducing this particular intermediate distribution \( \tilde{\gamma} \) is the key step for our Wasserstein bounds between \( \gamma \) and \( \tilde{\gamma} \). Because \( \tilde{\gamma} \) conditions on all \( y_t \) after \( y_{S^*} \), \( \tilde{\gamma} \) and \( \gamma \) have identical backward messages \( \beta_t \) and therefore identically distributed forward random maps \( f_t \). Similarly, because \( \tilde{\gamma} \) does not condition on \( y_t \) before \( y_{S^*} \), \( \tilde{\gamma} \) and \( \gamma \) have identical forward messages \( \alpha_t \) and identically distributed backward random maps \( \tilde{b}_t \). Therefore, we can bound \( W_p(\gamma, \tilde{\gamma}) \) using \( f_t \) and bound \( W_p(\tilde{\gamma}, \gamma) \) using \( \tilde{b}_t \) with the contraction trick Eq. (29) giving us Lemma 3.

**Lemma 3.** If there exists \( L_f, L_b < 1 \) such that for all \( t \in S^* \), \( \|f_t\|_{\text{Lip}} < L_f \) and \( \|\tilde{b}_t\|_{\text{Lip}} < L_b \), then for all \( t \in S \) we have

\[
W_p(\gamma_{t-1:t}, \tilde{\gamma}_{t-1:t}) \leq (1 + L_f^{t-1} \cdot L_b) \cdot W_p(\gamma_{t-1:t}, \tilde{\gamma}_{t-1:t})
\]

We show sufficient conditions for the random maps to be contractions (i.e. \( L_f, L_b < 1 \)) for specific models in Section 5.1.1 (HMMs) and 5.3.1 (LGSSMs).

### 4.3 Proof of Main Theorems

Putting together the results of the previous two subsections gives us our geometric error bounds: Theorem 1 when the gradient terms are Lipschitz in \( u \) and Theorem 2 when the gradient terms are Lipschitz in \( uu^T \). Both theorems require the random maps of the forward and backward smoothing kernels are contractions. We first prove Theorem 1.

**Proof of Theorem 1.** Combining Lemmas 1 and 3 with some algebra

\[
\|\nabla U(\theta) - \nabla \tilde{U}(\theta)\|_2 \leq \frac{|T|}{S} \cdot L_U \cdot \sum_{t \in S} W_1(\gamma_{t-1:t}, \tilde{\gamma}_{t-1:t})
\]

\[
\leq \frac{|T|}{S} \cdot L_U \cdot \sum_{t=1}^{S} W_1(\gamma_{t-1:t}, \tilde{\gamma}_{t-1:t}) + W_1(\gamma_{t-1:t}, \tilde{\gamma}_{t-1:t})
\]

\[
\leq \frac{|T|}{S} \cdot L_U \cdot \sum_{t=1}^{S} (1 + L_f) L_f^{t-1} \cdot (1 + L_b) L_b^{S-t} \cdot \epsilon_1
\]

\[
\leq |T| \cdot L_U \cdot \frac{1 + L_f}{1 - L} \cdot \frac{1 - L^S}{S} \cdot \frac{1}{L^2} \cdot 2 \epsilon_1,
\]

where \( \max\{W_1(\gamma_{t-1:t}, \tilde{\gamma}_{t-1:t}), W_1(\tilde{\gamma}_{t-1:t}, \tilde{\gamma}_{t-1:t})\} = \max\{\epsilon_\gamma, \epsilon_{\tilde{\gamma}}\} = \epsilon_1. \)

We now prove a similar result for when \( \nabla \log \Pr(y_t, u_t | u_{t-1}) \) is Lipschitz in \( uu^T \).

**Theorem 2.** Let \( \epsilon_2 = \max\{W_2(\gamma_{t-1:t}, \tilde{\gamma}_{t-1:t}), W_2(\tilde{\gamma}_{t-1:t}, \tilde{\gamma}_{t-1:t})\} \). If the gradients \( \nabla \log \Pr(y_t, u_t | u_{t-1}, \theta) \) are Lipschitz in \( uu^T \) with constant \( L_U \), and there exists \( L_f, L_b < 1 \) for Lemma 3, then with \( L = \max\{L_f, L_b\} \) and \( L_U = (2 \sqrt{\E_{\gamma}[u]} + 1) L_U \)

\[
\|\nabla U(\theta) - \nabla \tilde{U}(\theta)\|_2 \leq |T| \cdot L_U \cdot \frac{\sqrt{1 + L_f^2}}{1 - L_f^2} \cdot \frac{1 - L_f^S}{S^2} \cdot \frac{1}{L^2} \cdot \max_{r \in \{1/2, 1\}} (2 \epsilon_2)^r.
\]

Similar to Theorem 1, Theorem 2 states that the squared error of the buffered gradient estimator decays geometrically if the complete-data loglikelihood is Lipschitz in \( uu^T \) instead of \( u \). However, the price we pay is a square-root: the error decays \( O(L^2/2) \) instead of \( O(L^2) \).
We consider discrete latent state HMMs with Gaussian emissions. The complete data

\[\Pr(y, z | \theta) = \prod_{t=1}^{T} \Pi_{z_{t-1}, z_t} \cdot \mathcal{N}(y_t | \mu_{z_t}, \Sigma_{z_k}) , \tag{35}\]

where \(y_t \in \mathbb{R}^m\) are the observations, \(u_t \equiv z_t \in \{1, \ldots, K\}\) are the discrete latent variables, and \(\theta = \{\Pi, \mu, \Sigma\}\) are the parameters with \(\Pi_k \in \Delta^K\) (simplex over \(K\) states), \(\mu_k \in \mathbb{R}^m\), \(\Sigma_k \in \mathbb{S}_+^m\) (positive definite matrices) for \(k = 1, \ldots, K\). In practice, we use the expanded mean parameters of \(\Pi\) instead of \(\Pi\) (as in [52]) and the Cholesky decomposition of \(\Sigma_k^{-1}\) instead of \(\Sigma_k\) to ensure positive definiteness. As the latent states are discrete over a finite space, the forward backward algorithm for an HMM can be done in closed-form; thus, pairwise latent marginals \(\gamma_{t-1,t}(z_{t-1}, z_t)\), gradients \(\nabla U(\theta)\) and preconditioning terms \(D(\theta)\) and \(\Gamma(\theta)\) are straightforward to calculate. Complete details are provided in the Supplement.

5 Example Models

In this section, we provide examples of how to apply the generic framework of Section 3 and bounds of Section 4 to common SSMs.

5.1 Gaussian HMM

We consider discrete latent state HMMs with Gaussian emissions. The complete data

\[\Pr(y, z | \theta) = \prod_{t=1}^{T} \Pi_{z_{t-1}, z_t} \cdot \mathcal{N}(y_t | \mu_{z_t}, \Sigma_{z_k}) , \tag{35}\]

where \(y_t \in \mathbb{R}^m\) are the observations, \(u_t \equiv z_t \in \{1, \ldots, K\}\) are the discrete latent variables, and \(\theta = \{\Pi, \mu, \Sigma\}\) are the parameters with \(\Pi_k \in \Delta^K\) (simplex over \(K\) states), \(\mu_k \in \mathbb{R}^m\), \(\Sigma_k \in \mathbb{S}_+^m\) (positive definite matrices) for \(k = 1, \ldots, K\). In practice, we use the expanded mean parameters of \(\Pi\) instead of \(\Pi\) (as in [52]) and the Cholesky decomposition of \(\Sigma_k^{-1}\) instead of \(\Sigma_k\) to ensure positive definiteness. As the latent states are discrete over a finite space, the forward backward algorithm for an HMM can be done in closed-form; thus, pairwise latent marginals \(\gamma_{t-1,t}(z_{t-1}, z_t)\), gradients \(\nabla U(\theta)\) and preconditioning terms \(D(\theta)\) and \(\Gamma(\theta)\) are straightforward to calculate. Complete details are provided in the Supplement.

5.1.1 Error Bound Coefficients

In the finite discrete variable case, conditions for bounding the Lipschitz coefficient of the smoothing kernels \(F_t, B_t\) (as needed for Section 4.2) are equivalent to conditions for bounding their Dobrushin coefficients [9, 17]. The Dobrushin coefficient for a transition kernel \(Q\) is

\[\delta(Q) = \sup_{z, z'} \frac{1}{2} \|Q(z, \cdot) - Q(z', \cdot)\|_{TV} = \frac{\|Q(z, \cdot) - Q(z', \cdot)\|_{TV}}{\|\delta_z - \delta_{z'}\|_{TV}} . \tag{36}\]

The final term of Eq. (36) show the connection between Dobrushin coefficients and Lipschitz coefficients: it is the ratio of the distance of between kernels \(Q(z, \cdot), Q(z', \cdot)\) with the distance
between point masses at \( z \) and \( z' \). Therefore for discrete latent states, \( L_f = \max \delta(F_t) \) and \( L_b = \max \delta(B_t) \).

In the discrete case, sufficient conditions for \( L_f, L_b < 1 \) are well known (See [9] Chapter 4.3). If the transition matrix \( \Pi \) satisfies the strong mixing condition, that is, there exists constants \( \sigma^- \) and \( \sigma^+ \) with \( 0 < \sigma^- \leq \sigma^+ \) and a probability distribution \( \kappa \in \Delta^K \) over \( z \) such that \( \sigma^- \kappa(z') \leq \Pi_{z,z'} \leq \sigma^+ \kappa(z') \) and \( \mathbb{E}_z[\Pr(y \mid z)] < \infty \), then the Dobrushin coefficients are bounded by \( L = 1 - \sigma^- / \sigma^+ \). Relaxations of this condition can be found in [9, 17]. Alternatively, we can obtain tighter bounds for HMMs via estimating the Lyapunov exponents for the underlying random dynamical systems defined by random maps \( f_t \) and \( b_t \) [72, 48].

Finally, the Lipschitz constant \( L_U \) for Lemma 1 is

\[
L_U = \max_{t \in S} \| \nabla \log \Pr(y_t, z_t \mid z_{t-1} \theta) - \nabla \log \Pr(y_t, z'_t \mid z'_{t-1} \theta) \|. \tag{37}
\]

This is easy to compute since at each iteration \( y \) and \( \theta = \theta^{(s)} \) are fixed. Given these bounds on \( L_U \) and \( L \), we can use Theorem 1 to select the buffer size \( B \) to ensure approximate convergence to the stationary distribution.

### 5.2 Autoregressive HMM

We now consider ARHMMs, a generalization of the discrete state HMM where each observation depends not only on the latent state, but also on the last \( p \) observations. Specifically, the discrete latent state \( z_t \) determines which AR(\( p \)) process models the dynamics of \( y \) at time \( t \). The complete data likelihood of an ARHMM is as follows

\[
\Pr(y, z \mid \theta) = \prod_{t=1}^T \Pi_{z_{t-1}, z_t} \cdot \mathcal{N}(y_t \mid A z_t, \Sigma_y) \tag{38}
\]

where \( y_t \in \mathbb{R}^m \) are the observations, \( \overline{x} = y_{t-p+1:t} \) are the \( p \)-lagged observations, \( u_t \equiv z_t \in \{1, \ldots, K\} \) are the discrete latent variables, and \( \theta = \{\Pi, A, Q\} \) are the parameters with \( \Pi_k \in \Delta^K, A_k \in \mathbb{R}^{m \times mp}, Q_k \in S^m \) for \( k = 1, \ldots, K \). From Eq. (38), we see that the ARHMM is a time-dependent mixture of \( K \) AR processes of order \( p \). The pairwise latent marginals, gradients, and preconditioning terms for an ARHMM are calculated similarly to the Gaussian HMM. Further details are provided in the Supplement. The theory and constants for the error bounds of Section 4 are identical to those presented for the Gaussian HMM.

### 5.3 Linear Gaussian SSM

A linear Gaussian SSM (LGSSM), also called a linear dynamical system (LDS), consists of a latent Gaussian (vector) autoregressive process over states \( u_t \equiv x_t \in \mathbb{R}^n \) and conditionally Gaussian emissions \( y_t \in \mathbb{R}^m \) [7, 46]. Specifically,

\[
\Pr(y, x \mid \theta) = \prod_{t=1}^T \mathcal{N}(x_t \mid A x_{t-1}, Q) \cdot \mathcal{N}(y_t \mid C x_t, R) \tag{39}
\]

where \( A \in \mathbb{R}^{n \times n} \) is the latent state transition matrix, \( Q \in S^m_+ \) is the transition noise covariance, \( C \in \mathbb{R}^{m \times n} \) is the emission matrix, and \( R \in S^m_+ \) is the emission noise covariance. Together \( A, Q, C, R \) are the model parameters \( \theta \). The matrices \( A, C, \) and \( Q \) are unidentifiable without additional restriction, as applying an orthonormal transformation \( M \) gives an equivalent representation \( \tilde{A} = MAM^{-1}, \tilde{C} = CM^{-1}, \tilde{Q} = MQM^T \). To enforce identifiability, we choose to restrict the first \( \min(n, m) \) rows and columns of \( C \) to the identity matrix. In
practice, we use the Cholesky decompositions \( \psi_Q, \psi_R \) of \( Q^{-1}, R^{-1} \) (respectively) instead of \( Q, R \). The recursions for the forward backward algorithm for LGSSMs is known as the Kalman smoother [9, 7, 29]. Because the transition and emission processes are linear Gaussian, all forward messages, backward messages, and pairwise latent marginals \( \gamma_{t-1,t}(x_{t-1}, x_t) \) are Gaussian; therefore, the gradients and preconditioning matrix can be calculated analytically. Further details are provided in the Supplement.

5.3.1 Error Bound Coefficients

The forward and backward maps of an LGSSM are strict contractions under mild conditions (i.e. \( \|A\|_2 < 1 \) (Lemmas 4, 5) and the gradients \( \nabla \log \Pr(y_t, x_t | x_{t-1}, \theta) \) are Lipschitz in \( xx^T \) (Lemma 6). Therefore, Theorem 2 applies.

**Lemma 4.** The forward random maps of an LGSSM are Gaussian linear maps. Specifically, \( f_t(x_t) = F_t^x x_t + \zeta_t^f \), where \( \zeta_t^f \) is a Gaussian random intercept and \( F_t^x \) is a matrix function of \( \theta \) and \( y_{t>1} \). As a linear map, the Lipschitz constant of \( f_t \) is

\[
\|f_t\|_{Lip} = \|F_t^x\|_2 \leq \|A(I_n + QC^T R^{-1} C)^{-1}\|_2 = L_f
\]

As \( \|(I_n + QC^T R^{-1} C)^{-1}\|_2 < 1 \), if \( \|A\|_2 < 1 \), then \( \|f_t\|_{Lip} \leq L_f < 1 \) for all \( t \).

**Lemma 5.** The backward random maps of an LGSSM are Gaussian linear maps. Specifically, \( b_t(x_t) = F_t^b x_t + \zeta_t^b \), where \( \zeta_t^b \) is a Gaussian random intercept and \( F_t^b \) is a matrix function of \( \theta \) and \( y_{t<1} \). As a linear map, the Lipschitz constant of \( b_t \) is

\[
\|b_t\|_{Lip} = \|F_t^b\|_2 \leq \|A(I_n + Q(A^T (C^T R^{-1} C)^{-1} A)^{-1})^{-1}\|_2 = L_b
\]

As \( \|(I_n + Q(A^T (C^T R^{-1} C)^{-1} A)^{-1})^{-1}\|_2 < 1 \), if \( \|A\|_2 < 1 \), then \( \|b_t\|_{Lip} \leq L_b < 1 \).

Lemmas 4 and 5 agree with intuition, when \( \|A\|_2 \approx 0 \) (no connection between \( x_{t-1} \) and \( x_t \)) or \( \|Q\|_2 \gg \|R\|_2 \) (transition noise is much larger than emission noise), then \( L_f, L_b \approx 0 \) (observations can be treated independently). Conversely, when \( \|A\|_2 \approx 1 \) and \( \|Q\|_2 \ll \|R\|_2 \), then \( L_f, L_b \approx 1 \) and buffering is necessary.

**Lemma 6.** As \( x, y \) are jointly Gaussian in the LGSSM, the gradient of the complete data loglikelihood is a quadratic form in \( xx^T \) with matrices

\[
\Omega = \{ I_n \otimes Q^{-1}, I_n \otimes Q^{-1} A, Q^{-1/2} \otimes I_n, Q^{-1/2} A \otimes I_n, Q^{-1/2} A \otimes A, I_n \otimes R^{-1}, I_n \otimes R^{-1} C, R^{-1/2} C \otimes C \},
\]

where \( Q^{-1/2} = \psi_Q \) and \( R^{-1/2} = \psi_R \). Therefore a bound for the Lipschitz constant is

\[
L^*_U = \max_{x \in \Omega} \|\omega\|_2. \text{ This bound grows in } \|A\|, \|C\|, \|Q\|^{-1}, \|R\|^{-1}.
\]

The proofs and complete form of \( F^f_t, F^b_t, \zeta^f_t \) and \( \zeta^b_t \) can be found in the Supplement.

5.4 Switching Linear Dynamical System (SLDS)

Switching linear dynamical systems (SLDSs) are an example of a state space model with both discrete and continuous latent variables. The form of SLDS models that we consider is

\[
\Pr(y, x | z, \theta) = \prod_{t=1}^{T} \Pi_{z_{t-1}, z_t} \cdot \mathcal{N}(x_t | A_{z_t} x_{t-1}, Q_{z_t}) \cdot \mathcal{N}(y_t | C x_t, R), \quad (43)
\]
Figure 3: Graphical Model of a SLDS.

where \( y_t \in \mathbb{R}^m \) are the observations, \( u_t \equiv (x_t, z_t) \in \mathbb{R}^n \times \{1, \ldots, K\} \) are the mixed-type latent state sequence, and \( \theta = \{ \Pi, A, Q, C, R \} \) the model parameters with \( \Pi_k \in \Delta^K \), \( A_k \in \mathbb{R}^{n \times n} \), \( Q_k \in S^n_+ \) for \( k = 1, \ldots, K \), \( C \in \mathbb{R}^{m \times n} \) and \( R \in S^m_+ \). The SLDS of Eq. (43) can be viewed either as a latent AR(1)-HMM with conditional Gaussian emissions or as hidden Markov switches of a LGSSM. As an extension of the ARHMM, the latent continuous state sequence \( x_t \) can smooth noisy observations. As an extension of the LGSSM, the latent discrete state sequence \( z_t \) allows modeling of more complex dynamics by switching between different states (or regimes).

5.4.1 Gradient Estimators

Unlike previous models, the forward-backward algorithm for the latent variables \((x, z)\) in an SLDS does not have a closed form. Specifically, the transition kernel for \( x \) is a Gaussian mixture, so the forward and backward messages of \( x \) are Gaussian mixtures with an exponentially increasing number of components (e.g. \( \alpha_t \) has \( K^t \) components). Because the forward-backward algorithm is intractable for SLDSs, we rely on sampling \((x, z)\) and forming a Monte Carlo estimate of the expectation in Fisher’s identity Eq. (16). We consider various options of this Monte Carlo estimate below. To sample \((x, z)\), we use a blocked Gibbs scheme as in [28], detailed in the Supplement.

Given a collection of \( N \) samples from blocked Gibbs \( \{x^{(r)}(r), z^{(r)}(r)\} \sim x, z \mid y, \theta \), we construct three different estimators for the marginal loglikelihood. The first estimator, replaces the expectation in Eq. (16) with a Monte Carlo average

\[
E_{x,z|y,\theta}[\nabla \log Pr(y, x, z | \theta)] \approx \frac{1}{N} \sum_{r=1}^{N} \nabla \log Pr(y, x^{(r)}, z^{(r)} | \theta) .
\]  

(44)

We construct two additional estimators by analytically integrating out either one of the two latent variables. These estimators are the Rao-Blackwellization of the naive Monte Carlo estimate [9]. Integrating out either \( x \) or \( z \), gives us

\[
E_{x,z|y,\theta}[\nabla \log Pr(y, x, z | \theta)] = \frac{1}{N} \sum_{r=1}^{N} E_{z|x^{(r)},\theta}[\nabla \log Pr(y, x^{(r)}, z^{(r)} | \theta)]
\]  

(45)

\[
E_{x,z|y,\theta}[\nabla \log Pr(y, x, z | \theta)] = \frac{1}{N} \sum_{r=1}^{N} E_{x|z^{(r)},\theta}[\nabla \log Pr(y, x^{(r)}, z | \theta)].
\]  

(46)

Because Eq. (45) integrates out \( x \), it has lower variance for the gradient terms involving \( x \) (i.e. \( A, Q R \)). Similarly, because Eq. (46) integrates out \( z \), it has lower variance for the gradient terms involving \( z \) (i.e. \( \Pi \)).
Selecting one of the above Monte Carlo estimates of \( \nabla U(\theta) \), we can deploy the same buffered subsampling estimator Eq. (16), obtaining Algorithm 3. Algorithm 3 replaces the forward-backward subroutine in Algorithm 2 with blocked Gibbs sampling over \( S^* \). Although this is more computationally costly than the exact forward-backward algorithms of the previous sections, it still provides memory saving and runtime speed ups compared to running a full blocked Gibbs sampler over \( T \). The explicit forms of Eqs. (44)-(46), precondition matrix \( D(\theta) \), and correction term \( \Gamma(\theta) \) for SLDS used in Alg. 1 are a combination of those for ARHMMs and LGSSMs. Complete details are provided in the Supplement.

### Algorithm 3 NoisyGradient using blocked Gibbs (SLDS)

```
input: data \( y \), parameters \( \theta \), subsequence length \( S \), error tolerance \( \epsilon \),
\( B = \text{BufferLength}(\theta, S, \epsilon) \)  // From Theory or Adaptive
\( S, S^* = \text{GetBufferedSubsequence}(y, S, B) \)  // With ‘burn-in’
\( z_{S^*}^{(0)} = \text{InitLatent}(S^*, \theta) \)
for \( r = 1, 2, \ldots, N \) do
  sample \( x_{S^*}^{(r)} \sim x_{S^*} | y_{S^*}, z_{S^*}^{(r-1)} \)  // Blocked Gibbs
  sample \( z_{S^*}^{(r)} \sim z_{S^*} | y_{S^*}, x_{S^*}^{(r)} \)
end for
calculate \( \tilde{U}(\theta) \) using a Monte Carlo estimate  // Eq. (44), (45), or (46)
return \( \nabla \tilde{U}(\theta) \)
```

#### 5.4.2 Error Bounds

There are two primary challenges for the error analysis of the SLDS: (i) the forward and backward smoothing kernels for the SLDS are mixtures and (ii) the error from the finite-step blocked Gibbs sampler needs to be quantified. Conditions for contraction in the forward and backward smoothing random maps of switching models may follow from the conditions in [14]. Combining the convergence rate of the blocked Gibbs sampler with the error bound is an area we leave for future work. Our experiments in Section 6.2 provide empirical evidence of the potential benefits of the algorithm.

### 6 Experiments

We evaluate the performance of our proposed SGRLD algorithm (Section 3) using both synthetic and real data. We organize our experiments by the corresponding models of Section 5. Our evaluation focuses on the following three topics: (1) the computational speed-up of SGMCMC over batch MCMC, (2) the effectiveness of buffering in correcting bias, and (3) the effectiveness of the complete-data Fisher information preconditioning of SGRLD over SGLD.

To assess the performance of our samplers, we measure the marginal loglikelihood of samples \( \theta^{(s)} \) at different runtimes on a heldout test sequence. In synthetic data, where the true parameter \( \theta^* \) is known, we also measure the mean-squared error (MSE) of the sample average \( \bar{\theta}^{(s)} = \frac{1}{s} \sum_{i \leq s} \theta^{(i)} \) to \( \theta^* \). To assess the quality of our MCMC samples at approximating the posterior \( \Pr(\theta | y) \), we measure the kernel Stein discrepancy (KSD) of each chain after burn-in given equal computation time [34, 45], rather than effective sample size (ESS) [8, 30], as KSD accounts for bias in the samples. As with all gradient-based methods, our SGMCMC methods require a hyper-parameter search over the fixed step-size tuning parameters.
We present results for the best step-size as assessed via heldout loglikelihood on a validation set. As the potential $U(\theta)$ for SSMs is non-convex, initialization is important. For the HMM and ARHMM, we initialize the parameters $\Pi, A, Q$ using $z$ given from $K$-means clustering of the observations $y$ (or $y_{t-p:t}$). For the LGSSM, we initialize the parameters from the prior. For the mixed-type SLDS, we first sample $R$ from the prior and initialize $\Pi, A, Q$ using $z$ from $K$-means. Finally, in our experiments, we use flat and non-informative priors for $\theta$. For complete details see the Supplement.

### 6.1 Gaussian HMM & ARHMM

#### 6.1.1 Synthetic ARHMM

We first consider synthetic data generated from a 2-state ARHMM in two dimensions $m = 2$. The true model parameters $\theta^*$ are

\[
\Pi = \begin{bmatrix}
0.1 & 0.9 \\
0.9 & 0.1
\end{bmatrix}, \quad Q_1 = Q_2 = 0.1 \cdot \begin{bmatrix} 1 & 0 \\
0 & 1 \end{bmatrix}
\]

\[
A_1 = 0.9 \cdot \begin{bmatrix}
\cos(-\vartheta) & -\sin(-\vartheta) \\
\sin(-\vartheta) & \cos(-\vartheta)
\end{bmatrix}, \quad A_2 = 0.9 \cdot \begin{bmatrix}
\cos(\vartheta) & -\sin(\vartheta) \\
\sin(\vartheta) & \cos(\vartheta)
\end{bmatrix}
\]

The model’s two states are alternating rotations of $y \in \mathbb{R}^2$ with angle $\vartheta = \pi/4$ and the latent state sequence has a high transition rate $\Pr(z_t \neq z_{t-1}) = 0.9$. From this model we generate time series of length $|T| = 10^4$.

![Stochastic gradient error of transition matrix II](image)

**Figure 4**: Stochastic gradient error of transition matrix $\Pi$. (Left) stochastic gradient error varying subsequence length $S$ for no-buffer $B = 0$ and buffer $B = 10$. (Right) stochastic gradient error varying buffer size $B$ for small $S = 2$ and long $S = 50$ subsequences. Error bars are SD over $10^4$ samples.

Figure 4 are plots of the stochastic gradient error $\nabla \tilde{U}(\theta) - \nabla U(\theta)$ of the transition matrix $\Pi$ evaluated at the true model parameters $\theta = \theta^*$. From Figure 4 (left), we see that the stochastic gradients are heavily biased without buffering (orange) for small subsequence lengths; however buffering (blue) corrects the bias. From Figure 4 (right), we see that for a small subsequence length $S = 2$ (purple) buffering is necessary to correct for the bias. However, for a larger subsequence length $S = 50$ (green), buffering is not needed as the latent state of the endpoints can be well estimated from the subsequence alone. This agrees with intuition: for this HMM, inferring the marginal posterior given a few observations is easy; therefore messages from buffering are not required for large subsequence sizes. The bias in the stochastic gradients of AR-parameters $(A, Q)$ is less extreme than for the transition matrix $\Pi$ associated with the latent states; we include their error plots in the Supplement.
Figure 5: Metrics vs Runtime on synthetic ARHMM data with $|\mathcal{T}| = 10^4$ (left), $|\mathcal{T}| = 10^6$ (center), $|\mathcal{T}| = 10^8$ (right), for different inference methods: Gibbs, SGLD, and SGRLD. For SGMCMC methods, solid (—) and dashed (·-) lines indicate buffering and no buffering respectively. The different metrics are: (top) heldout loglikelihood and (bottom) transition matrix estimation error $MSE(\hat{\Pi}(s), \Pi^*)$. Note that Gibbs is computationally intractable for $|\mathcal{T}| = 10^8$.

In Figure 5, we compare SGLD (no-buffer and buffer), SGRLD (no-buffer and buffer), and Gibbs. We fit our samplers on one training sequence and evaluate performance on one test sequence. We consider sequence lengths of $|\mathcal{T}| = 10^4$, $|\mathcal{T}| = 10^6$, and $|\mathcal{T}| = 10^8$. For the SGMCMC methods we use a subsequence size of $S = 2$ and a buffer size of $B = 0$ (no-buffer) or $B = 2$ (buffer). From Figure 5, we see that preconditioning helps convergence and mixing as SGRLD outperforms SGLD. We also see that buffering is necessary to properly estimate $\Pi$. Finally, although Gibbs outperforms SGRLD for $|\mathcal{T}| = 10^4$, Gibbs performs worse for $|\mathcal{T}| = 10^6$, as Gibbs only draws $\approx 60$ samples in 10 hours, and is intractable for $|\mathcal{T}| = 10^8$.

Table 1 displays the KSD of the samples to the posterior after discarding half the samples as burn-in. Although Gibbs performs well for small $|\mathcal{T}|$, it performs worse for larger $|\mathcal{T}|$ due to the limited number of drawn samples. We also see that the non-buffered methods do poorly for all $|\mathcal{T}|$ due to sampling from the incorrect distribution. Although SGLD (buffer) and SGRLD (buffer) perform comparably after burn-in, Figure 5 suggests SGRLD converges quicker.

In the Supplement, we present a synthetic data experiment for the Gaussian HMM, and find similar results.
Table 1: $\log_{10}(\text{KSD})$ by variable of MCMC samplers. Mean and (SD) over runs in Figure 5.

| Sampler       | $\pi$ (SD) | $\mu$ (SD) | $\Sigma$ (SD) |
|---------------|------------|------------|---------------|
| $|T|=10^4$     |            |            |               |
| Gibbs (Full)  | 0.28 (0.10)| 1.33 (0.09)| 0.6 (0.05)    |
| SGLD (Buffer) | 0.18 (0.03)| 1.41 (0.12)| 0.74 (0.12)   |
| SGLD (Buffer) | 0.22 (0.08)| 1.42 (0.04)| 0.71 (0.11)   |
| SGLD (No Buffer) | 2.76 (0.69)| 2.17 (0.04)| 1.77 (0.17)   |
| SGLD (No Buffer) | 1.79 (0.03)| 2.00 (0.09)| 1.39 (0.31)   |
| $|T|=10^6$     |            |            |               |
| Gibbs (Full)  | 2.08 (0.26)| 3.80 (0.16)| 2.95 (0.26)   |
| SGLD (Buffer) | 1.55 (0.48)| 3.21 (0.05)| 2.50 (0.05)   |
| SGLD (Buffer) | 1.50 (0.10)| 3.26 (0.02)| 2.45 (0.08)   |
| SGLD (No Buffer) | 5.08 (0.65)| 4.08 (0.07)| 3.49 (0.2)    |
| SGLD (No Buffer) | 5.40 (0.02)| 3.96 (0.15)| 3.62 (0.19)   |
| $|T|=10^8$     |            |            |               |
| Gibbs         | –          | –          | –             |
| SGLD (Buffer) | 3.82 (0.28)| 5.49 (0.10)| 4.60 (0.11)   |
| SGLD (Buffer) | 3.79 (0.20)| 5.56 (0.09)| 4.70 (0.18)   |
| SGLD (No Buffer) | 7.38 (0.02)| 6.13 (0.11)| 5.45 (0.40)   |
| SGLD (No Buffer) | 7.40 (0.02)| 6.06 (0.12)| 5.63 (0.11)   |

6.1.2 Ion Channel Recordings

We investigate the behavior of the SGMCMC samplers on ion channel recording data. In particular, we consider a 1MHz recording of a single alamethicin channel [56]. This data was previously investigated using a Bayesian nonparametric HMM in [51] and [63]. In that work, the authors downsample the data by a factor of 100 and only used 10,000 and 2,000 observations due to the challenge of scaling computations to the full sequence. We present the results on the data without downsampling (10 million observations), where Gibbs sampling runs into memory issues. Figure 6 presents our results, after applying a log-transform and normalizing the observations. We train on the first 90% and evaluate on the last 10%. For our SGMCMC methods we use a subsequence size of $S = 10$ and a buffer size of $B = 0$ (no-buffer) or $B = 10$ (buffer). In addition to heldout loglikelihood, we also evaluate on 10-step ahead predictive loglikelihood $\sum_t \log \Pr(y_{t+10} | \theta, y_{\leq t})$, which is more sensitive to $\Pi$.

We see that SGRLD quickly converges compared to SGLD. Although the buffered methods take twice as long to compute ($S + B = 20$ vs $S = 10$), we see that buffering is necessary to perform well. In the Supplement, we present results comparing SGMCMC methods with Gibbs sampling on a downsampled version.

6.1.3 Canine Seizure iEEG

We now consider applying SGMCMC samplers to intracranial EEG (iEEG) data. In particular, we consider data from a study on canines with epilepsy available at ieeeg.org [16]. We focus on one canine, which over the course of 45.1 days was continuously monitored at 200Hz over 16 channels and recorded 90 seizures. This data was analyzed in prior work that compared a baseline ARHMM to nonparametric extensions using Gibbs sampling [69]. Following [69], we process the data into 4 minute windows around each seizure to focus on the seizure dynamics resulting in 90 time series of 48,000 points in $\mathbb{R}^{16}$. We use an ARHMM with $K = 5$ latent states and $p = 5$ lags treating each channel independently. We perform an 80-20 train-test split over 90 seizures, running inference on the training set and evaluating log-likelihood on the heldout test set. We compare SGLD and SGRLD samplers with $S = 100$. 

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and \( B = 10 \) with the baseline Gibbs sampler on the full data set. Because of the large data size, we also consider a subset Gibbs sampler that only uses 10\% of the training set seizures.

In Figure 7, we see that SGLRD converges much more rapidly than the other methods. As each iteration of the Gibbs sampler takes 6 hours, it takes a couple weeks for the Gibbs sampler to converge to the solution SGLRD converges to in a few hours. Although the subset Gibbs sampler is 10\% faster than Gibbs, it does not converge to the full data posterior and its generalization error to the heldout test set is poorer than the other methods. From this experiment we see that SGMCMC methods provide order of magnitude improvements (compared to subsetting the data).

### 6.2 LGSSM and SLDS

We first validate the LGSSM (SLDS with \( K = 1 \)) on synthetic data. We then consider the SLDS sampler on a synthetic dataset and two real datasets: the seizure data of Section 6.1.3 and a weather dataset.
6.2.1 Synthetic LGSSM

We consider synthetic data from a LGSSM with observations and latent state dimension \( m = n = 2 \). In particular, we consider, a rotating state sequence with noisy observations. The true model parameter \( \theta^* \) are

\[
A = 0.7 \cdot \begin{bmatrix} \cos(\vartheta) & -\sin(\vartheta) \\ \sin(\vartheta) & \cos(\vartheta) \end{bmatrix}, \quad Q = 0.1 \cdot \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad C = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad R = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix},
\]

where \( \vartheta = \pi/4 \). Because the transition error \( Q \) is smaller than the emission error \( R \), inclusion of previous and future observations is necessary to accurately infer the continuous latent state \( x_t \).

![Graphs showing error and loglikelihood over time for different methods and subsequence lengths.](image)

Figure 8: Synthetic LGSSM plots. (Top-left) stochastic gradient error varying subsequence length \( S \) for no-buffer \( B = 0 \) and buffer \( B = 10 \). (Top-right) stochastic gradient error varying buffer size \( B \) for small \( S = 10 \) and long \( S = 100 \) subsequences. Error bars are SD over 10^4 samples. (Bottom-left) heldout loglikelihood vs runtime. (Bottom-right) transition matrix estimation error \( \text{MSE}(\hat{A}(\theta), A^*) \). The MCMC methods compared are Gibbs, SGLD, and SGLRD, where solid (—) and dashed (---) lines indicate buffering and no buffering respectively.

Figure 8 (top) are plots of the stochastic gradient error \( \nabla \hat{U}(\theta) - \nabla U(\theta) \) for the latent state transition matrix \( A \) for random subsequences evaluated at \( \theta = \theta^* \). Figure 8 (top left) shows there is clear bias in the gradient of \( A \) without buffering (orange), but buffering (blue) corrects for the bias. Figure 8 (top right) shows that buffering is necessary to correct for bias with small subsequences (purple). Unlike for HMMs, even long subsequences (green) have noticeable bias. This is because the marginal posterior of LGSSM’s continuous latent state
sequence \( x \) requires accurate messages to calculate the mean and variance. Without a buffer, the inferred variance of \( x_t \) near the ends of \( S \) is higher, as it ignores observations before and after the subsequence. As a result, SGMCMC methods without buffering overestimate the transition noise covariance \( Q \) and underestimate the emission covariance \( R \), as \( x \) appears to be noisier. We can expect this behavior in any stable LGSSM where message passing is required to infer \( x \) (e.g. whenever \( \|A\|_2 \) and \( \|R\|_2/\|Q\|_2 \) are not close to zero). The stochastic gradient error for parameters \((R,Q)\) are similar can be found in the Supplement.

In Figure 8 (bottom), we again compare SGLD (no-buffer and buffer), SGRLD (no-buffer and buffer), and a blocked Gibb sampler. We run our samplers on one training sequence and evaluate performance on another test sequence (both with \(|T| = 10^4\)). For the SGMCMC methods, we use a large subsequence size of \( S = 100 \) with \( B = 0 \) (no buffer) and \( B = 10 \) (buffer). We see that even with a large subsequence size, buffering is crucial for accurate inference as SGMCMC methods without buffering converge to a different stationary distribution than the posterior.

In Table 2, we evaluate the KSD of the different MCMC methods. We find that SGRLD performs as well as Gibbs even for \(|T| = 10^4\), as the forward-backward algorithm was more computationally expensive for the LGSSM than for HMMs.

### Table 2: \( \log_{10}(\text{KSD}) \) by variable of MCMC samplers. Mean and (SD) over runs in Figure 8.

| Sampler                        | \( A \)   | \( Q \)   | \( R \)   |
|-------------------------------|-----------|-----------|-----------|
| Gibbs                         | 0.59 (0.27) | 0.29 (0.12) | 0.81 (0.02) |
| SGLD (Buffer)                 | 0.80 (0.15) | 0.27 (0.19) | 1.01 (0.13) |
| SGRLD (Buffer)                | 0.64 (0.07) | 0.28 (0.02) | 0.78 (0.04) |
| SGLD (No Buffer)              | 1.96 (0.09) | 1.02 (0.16) | 1.17 (0.08) |
| SGRLD (No Buffer)             | 2.00 (0.05) | 0.77 (0.27) | 0.94 (0.08) |

#### 6.2.2 Synthetic SLDS

We now consider synthetic data from a model we can view as switching extension of the LGSSM in Section 6.2.1 or as a noisy version of the ARHMM in the Supplement. The true model parameters \( \theta^* \) are

\[
\Pi = \begin{bmatrix} 0.9 & 0.1 \\ 0.1 & 0.9 \end{bmatrix}, \quad Q_1 = Q_2 = 0.1 \cdot \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad C = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad R = 0.1 \cdot \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix},
\]

\[
A_1 = 0.9 \cdot \begin{bmatrix} \cos(-\vartheta) & -\sin(-\vartheta) \\ \sin(-\vartheta) & \cos(-\vartheta) \end{bmatrix}, \quad A_2 = 0.9 \cdot \begin{bmatrix} \cos(\vartheta) & -\sin(\vartheta) \\ \sin(\vartheta) & \cos(\vartheta) \end{bmatrix},
\]

where again \( \vartheta = \pi/4 \). We generate sequences of length \(|T| = 10^4 \) and \( 10^6 \).

We first compare the variance of the three difference Monte-Carlo gradient estimators for SLDS: using \((x,z)\) samples (\(xz\ Gradient\)) as in Eq. (44), only using \( z \) samples (\(z\ Gradient\)) as in Eq. (45), and only using \( x \) samples (\(x\ Gradient\)) as in Eq. (46). Figure 9 presents boxplots of \( \nabla U(\theta) - E \nabla U(\theta) \) for the three different estimators at \( \theta = \theta^* \). From Figure 9 (left), we see that \( z\ Gradient \) (blue) has much lower variance than the other two estimators for the gradient of \( A \). This also holds for the gradients of \( Q \) and \( R \) (see Supplement). From Figure 9 (right), we see that all three estimators have similar variance for the gradient of \( \Pi \) (with \( x\ Gradient \) (green) slightly better than the other two). This agrees with intuition described in Section 5.4.1. Because \( z\ Gradient \) has lower variance than the other two estimators, we can use larger step-sizes, leading to faster convergence and mixing.
Figure 9: SLDS gradient error for the different estimators Eqs. (44)-(46). (Left) Boxplots of $\nabla_A U(\theta) - E \nabla_A U(\theta)$. (Right) Boxplots of $\nabla_{\Pi} U(\theta) - E \nabla_{\Pi} U(\theta)$.

Figure 10: SLDS stochastic gradient error for z Gradient. (Left) error varying subsequence length $S$ for no-buffer $B = 0$ and buffer $B = 10$. (Right) error varying buffer size $B$ for small $S = 2$ and long $S = 50$ subsequences. Error bars are SD over $10^4$ samples.

Figure 10 plots the stochastic gradient error $\nabla U(\theta) - \nabla U(\theta)$ for $A_0$, $A_1$, $\Pi$ evaluated at $\theta = \theta^*$. We see that buffering is necessary to correct for subsampling bias. Similar to the results for HMM and LGSSM, we also see that the bias for the discrete-state transition matrix $\Pi$ decays quickly with subsequence length $S$, but does not decay quickly for the continuous-state transition matrix $A$.

In Figure 11, we compare SGRDL (with buffer) using each of the gradient estimators Eqs. (44)-(46), and a blocked Gibbs sampler. We run our samplers on one training sequence and evaluate performance on another test sequence. For all SGRDL samplers, we used subsequence size of $S = 10$ and $B = 10$. As the marginal loglikelihood is not available in closed form for SLDSs, we instead use a Monte Carlo approximation of the EM lower bound $\log \Pr(y | \theta) \geq E_{x,z | y,\theta} [\log \Pr(y, x, z | \theta)]$ where the expectation is approximated with samples of $x, z$ drawn using blocked Gibbs for each fixed $\theta$. From Figure 11, we see that SGRDL methods perform similarly to Gibbs for $|T| = 10^4$, but vastly outperform Gibbs for $|T| = 10^6$. 

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6.2.3 Canine Seizure iEEG

Recall the data from Section 6.1.3. For our SLDS analysis, we set the continuous latent variable dimension to $n = 1$. The number of latent states remains $K = 5$. We again compare SGLD and SGRLD samplers with $S = 100$ and $B = 10$ to Gibbs samplers on both the full data set and a 10% subset of seizures. In Figure 12, we see again that the SGRLD sampler converges much more rapidly than the other methods. In comparison to Figure 7, we also see that the SLDS is a better model for this data than the ARHMM (as measured by heldout likelihood). Qualitatively, the SLDS segmentations of seizures (Figure 12 (right)) is more contiguous than the ARHMM segmentation (Figure 7 (right)).

6.2.4 Historical Cities Weather Data

We apply SGMCMC to historical city weather data from Kaggle [6]. The data consists of hourly temperature, pressure and humidity measurements ($m = 3$) for 20 US cities over 5 years with $T = 44,000$ hourly observations per city. We fit SLDS models with $n = 3$ and $K = 4$ to both the hourly and daily average observations, treating the cities independently. For both sets of observations, we perform an 80-20 train-test split over 20 cities, running inference on the training set (16 cities) and evaluating loglikelihood on the test set (4 cities).

Figure 13 (top-left) shows the heldout loglikelihood vs the runtime for the different samplers on the daily data. From this plot, we see that SGRLD clearly outperforms Gibbs. Although Gibbs converges quickly on the daily data, it gets stuck in local optima. In particular, the Gibbs runs converge to a suboptimal parametrization that mixes over three states, while SGRLD converges to a two state (summer-winter) solution (with the remaining
Figure 12: SLDS Canine Seizure Data: (left) heldout loglikelihood vs time, (center) heldout loglikelihood vs time on log-scale (right) example segmentation by ARHMM fit with SGRLD. The MCMC methods compared are Gibbs, Subset Gibbs, SGLD, and SGLRD.

states for sudden shifts or jumps). For example, Figure 13 (top-center and right) are fits of the daily model to the Houston time series for both Gibbs and SGRLD respectively. Figure 13 (bottom-left) shows the heldout loglikelihood vs the runtime of the different samplers for the hourly data. SGRLD again outperforms Gibbs and, for the hourly data, the Gibbs sampler is significantly slower than the SGMCMC samplers.

7 Conclusion

In this work, we developed stochastic gradient MCMC samplers for state space models of sequential data. Our key contribution is a buffered gradient estimator $\nabla \tilde{U}(\theta)$ for general discrete-time SSMs based on Fisher’s identity. We developed bounds for the error of this buffered gradient estimator and showed that the error decays geometrically in the buffer size under mild conditions. Using this estimator and bound, we developed SGRLD samplers for discrete (Gaussian HMM, ARHMM), continuous (LGSSM), and mixed-type (SLDS) state space models. In our experiments, we find that our methods can provide orders of magnitude run-time speed ups compared to Gibbs sampling, control bias with modest buffer size, and converge and mix more rapidly using preconditioning. In particular, our SGRLD method only uses subsequences at each iteration and is able to take advantage of geometric structure using the complete-data Fisher information matrix.

There are many interesting directions for future work. This buffered gradient estimator for sequential data could be applied to other stochastic gradient methods such as maximum likelihood estimation or variational inference [3, 41]. The approach could also be extended to non-linear continuous SSMs (e.g. stochastic volatility models) replacing message passing with particle filtering [2, 9, 21, 50]. The buffered gradient estimator could likewise be applied to diffusions with augmented dynamics, such as using momentum (SGHMC) [13] or temperature (SGNHT) [19]. In terms of analysis, the standard SGLD error analysis could be extended to analyze the optimal trade-off between buffer size and subsequence length.

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Figure 13: SLDS Weather Data. (Top) daily aggregated data, (bottom) hourly data. (Left) heldout loglikelihood vs runtime, (center) Gibbs Houston fit, (right) SGRLD Houston fit.

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Supplement

This supplement is organized as follows. In Section A, we review how to randomly sample subsequences \( S \). In Section B, we provide the proofs of Lemmas for Section 4. In Section C, we provide additional details for how to calculate the forward backward messages, gradients, and preconditioning terms for the models in Section 5. In particular, in C.3.4, we provide the proofs of the error bound lemmas from Section 5.3.1. Finally, in Section D, we provide additional details and figures of experiments.

A Subsequence Sampling Procedure

In this section, we describe how to sample the subsequences used to compute stochastic gradients.

Without loss of generality, we consider the case of sampling a single subsequence \( S \) from a long time series \( T \). If we are given multiple, independent time series \( \{T_n\} \), then our procedure can be applied by sampling a subsequence from each series. If we wish to sample multiple subsequences from a single time series, we can sample \( S \) with replacement or require a minimum gap size between subsequences as in [48]. In our experiments, we sampled a single subsequence (from each independent time series in the case of multiple series) for each stochastic gradient estimate.

The naive sampling method is to sample \( S \) from all subsequences of length \( S \) of \( T \) with \( \Pr(S) = 1/(|T| - |S|) \). As observations can appear in multiple subsequences, each time point must be weighted by the number of subsequences it appears in (e.g. \( \Pr(t \in S) \)); points in the center are scaled by \( |S|/(|T| - |S|) \), while end points are scaled by \( 1/(|T| - |S|) \). This leads to a different correction term for each observation \( t \in S \). This is slightly different than what is presented in the paper Eq. (16), as the unbiased gradient estimates take the form

\[
\nabla \hat{U}(\theta) = -\sum_{t \in S} \frac{|T| - |S|}{\#(t, S)} E_{u|y_{S^*}, \theta} [\nabla \log \Pr(y_t, u_t | u_{t-1}, \theta)] - \nabla \log \Pr(\theta) \ . \quad (A.47)
\]

where \( \#(t, S) \) is the number of subsequences of length \( S \) containing \( t \). The difference in correction terms is negligible when \( |S| << |T| \) as \( \#(t, S) = S \) for most \( t \); however it is easy to obtain constant correction terms with next sampling method.

A strict partition sampling method corrects this by splitting \( T \) into \( |T|/S \) separate subsequences (where \( S = |S| \)). If \( |T| \) is not perfectly divisible by \( S \), then the last subsequence will be shorter than the target length \( S \). We sample a subsequence from this partition proportional to the subsequence length; that is \( \Pr(S) = |S|/|T| \), thus our gradient estimate is the same form as Eq. (16)

\[
\nabla \hat{U}(\theta) = -\frac{|T|}{|S|} \sum_{t \in S} E_{u|y_{S^*}, \theta} [\nabla \log \Pr(y_t, u_t | u_{t-1}, \theta)] - \nabla \log \Pr(\theta) \ . \quad (A.48)
\]

To avoid high variance due to fixing the partition (i.e. every \( S \) points are always grouped together), one can randomly sample the first subsequence length from \([1, S]\). In practice, when the endpoint subsequences have length less than \( S/2 \), we append them to the next (or previous) subsequence, so that all subsequences have length in \([S/2, 3S/2]\). We used this second method in the experiments.

To obtain a buffered subsequence \( S^* \), we take \( B \) points to the left and right of \( S \). If we reach the beginning or end of the sequence, then we stop early (as the approximate and
exact messages are equal at the end points: \( \alpha_T = \tilde{\alpha}_T \) and \( \beta_T = \tilde{\beta}_T \). Because \( S^* \) are only used in calculating the pairwise marginal posterior of the latent states, we do not need consider the size of the buffer \( B \) when sampling \( S \).

## B Proof of Lemmas in Section 4

We now provide proofs to the Lemmas in section 4.

We first present a proof of Lemma 1 that relates the error in the difference of expectations in Eq. (26) to Wasserstein distance.

**Proof of Lemma 1.** Let \( \nabla U_t(u_{t-1:t}) = \nabla \log \Pr(y_t, u_t | u_{t-1}, \theta) \).

Recall \( \| \nabla U_t(u_{t-1:t}) \|_{Lip} \leq L_U \) for all \( t \) by assumption. Then, by the Kantorovich-Rubinstein duality formula Eq. (25), we have

\[
\left\| \mathbb{E}_{\gamma_{t-1}} [U_t(u_{t-1:t})] - \mathbb{E}_{\tilde{\gamma}_{t-1}} [U_t(u_{t-1:t})] \right\|_2 \leq L_U \cdot \mathcal{W}_1(\gamma_{t-1}, \tilde{\gamma}_{t-1}) \, . \tag{B.49}
\]

Therefore,

\[
\| \nabla U(\theta) - \nabla \tilde{U}(\theta) \|_2 \leq \left\| \frac{T}{S} \sum_{t \in S} \mathbb{E}_{\gamma_{t-1}} [\nabla U_t(u_{t-1:t})] - \mathbb{E}_{\tilde{\gamma}_{t-1}} [\nabla U_t(u_{t-1:t})] \right\|_2 \tag{B.50}
\]

\[
\leq \left\| \frac{T}{S} \sum_{t \in S} \mathbb{E}_{\gamma_{t-1}} [\nabla U_t(u_{t-1:t})] - \mathbb{E}_{\tilde{\gamma}_{t-1}} [\nabla U_t(u_{t-1:t})] \right\|_2 \cdot L_U \cdot \sum_{t \in S} \mathcal{W}_1(\gamma_{t-1}, \tilde{\gamma}_{t-1}) \, . \tag{B.51}
\]

We now present the proof of Lemma 2 that relates the 1-Wasserstein distance between distributions \((\gamma', \tilde{\gamma}')\) of \( uu^T \) to the 2-Wasserstein distance between \((\gamma, \tilde{\gamma})\) over \( u \).

**Proof of Lemma 2.** Let \( \xi \) be a joint distribution over \( u \) and \( \tilde{u} \) with marginals \( \gamma \) and \( \tilde{\gamma} \). Let \( w := \tilde{u} - u \), which implies \( \tilde{u} = u + w \).

Then we have

\[
\mathbb{E} \| \tilde{u}u^T - uu^T \|_F = \mathbb{E} \| uu^T + wu^T + uw^T \|_F \tag{B.53}
\]

\[
\leq \mathbb{E} \| uu^T \|_F + \mathbb{E} \| uw^T \|_F + \mathbb{E} \| uw^T \|_F \tag{B.54}
\]

\[
= 2\mathbb{E} \| u^T w \| + \mathbb{E} \| w \|^2 \tag{B.55}
\]

\[
\leq 2\sqrt{\mathbb{E} \| w \|^2} \mathbb{E} \| ||w||^2 \| + \mathbb{E} \| ||w||^2 \| \tag{B.56}
\]

\[
\leq (2\sqrt{M} + 1) \max \{ \mathbb{E} \| u \|_2^{1/2}, \mathbb{E} \| ||w||^2 \| \} \tag{B.57}
\]

\[
= (2\sqrt{M} + 1) \max \{ \mathbb{E} \| \tilde{u} - u \|_2^{1/2}, \mathbb{E} \| ||\tilde{u} - u||^2 \| \} \tag{B.58}
\]

where we observe \( \|xx^T\|_F = \|xx^T\|_2 = ||x||_2^2 = x^Tx \) and we use Cauchy-Schwartz.
Taking the infimum over all $\xi$ gives the result

\[
W_1(\gamma', \tilde{\gamma}') = \inf_{\xi} \mathbb{E}[\tilde{\mu}^T - u u^T]_F \tag{B.59}
\]

\[
\leq \inf_{\xi} \left(2 \sqrt{M + 1} \max \left\{ \mathbb{E}[\|\tilde{\mu} - u\|^2]^{1/2}, \mathbb{E}[\|\tilde{\mu} - u\|^2] \right\} \right) \tag{B.60}
\]

\[
= (2 \sqrt{M + 1}) \max_{\xi} \left\{ \inf \mathbb{E}[\|\tilde{\mu} - u\|^2]^{1/2}, \inf \mathbb{E}[\|\tilde{\mu} - u\|^2] \right\} \tag{B.61}
\]

\[
= (2 \sqrt{M + 1}) \cdot \max_{r \in 1/2} W_2(\gamma, \tilde{\gamma})'. \tag{B.62}
\]

\[\square\]

We now prove Lemma 3 that bounds $W_p(\gamma_{t-1:t}, \tilde{\gamma}_{t-1:t})$ in terms of buffer size, if the forward and backward random maps $f_t, b_t$ are Lipschitz.

**Proof of Lemma 3.** We will first prove Eq. (33). Recall $f_t$ is Lipschitz with constant $L_f < 1$ for all $t \in S^*$.

Let $\xi_{t:t+1}$ be a joint distribution over $u_{t,t+1}$ and $\tilde{u}_{t:t+1}$ with marginals $\gamma_{t:t+1}$ and $\tilde{\gamma}_{t:t+1}$. Let $\xi_t$ be a joint distribution over $u_t$ and $\tilde{u}_t$ with marginals $\gamma_t$ and $\tilde{\gamma}_t$. Then for all $t \in S$, we have

\[
W_p(\gamma_{t:t+1}, \tilde{\gamma}_{t:t+1})^p \leq \inf_{\xi_{t:t+1}} \int \|u_t - \tilde{u}_t\|_2^p + \|u_{t+1} - \tilde{u}_{t+1}\|_2^p d\xi_{t:t+1}(u_{t:t+1}, \tilde{u}_{t:t+1}) \tag{B.63}
\]

\[
\leq \inf_{\xi_t} \int \|u_t - \tilde{u}_t\|_2^p + \|f_t(u_t) - f_t(\tilde{u}_t)\|_2^p d\xi(u_t, \tilde{u}_t) d\xi_t \tag{B.64}
\]

\[
\leq \inf_{\xi_t} \int \|u_t - \tilde{u}_t\|_2^p + L_f^p \cdot \|u_t - \tilde{u}_t\|_2^p d\xi_t(u_t, \tilde{u}_t) \tag{B.65}
\]

\[
\leq (1 + L_f^p) \cdot W_p(\gamma_t, \tilde{\gamma}_t)^p \tag{B.66}
\]

Repeatedly applying Eq. (29) completes the proof for Eq. (33)

\[
W_p(\gamma_{t-1:t}, \tilde{\gamma}_{t-1:t}) \leq (1 + L_f^p)^{1/p} \cdot W_p(\gamma_{t-1}, \tilde{\gamma}_{t-1}) \tag{B.67}
\]

\[
\leq (1 + L_f^p)^{1/p} \cdot L_f \cdot W_p(\gamma_{t-2}, \tilde{\gamma}_{t-2}) \tag{B.68}
\]

\[
\leq (1 + L_f^p)^{1/p} \cdot L_f^2 \cdot W_p(\gamma_{t-3}, \tilde{\gamma}_{t-3}) \tag{B.69}
\]

\[
\leq \ldots
\]

\[
\leq (1 + L_f^p)^{1/p} \cdot L_f^{p+t-1} \cdot W_p(\gamma_{-B}, \tilde{\gamma}_{-B}) \tag{B.71}
\]

The proof of Eq. (34) is identical.  \[\square\]

**C Additional Model Details**

**C.1 Gaussian HMM**

See Sections 5.1 for notation.
With some algebra, the Fisher information matrix, precondition matrices, and correction terms are

\[
\alpha_t := \Pr(z_t, y_{\leq t}) = \alpha_{t-1} \cdot \Pi \cdot P_t \\
\beta_t := \Pr(y_{> t} | z_t) = \Pi \cdot P_{t+1} \beta_{t+1} ,
\]

where \( \alpha_{-T} = 1/K \), \( \beta_T = 1 \), and

\[
P_t := \text{diag}\{N(y_t | \mu_k, \Sigma_k)\}_k=1^K .
\]

C.1.1 Forward Backward

The forward and backward recursions (Eqs. (4) and (5)) for an HMM are

\[
\alpha_t := \Pr(z_t, y_{\leq t}) = \alpha_{t-1} \cdot \Pi \cdot P_t \\
\beta_t := \Pr(y_{> t} | z_t) = \Pi \cdot P_{t+1} \beta_{t+1} ,
\]

where \( \alpha_{-T} = 1/K \), \( \beta_T = 1 \), and

\[
P_t := \text{diag}\{N(y_t | \mu_k, \Sigma_k)\}_k=1^K .
\]

C.1.2 Gradient Estimator

As stated in Sec. 5.1, we use the ‘expanded mean’ parameters of \( \Pi \) instead of \( \Pi \) (as in [52]) and the Cholesky decomposition of \( \Sigma_k^{-1} \) instead of \( \Sigma_k \) to ensure positive definiteness. The expanded mean parametrization is \( \phi \in \mathbb{R}^{K \times K} \) where \( \Pi_k = \phi_k / \sum_k \phi_{k,k'} \). The Cholesky decomposition of the precision \( \Sigma_k^{-1} \) is \( \psi_{\Sigma_k} \) such that \( \psi_{\Sigma_k} \psi_{\Sigma_k}^T = \Sigma_k^{-1} \).

The gradient of the marginal loglikelihood takes the form

\[
\nabla_{\phi_k} \log \Pr(y | \theta) = \sum_{t \in T} \mathbb{E}_{z_t, z_{t-1} | y} [I(z_{t-1} = k) \cdot \phi_k^{-1} \circ (\bar{c}_{z_t} - \Pi_k)]
\]

\[
\nabla_{\mu} \log \Pr(y | \theta) = \sum_{t=1}^T \mathbb{E}_{z_t | y} [\Sigma^{-1}_{z_t} (y_t - \mu_{z_t})]
\]

\[
\nabla_{\psi_{\Sigma_k}} \log \Pr(y | \theta) = \sum_{t \in T} \mathbb{E}_{z_t | y} [(\Sigma_{z_t} - (y_t - \mu_{z_t})(y_t - \mu_{z_t})^T) \psi_{\Sigma_{z_t}}] .
\]

As \( z \) is discrete and these expectations only involve pairwise elements of \( z \), they can be tractably computed as weighted average using \( \gamma(z_t, z_{t-1}) \) from forward backward.

C.1.3 Preconditioning

For the Gaussian HMM, the complete-data Fisher information matrix is block diagonal. With some algebra, the Fisher information matrix, precondition matrices, and correction term are

\[
\mathcal{I}_{\phi_k} = (\text{diag}(\Pi_k) - 11^T) \cdot (1^T \phi_k)^{-2} \Rightarrow D(\theta)_{\phi_k} = \text{diag}(\phi_k) \quad \text{and} \quad \Gamma(\theta)_{\phi_k} = 1
\]

\[
\mathcal{I}_{\mu_k} = \Sigma_k^{-1} \Rightarrow D(\theta)_{\mu_k} = \Sigma_k \quad \text{and} \quad \Gamma(\theta)_{\mu_k} = 0
\]

\[
\mathcal{I}_{\psi_{\Sigma_k}} = 2(I_m \otimes \Sigma_k) \Rightarrow D(\theta)_{\psi_{\Sigma_k}} = \frac{1}{2}(I_m \otimes \Sigma_k^{-1}) \quad \text{and} \quad \Gamma(\theta)_{\psi_{\Sigma_k}} = \psi_{\Sigma_k}
\]

For \( \phi_k \), we use \( D(\theta)_{\phi_k} = \text{diag}(\phi_k) \) and \( \Gamma(\theta)_{\phi_k} = 1 \), following past work [52, 48]. However, we observed that \( \phi_k \) will be absorbed at 0, whenever \( \phi_k \) approaches to closely to 0. To fix this we recommend adding a small identity matrix \( \nu_{\phi} I_K \) (for some \( \nu_{\phi} > 0 \)) to \( D(\theta)_{\phi} \).
C.2 ARHMM

See Section 5.2 for notation.

C.2.1 Forward Backward

The forward backward recursions for the ARHMM are identical to the Gaussian HMM Eqs. (C.72)-(C.76), where
\[ P_t := \text{diag}\{N(y_t | A_k \eta_t, Q_k)\}^K_{k=1}. \] (C.83)

C.2.2 Gradient Estimator

The gradient of the marginal loglikelihood is similar to the Gaussian HMM Eqs. (C.77)-(C.79) with \( \mu_k \) replaced with \( A_k \eta_t \)
\[
\nabla_{\phi_k} \log \Pr(y | \theta) = \sum_{t \in T} \mathbb{E}_{z_t, z_{t-1} | y}[\epsilon(z_{t-1} = k) \cdot \phi_k^{-1} \odot (\epsilon_{z_t} - \Pi_k)]
\] (C.84)
\[
\nabla_{A_k} \log \Pr(y | \theta) = \sum_{t = 1}^{T} \mathbb{E}_{z_t | y} [Q_{z_t}^{-1} (y_t - A_{z_t} \eta_t) \eta_t^T]
\] (C.85)
\[
\nabla_{\psi_{Q_k}} \log \Pr(y | \theta) = \sum_{t \in T} \mathbb{E}_{z_t | y} \left[ (Q_{z_t} - (y_t - A_{z_t} \eta_t)(y_t - A_{z_t} \eta_t)^T) \psi_{z_t} \right].
\] (C.86)

C.2.3 Preconditioning

The preconditioning terms for the ARHMM is similar to the Gaussian HMM
\[
I_{\phi_k} = (\text{diag}(\Pi_k) - 11^T) \cdot (1^T \phi_k)^{-2} \Rightarrow D(\theta)_{\phi_k} = \text{diag}(\phi_k) \quad \text{and} \quad \Gamma(\theta)_{\phi_k} = 1
\] (C.87)
\[
I_{A_k} = \mathbb{E}_{y,z | [\eta_t, \eta_t^T]} \odot Q_k^{-1} \Rightarrow D(\theta)_{A_k} = I_m \odot Q_k \quad \text{and} \quad \Gamma(\theta)_{A_k} = 0
\] (C.88)
\[
I_{\psi_{Q_k}} = 2(I_m \odot Q_k) \Rightarrow D(\theta)_{\psi_{Q_k}} = \frac{1}{2} (I_m \odot Q_k^{-1}) \quad \text{and} \quad \Gamma(\theta)_{\psi_{Q_k}} = \psi_{Q_k}
\] (C.89)

The expectation \( \mathbb{E}[\eta_t, \eta_t^T] \) does not have a closed form as the expectation is over \( z \) is a combinatorial sum. Therefore, we choose to replace \( \mathbb{E}[\eta_t, \eta_t^T] \) with the identity matrix \( I_m \) in our preconditioning matrix \( D(\theta)_{A} \).

C.3 LGSSM

See Section 5.3 for notation.

C.3.1 Forward Backward

The recursions for the forward backward algorithm for LGSSMs is known as the Kalman smoother [9, 7, 29]. Because the transition and emission processes are linear Gaussian, all forward messages, backward messages, and pairwise latent marginals \( \gamma(x_t, x_{t-1}) \) are Gaussian.
\[
\alpha_t := \Pr(x_t, y_{\leq t}) = N(x_t | \mu_{\alpha_t} = \Lambda_{\alpha_t}^{-1} h_{\alpha_t}, \Sigma_{\alpha_t} = \Lambda_{\alpha_t}^{-1})
\] (C.90)
\[
\beta_t := \Pr(y_{> t} | x_t) \propto N(x_t | \mu_{\beta_t} = \Lambda_{\beta_t}^{-1} h_{\beta_t}, \Sigma_{\beta_t} = \Lambda_{\beta_t}^{-1})
\] (C.91)
where $h_{\alpha_t}, \Lambda_{\alpha_t}$ are the Gaussian natural parameters of $\alpha$ that satisfy the recursion

$$
\Lambda_{\alpha_t} = C^T R^{-1} C + (Q + C A_{\alpha_{t-1}} A^T)^{-1} \quad (C.92)
$$

$$
h_{\alpha_t} = C^T R^{-1} y_t + (Q + C A_{\alpha_{t-1}} A^T)^{-1} A \Lambda_{\alpha_{t-1}} h_{\alpha_{t-1}}, \quad (C.93)
$$

and $h_{\beta_t}, \Lambda_{\beta_t}$ are the Gaussian natural parameters of $\beta$ that satisfy the recursion

$$
\Lambda_{\beta_t} = A^T Q^{-1} A - A^T Q^{-1} (Q^1 + C^T R^{-1} C + \Lambda_{\beta_{t+1}})^{-1} Q^{-1} A \quad (C.94)
$$

$$
h_{\beta_t} = A^T Q^{-1} (Q^1 + C^T R^{-1} C + \Lambda_{\beta_{t+1}})^{-1} (C^T R^{-1} y_{t+1} + h_{\beta_{t+1}}). \quad (C.95)
$$

Given the messages $\alpha_t, \beta_t$ the marginal and pairwise posteriors of the latent states $x_t$ and $(x_{t-1}, x_t)$ are computed as

$$
\gamma_t(x_t) := \Pr(x_t | y) \propto \alpha_t(x_t) \beta_t(x_t)
$$

$$
\alpha_{t-1}(x_{t-1}) := \Pr(x_{t-1} | y) \propto \alpha_{t-1}(x_{t-1}) \Pr(y_t, x_t | x_{t-1}) \beta_t(x_t) \quad (C.96)
$$

$$
\gamma_{t-1,t}(x_{t-1}, x_t) := \Pr(x_{t-1}, x_t | y) \propto \alpha_{t-1}(x_{t-1}) \Pr(y_t, x_t | x_{t-1}) \beta_t(x_t) \quad (C.97)
$$

$$
\propto \mathcal{N}\left( \begin{bmatrix} x_{t-1} \\ x_t \end{bmatrix} ; \mu = \Sigma \begin{bmatrix} h_{\alpha_{t-1}} \\ C^T R_{t-1} y_t + h_{\beta_t} \end{bmatrix}, \Sigma = \begin{bmatrix} \Lambda_{\alpha_{t-1}} + A^T Q^{-1} A & A^T Q^{-1} \\ Q^{-1} & C^T R^{-1} C + Q^{-1} + \Lambda_{\beta_t} \end{bmatrix} \right)^{-1} \right). \quad (C.98)
$$

### C.3.2 Gradient Estimator

We compute the gradient of marginal loglikelihood via Fisher’s identity

$$
\nabla_A \log \Pr(y | \theta) = \sum_{t=1}^{T} \mathbb{E}_{x_t | y} \left[ (Q^{-1}(x_t - Ax_{t-1}) x_{t-1}^T) \right] \quad (C.99)
$$

$$
\nabla_{\psi_Q} \log \Pr(y | \theta) = \sum_{t=1}^{T} \mathbb{E}_{x_t | y} \left[ (Q - (x_t - Ax_{t-1}) (x_t - Ax_{t-1})^T) \psi_Q \right] \quad (C.100)
$$

$$
\nabla_C \log \Pr(y | \theta) = \sum_{t=1}^{T} \mathbb{E}_{x_t | y} \left[ R^{-1}(y_t - C x_t) x_{t}^T \right] \quad (C.101)
$$

$$
\nabla_{\psi_R} \log \Pr(y | \theta) = \sum_{t=1}^{T} \mathbb{E}_{x_t | y} \left[ (R - (y_t - C x_t) (y_t - C x_t)^T) \psi_R \right] \quad (C.102)
$$

Because each gradient is linear with respect to first and second order terms (e.g. $x_t, x_t x_{t-1}^T$ and $x_t x_{t-1}^{T_{t-1}}$), their expectation of each of these terms is easily computable given $\gamma(x_t, x_{t-1})$.

Let $\gamma_{t-1,t}(x_{t-1}, x_t)$ be the Gaussian pairwise marginal posterior from forward backward (see Eq. (C.97))

$$
\gamma_{t-1,t}(x_{t-1}, x_t) = \mathcal{N}\left( \begin{bmatrix} x_{t-1} \\ x_t \end{bmatrix} ; \mu = \begin{bmatrix} \mu_{t-1} \\ \mu_t \end{bmatrix}, \Sigma = \begin{bmatrix} \Sigma_{t-1,t-1} & \Sigma_{t-1,t} \\ \Sigma_{t,t-1} & \Sigma_{t,t} \end{bmatrix} \right). \quad (C.103)
$$

Let $M = \Sigma + \mu \mu^T$ be the second moment of $\gamma_{t-1,t}$, that is $M_{t,t'} := \mathbb{E}[x_t, x_{t'}^T]$.  

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Then the expectations in the summations of Eqs. (C.98)-(C.101) are
\[ E_{x|y} [(x_t - Ax_{t-1})x_{t-1}^T] = M_{t,t-1} - AM_{t-1,t-1} \]  
(C.103)
\[ E_{x|y} [(x_t - Ax_{t-1})(x_t - Ax_{t-1})^T] = M_{t,t} - AM_{t-1,t} - M_{t,t-1}A^T + AM_{t-1,t-1}A^T \]  
(C.104)
\[ E_{x|y} [(y_t - Cx_t)x_t^T] = y_t\mu_t^T - CM_{t,t} \]  
(C.105)
\[ E_{x|y} [(y_t - Cx_t)(y_t - Cx_t)^T] = y_ty_t^T - C\mu_t\mu_t^T - y_t\mu_t^TC^T + CM_{t,t}C^T . \]  
(C.106)

C.3.3 Preconditioning

For the LGSSM, the complete data Fisher information matrix is block diagonal. With some algebra, the Fisher information matrix, precondition matrices, and correction term are
\[ I_A = E [x_t x_t]^T \otimes Q^{-1} \Rightarrow D_A = I_n \otimes Q \text{ and } \Gamma(\theta)_A = 0 \]  
(C.107)
\[ I_{\psi Q} = 2(I_n \otimes Q) \Rightarrow D_{\psi Q} = \frac{1}{2}(I_n \otimes Q^{-1}) \text{ and } \Gamma(\theta)_{\psi Q} = \psi_Q \]  
(C.108)
\[ I_C = E [x_t x_t]^T \otimes R^{-1} \Rightarrow D_C = I_n \otimes R \text{ and } \Gamma(\theta)_C = 0 \]  
(C.109)
\[ I_{\psi R} = 2(I_m \otimes R) \Rightarrow D_{\psi R} = \frac{1}{2}(I_m \otimes R^{-1}) \text{ and } \Gamma(\theta)_{\psi R} = \psi_R , \]  
(C.110)
where \( E [x_t x_t]^T = \sum_{x_t} A^t Q(A^t)^T \) for the LGSSM. In our experiments we chose to replace \( E [x_t x_t]^T \) with the identity matrix \( I_n \) to match the ARHMM setup.

C.3.4 Proof of Lemmas in Section 5.3.1

We now provide proofs to the Lemmas in section 5.3.1.

We first present a proof of Lemma 4 that shows the forward random maps \( f_t \) are contractions if \( \|A\| < 1 \).

\textbf{Proof of Lemma 4.} For an LGSSM, the forward smoothing kernel \( \mathcal{F}_t \) takes the form
\[ \mathcal{F}_t(x_{t+1}, x_t | y) \propto \beta_{t+1}(x_{t+1}) \frac{\Pr(y_{t+1} | x_{t+1}) \Pr(x_{t+1} | x_t)}{\Pr(y_{t+1} | x_{t+1})} \]  
(C.111)
where \( \beta_{t+1} \) is the backward message at time \( t+1 \) given by Eq. (C.91). The recursive formula for \( \beta_t \) can be extended to \( \Pr(y_{\geq t} | x_{t+1}) \propto \mathcal{N}(x_{t+1} | \Lambda_t^{-1} h_{t+1}, \Lambda_t^{-1}) \) with
\[ \Lambda_t = C^T R^{-1} C + A^T (Q + \Lambda_t^{-1})^{-1} A \]  
(C.112)
\[ h_t = C^T R^{-1} y_t + A^T (Q + \Lambda_t^{-1})^{-1} \Lambda_t h_{t+1} . \]  
(C.113)

With this parametrization, the forward smoothing kernel takes the form
\[ \mathcal{F}_t(x_{t+1} | x_t) = \mathcal{N}(x_{t+1} | (Q^{-1} + \Lambda_t)^{-1}(Q^{-1} A x_t + h_{t+1}), (Q^{-1} + \Lambda_t)^{-1}) . \]  
(C.114)

Therefore our random map \( f_t \) is
\[ f_t(x) = \left( Q^{-1} + \Lambda_t^{-1} \right)^{-1} Q^{-1} A x_t + \left( Q^{-1} + \Lambda_t^{-1} \right)^{-1} h_{t+1} + (Q^{-1} + \Lambda_t^{-1})^{-1/2} \nu_t , \]  
(C.115)
where \( \nu_t \sim \mathcal{N}(0, I) \) makes \( f_t \) a random map.
The Lipschitz constant for $f_t$ with respect to $x_t$ is $\|F_t^f\| = \|(Q^{-1} + \Lambda_{t+1})^{-1}Q^{-1}A\|$. From Eq. (C.112), $A_0 = C^TR^{-1}C$ is a lower bound on $\Lambda_t$ and it is tight when $\Lambda_{t+1} = 0$ (at the very beginning of the recursion).

Therefore we have a uniform bound on the Lipschitz constants of $f_t$:

$$\|F_t^f\| = \|(Q^{-1} + \Lambda_{t+1})^{-1}Q^{-1}A\| < \|(Q^{-1} + A_0)^{-1}Q^{-1}A\| = L_f .$$  \hfill (C.116)

We now present a proof of Lemma 5 that similarly shows the backward random maps $b_t$ are contradictions if $\|A\| < 1$.

**Proof of Lemma 5.** The backward smoothing kernel $B_t$ takes the form

$$B_t(x_{t-1}, x_t \mid y) \propto \Pr(x_t \mid x_{t-1}) \alpha_{t-1}(x_{t-1})$$

where $\alpha_{t-1}$ is the forward message at time $t-1$. Recall from Eq. (C.90) the forward messages are $\alpha_t(x_t) \propto \mathcal{N}(x_t | \Lambda_t^{-1}h_{t-1}, \Lambda_{t-1})$. With this parametrization, the backward smoothing kernel takes the form

$$B_t(x_{t-1}, x_t \mid y) = \mathcal{N}(x_{t-1} \mid (A^TQ^{-1}A + \Lambda_{n-1})^{-1}(A^TQ^{-1}x_t + h_{n-1}), (A^TQ^{-1}A + \Lambda_{n-1})^{-1}) .$$

Our backward random map $b_t$ is thus

$$b_t(x_t) = (A^TQ^{-1}A + \Lambda_{n-1})^{-1}(A^TQ^{-1}x_t + h_{n-1}) + (A^TQ^{-1}A + \Lambda_{n-1})^{-1/2}\nu_t ,$$

where $\nu_t \sim \mathcal{N}(0, I)$ with

$$F_t^b = (A^TQ^{-1}A + \Lambda_{n-1})^{-1}A^TQ^{-1}$$

$$\zeta_t^b = (A^TQ^{-1}A + \Lambda_{n-1})^{-1}h_{n-1} + (A^TQ^{-1}A + \Lambda_{n-1})^{-1/2}\nu_t .$$  \hfill (C.117)

The Lipschitz constant for $b_t$ with respect to $x_t$ is

$$\|F_t^b\| = \|(A^TQ^{-1}A + \Lambda_{n-1})^{-1}A^TQ^{-1}\| = \|A(I_n + Q(A^T\Lambda_{n-1}A)^{-1})^{-1}\| .$$

From Eq. (C.92), $A_0 = C^TR^{-1}C$ is a lower bound on $\Lambda_{n}$ and it is tight when $\Lambda_{n-1} = 0$ (at the very beginning of the recursion). Therefore we have a uniform bound on the Lipschitz constants of $b_t$ for Lemma 3:

$$\|F_t^b\| = \|A(I_n + Q(A^T\Lambda_{n-1}A)^{-1})^{-1}\| \leq \|A(I_n + Q(A^T\Lambda_{0}A)^{-1})^{-1}\| = L_b .$$  \hfill (C.118)

Finally we prove Lemma 6 which bounds the Lipschitz constant for the complete data loglikelihood terms.

**Proof of Lemma 6.** The gradient of the complete data loglikelihood with respect to $\theta = (A, Q, C, R)$ is

$$\nabla_A \log \Pr(y, x_t \mid x_{t-1}, \theta) = Q^{-1}(x_t - Ax_{t-1})x_{t-1}^T$$

$$\nabla_Q \log \Pr(y, x_t \mid x_{t-1}, \theta) = (Q - (x_t - Ax_{t-1})(x_t - Ax_{t-1})^T)\psi_Q$$

$$\nabla_C \log \Pr(y, x_t \mid x_{t-1}, \theta) = R^{-1}(y_t - Cx_t)x_t^T$$

$$\nabla_R \log \Pr(y, x_t \mid x_{t-1}, \theta) = (R - (y_t - Cx_t)(y_t - Cx_t)^T)\psi_R .$$  \hfill (C.119)

From Eqs. (C.119)-(C.122) it is clear that the complete data loglikelihood are quadratic form in $xx^T$ with matrices given by $\Omega$ in Lemma 6.  \hfill \Box
C.4 SLDS

See Section 5.4 for notation. As the SLDS does not have a closed form forward-backward algorithm, we instead present the details for the blocked Gibbs sampling scheme (conditional distributions and Initialization) used in Algorithm 3.

C.4.1 Blocked Gibbs Conditional Distributions

The conditional posterior distribution of \( x \) given \( y \) and \( z \) follows a time-varying LGSSM. To sample \( x \), we can use the time-varying Kalman filter [35]. We first calculate the forward messages \( \alpha_t(x_t) \) using the Kalman filter recursion Eq. (C.90) with \( A_t = A_{z_t}, C_t = C, Q_t = Q_{z_t} \), and \( R_t = R \). Given \( \alpha_t(x_t) \propto \mathcal{N}(x_t | \mu_{\alpha_t}, \Sigma_{\alpha_t}) \), we sample \( x \) using the backward sampler (starting from \( t = T \) and descending)

\[
x_t | x_{t-1} \sim \begin{cases} \mathcal{N}(x_T | \mu = \mu_{\alpha_T}, \Sigma = \Sigma_{\alpha_T}) \text{ if } t = T , \\ \mathcal{N}(x_t | \mu = \Sigma(\Sigma_{\alpha_t}^{-1} \mu_{\alpha_t} + A_T^T Q_{z_{t+1}}^{-1} x_{t+1}), \Sigma = (\Sigma_{\alpha_t}^{-1} + A_T^T Q_{z_{t+1}}^{-1} A_{z_t})^{-1}) \end{cases} 
\]

(C.123)

The conditional posterior distribution of \( z \) given \( y \) and \( x \) follows the ARHMM. To sample \( z \), we apply a similar sampler for the ARHMM. We first calculate the backward messages \( \beta_t(z_t) \) using the ARHMM forward messages Eq. (C.73), replacing \( y \) with \( x \). Given \( \alpha_t(z_t) \), we then sample \( z \) sequentially in ascending order using the forward sampler

\[
\Pr(z_t = k | z_{t-1}, x, y) \propto \Pr(x_t, y_t | x_{t-1}, z_t = k, \theta) \circ \Pi_{z_{t-1}, k} \circ \beta_t(k) .
\]

(C.124)

Finally, the conditional posterior distribution of \( z_t \) given \( y \) and \( z_{\leq t} \) can be calculated using the forward backward algorithm to marginalize \( x \). Specifically,

\[
\Pr(z_t = k | z_{\leq t}, y) \propto \Pi_{z_{t-1}, k} \Pi_{k, z_t} \int \alpha_{t-1}(x_{t-1}) \Pr(y_t, x_t | x_{t-1}, z_t = k) \beta_t(x_t) dx_t dx_{t-1} ,
\]

(C.125)

where \( \alpha_t, \beta_t \) are calculated using Eqs. (C.90)-(C.91) with \( A_t = A_{z_t}, Q_t = Q_{z_t} \) for all \( t' \in \mathcal{S}^* \setminus \{ t \} \).

Note that Eq. (C.125) requires \( O(|\mathcal{S}^*|) \) time per time point \( z_t \); therefore one pass over \( z_\mathcal{S} \) requires \( O(|\mathcal{S}^*|^2) \).

C.4.2 Initialization of Blocked Gibbs Sampler

To sample \( z \) from the filtered process, we recursively sample from the conditional distribution \( z_t | y_t, z_{\leq t-1} \)

\[
\Pr(z_t = k | z_{t-1}, y_t) \propto \Pi_{z_{t-1}, k} \int \alpha_{t-1}(x_{t-1}) \Pr(y_t, x_t | x_{t-1}, z_t = k) dx_t dx_{t-1} ,
\]

(C.126)

where \( \alpha_{t-1} \) is calculated using Eq. (C.90) with \( A_t = A_{z_t}, Q_t = Q_{z_t} \) for all \( t' < t \). Because we do not condition on \( y_{>t} \) when \( z_t \) is sampled, we emphasize that this distribution is not the posterior \( z | y \) (it is the filtered distribution, not the smoothed distribution). However, it provides a better initialization point than sampling \( z \) from the prior.

Alternatively, when \( \dim(x) = n \leq \dim(y) = m \), we can initialize \( z^{(0)} \) by sampling \( z | x', y, \theta \) using Eq. (C.124) with \( x' = y \).

C.4.3 Gradient Estimator

For the SLDS, the gradients are similarly a combination of those for the ARHMM Eqs. (C.84)-(C.86) and the LGSSM Eqs. (C.101)-(C.101).
C.4.4 Preconditioning

For the SLDS, the precondition matrices are similarly a combination of those for the ARHMM Eqs. (C.87)-(C.89) and the LGSSM Eqs. (C.107)-(C.110).

\[ D(\theta)_{\phi_k} = \text{diag}(\phi_k) \text{ and } \Gamma(\theta)_{\phi_k} = 1 \]  
\[ D(\theta)_{A_k} = I_m \otimes Q_k \text{ and } \Gamma(\theta)_{A_k} = 0 \]  
\[ D(\theta)_{\psi_Q k} = \frac{1}{2} I_n \otimes Q_k^{-1} \text{ and } \Gamma(\theta)_{\psi_Q k} = \psi_Q k \]  
\[ D(\theta)_{\psi_R k} = \frac{1}{2} I_m \otimes R_k^{-1} \text{ and } \Gamma(\theta)_{\psi_R k} = \psi_R k . \]

D Additional Experiment Details

D.1 Priors

In our experiment we use the following (conjugate) priors for \( \theta \).

For the discrete latent state sequence transition matrix \( \Pi_k \), we use a flat-Dirichlet prior
\[ \Pr(\Pi_k) \propto \prod_k \Pi_{k,k'}^{\alpha_{k,k'} - 1}, \text{ where } \alpha_{k,k'} = 1. \]  
\[ \text{(D.132)} \]

For the continuous transition matrix \( A_k \), we use a matrix normal prior
\[ \Pr(A) \propto \exp\left(-\text{tr}\left[ V^{-1}(A - M)^T U^{-1}(A - M) \right]/2 \right), \]  
\[ \text{(D.133)} \]

with mean \( M = 0 \), diagonal column covariance \( V = 10^3 \cdot I_n \), and row variance \( U = Q \).

For the noise covariances \( Q \) and \( R \), we use flat Wishart priors over \( Q^{-1} \) and \( R^{-1} \)
\[ \Pr(Q^{-1}) \propto |Q|^{(n+1-\nu)/2}e^{-\text{tr}(\Psi Q^{-1})/2}, \quad \Pr(R^{-1}) \propto |R|^{(m+1-\nu)/2}e^{-\text{tr}(\Psi R^{-1})/2}, \]  
\[ \text{(D.134)} \]

where \( \Psi = \nu \cdot I \) and \( \nu = n + 1 \) or \( m + 1 \).

D.2 Additional Metric Details

To assess the ‘mixing’ rate of our MCMC samplers, we measure each sampled chain’s kernel Stein divergence (KSD) to the posterior [45, 34]. Given a chain of sampled \( \{\theta(i)\}^N \) (after burnin and thinning), let \( q(\theta) \) be the empirical distribution of the samples, that is
\[ q(\theta) = \frac{1}{N} \sum_{i=1}^{N} \delta_{\theta=\theta(i)} . \]  
\[ \text{(D.135)} \]

Then the KSD between \( q(\theta) \) and the posterior distribution \( p(\theta) \) is
\[ KSD(q, p) = \sum_{d=1}^{\dim(\theta)} \sqrt{\sum_{k=1}^{n} k(d, d)}^{\theta_k, \theta_{k'}}, \text{ where} \]  
\[ \text{(D.136)} \]

\[ k(d, d) = \nabla_{\theta_d} \log p(\theta) k(\theta, \theta) \nabla_{\theta_d} \log p(\theta) + \nabla \log p(\theta) \nabla_{\theta_d} k(\theta, \theta) + \nabla \nabla_{\theta_d} k(\theta, \theta) \]  
\[ \text{(D.137)} \]
and \( k(\cdot, \cdot) \) is a valid kernel function. Following [34], we use the inverse multiquadratic kernel (IMQ) \( k(x, y) = \frac{1}{(1 + ||x - y||^2)^{0.5}} \) in our experiments. As full gradient evaluations \( \nabla \log p(\theta) \) are computationally intractable for our long time series, we replace them with stochastic estimates based on Eq. (16).

To measure the recovery of discrete latent state variables \( z_t \) when the true latent states are known (e.g. in synthetic experiments), we use normalized mutual information (NMI). NMI is an information theoretic measure of similarity between discrete assignments [67].

\[
\text{NMI}(Z_i, Z_s) = \frac{I(Z_i, Z_s)}{\sqrt{H(Z_i)H(Z_s)}}, \quad \text{with} \quad Z_i = (z_1^{(i)}, \ldots, z_T^{(i)}),
\]

where \( I(X, Y) \) is mutual information and \( H(X) \) is entropy. NMI is maximized at 1 when the assignments are equal up to a permutation and minimized at 0 when the assignments share no information. This serves as ‘clustering’ or segmentation metric for measuring the coherence between our model’s inferred latent states and the true latent states.

To measure the recovery of continuous latent state variables \( x_t \) when the true latent states are known, we use root mean-squared error (RMSE) \( \text{RMSE}(x, x') = \sum ||x_t - x'_t||_2 \).

### D.3 Synthetic Gaussian HMM

Following [27, 48], we generate data from a Gaussian HMM with \( K = 8 \) latent states (see Figure 14 (left)). This reversed cycles (RC) dataset strongly transitions between two cycles over three states, each in opposite directions.

![Reversed Cycles](image)

Figure 14: (Left) Sample dataset; arrows indicate Markov transitions. Stochastic gradient error of select elements of transition matrix \( \Pi \): (center) varying subsequence size \( S \) for no-buffer \( B = 0 \) and buffer \( B = 5 \), (right) varying buffer size \( B \) for \( S = 2 \) and \( S = 50 \). Error bars are SD over \( 10^4 \) randomly drawn subsequences.

Figure 14 (right-pair) are plots of the stochastic gradient error \( \nabla \tilde{U}(\theta) - \nabla U(\theta) \) of the transition probabilities \( \Pi \) between the two cycles (dashed arrows in Figure 14 (left)) evaluated at the true model parameters \( \theta = \theta^* \). From Figure 14 (center), we see that the stochastic gradients are heavily biased without buffering (orange) for small subsequence lengths, as they fail to capture the structured transitions between states. However this bias disappears with buffering (blue). From Figure 14 (right), we see that the stochastic gradient decays quickly with increasing buffer size \( B \) for small subsequence \( S = 2 \) (purple). For larger subsequence \( S = 50 \) (green), buffering is not needed as the latent state of the endpoints can be well estimated from the subsequence alone. This agrees with intuition: for this HMM, inferring the marginal posterior given a few observations is easy; therefore messages from buffering are not required for large subsequence sizes. The bias in the stochastic gradients of observations parameters \( (\mu, \Sigma) \) is less extreme than for transition matrix \( \Pi \) which is associated with the latent states; we include their error plots in the Supplement.
In Figure 15, we compare SGLD (no-buffer and buffer), SGRLD (no-buffer and buffer), and Gibbs. We run our samplers on one training sequence and evaluate performance on another test sequence. We consider sequence lengths of $|\mathcal{T}| = 10^4$, $|\mathcal{T}| = 10^6$, and $|\mathcal{T}| = 10^8$. For the SGMCMC methods, we use a subsequence size of $S = 2$ and a buffer size of $B = 0$ (no-buffer) or $B = 2$ (buffer). From Figure 15, we again see that preconditioning helps convergence and mixing as SGRLD outperforms SGLD and that buffering is necessary to properly estimate $\Pi$. Although Gibbs outperforms SGRLD for $|\mathcal{T}| = 10^4$, Gibbs performs worse for $|\mathcal{T}| = 10^6$, as Gibbs only draws $\sim 30$ samples in 5 hours, and is computationally intractable for $|\mathcal{T}| = 10^8$.

Note that for the $|\mathcal{T}| = 10^4$ case, we observe that SGRLD underestimates the variance of $\Pi$ (Figure 15 bottom-left). This is due to the preconditioner $D(\theta)\Pi = \Pi$, creating absorbing states in the discretized dynamics (see comment in Section C.1.3).

Table 3 shows the KSD of different sampling methods for different components of $\theta$. Although Gibbs performs well for small $|\mathcal{T}|$, it performs worse for larger $|\mathcal{T}|$ due to the limited number of drawn samples. On the other hand, the SGMCMC methods perform comparably for all $|\mathcal{T}|$. We also see that buffered SGRLD outperforms the other SGMCMC methods on $\Pi$, as the non-buffered methods are sampling from the incorrect distribution and SGLD suffers from extreme autocorrelation.
Table 3: $\log_{10}(\text{KSD})$ by variable of MCMC samplers. Mean and (SD) over runs in Figure 15.

| Sampler          | $\pi$       | $\mu$       | $\Sigma$     |
|------------------|-------------|-------------|--------------|
| $10^4$           |             |             |              |
| Gibbs            | 1.03 (0.01) | 0.32 (0.03) | 1.93 (0.08)  |
| SGLD (Buffer)    | 0.93 (0.15) | 1.10 (0.07) | 1.96 (0.15)  |
| SGLD (Buffer)    | 0.58 (0.15) | 0.60 (0.11) | 2.21 (0.03)  |
| SGLD (No Buffer) | 1.64 (0.13) | 1.16 (0.08) | 2.06 (0.21)  |
| SGRLD (Buffer)   | 1.28 (0.03) | 0.63 (0.14) | 2.28 (0.08)  |
| $10^6$           |             |             |              |
| Gibbs            | 3.00 (0.17) | 3.04 (0.10) | 4.57 (0.15)  |
| SGLD (Buffer)    | 2.77 (0.19) | 2.37 (0.14) | 3.60 (0.04)  |
| SGR (Buffer)     | 2.58 (0.03) | 2.31 (0.11) | 3.77 (0.12)  |
| SGLD (No Buffer) | 3.50 (0.06) | 2.34 (0.12) | 4.00 (0.10)  |
| SGRLD (No Buffer)| 3.45 (0.13) | 2.43 (0.16) | 3.94 (0.09)  |

D.4 Downsampled Ion Channel Recordings

We now consider a downsampled version of the ion channel recording data presented in Section 6.1.2. In particular, we consider downsampling the data by a factor of 50 (as in [48]), resulting in $|T| = 209,634$ observations. We again train on the first 90% and evaluate on the last 10% after applying a log-transform and normalizing the observations to use Gaussian emissions. For our SGMCMC methods we again use a subsequence size of $S = 10$ and a buffer size of $B = 0$ (no-buffer) or $B = 10$ (buffer). Figure 16 presents our results including comparisons to Gibbs sampling (red). For this (shorter) downsampled data, Gibbs sampling outperforms the SGMCMC methods. We see that the performance of the SGMCMC method is similar to the full sample case (compare to Figure 6) and that SGRLD with buffering quickly reaches the same mode as Gibbs.

Figure 16: Ion Channel Recordings: (Left) predictive loglikelihood vs runtime. (Center) example segmentation using Gibbs (Right) example segmentation using SGRLD.
D.5 Additional Synthetic Experiment Plots

We now present additional plots for the synthetic data experiments. These plots show the MSE for ‘other’ components of $\theta$ to the true parameters of $\theta^*$ as well as other measures of fit such as predictive loglikelihood or recovery of the latent state sequence (NMI or RMSE).

D.5.1 Gaussian HMM

The parametrization of the RC data set is as follows:

$$
\Pi = \begin{bmatrix}
0.01 & 0.99 & 0 & 0 & 0 & 0 & 0 \\
0 & 0.01 & 0.99 & 0 & 0 & 0 & 0 \\
0 & 0 & 0.85 & 0.15 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0.01 & 0.99 & 0 \\
0 & 0 & 0 & 0 & 0 & 0.01 & 0.99 \\
0 & 0 & 0 & 0 & 0.85 & 0 & 0.15 \\
1 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
$$

with $\mu_{1:8} = \{(-50, 0); (30, -30); (30, 30); (-100, -10); (40, -40); (-65, 0); (40, 40); (100, 10)\}$,

and $\Sigma_k = 20 * I_2$ for all states $k = 1: K$. Figure 17 are plots of additional metrics for the Gaussian HMM experiment on the RC data set. We see a bigger difference between the buffered and non-buffered methods in predictive loglikelihood as it is more sensitive to $\Pi$. For RC data, there is less difference between the buffered and non-buffered methods for estimating $A$ and $Q$ (Figure 17 (bottom)).
Figure 17: Additional Metrics vs Runtime on RC data: (top) predictive loglikelihood and (bottom) estimation error $\|\theta(s) - \theta^*\|$. (left) $|T| = 10^4$, (center) $|T| = 10^6$, (right) $|T| = 10^8$. Different inference methods: Gibbs, SGLD, and SGLRD.
Figure 18: Stochastic gradient error of $\mu$ (top) and $\Sigma$ (bottom): (left) varying subsequence size $S$ for no-buffer $B = 0$ and buffer $B = 5$, (right) varying buffer size $B$ for $S = 2$ and $S = 50$. Error bars are SD over $10^4$ randomly drawn subsequences.
D.5.2 ARHMM

Figure 19 are plots of additional metrics for the ARHMM synthetic data.

Figure 19: Additional Metrics vs Runtime on ARHMM data: (top) NMI and (bottom) estimation error $\|\theta^{(s)} - \theta^*\|$. (left) $|T| = 10^4$, (center) $|T| = 10^6$, (right) $|T| = 10^8$. Different inference methods: Gibbs, SGLD, and SGLRD.
Figure 20: Stochastic gradient error of $A$ (top) and $Q$ (bottom): (left) varying subsequence size $S$ for no-buffer $B = 0$ and buffer $B = 10$, (right) varying buffer size $B$ for $S = 2$ and $S = 50$. Error bars are SD over $10^4$ randomly drawn subsequences.
D.5.3 LGSSM

Figure 21 are plots of additional metrics for the LDS synthetic data.

Figure 21: Additional Metrics vs Runtime on LGSSM data: (Left) root-mean square error (RMSE) between $\hat{x}$ and $x^*$, (Right) estimation error $\|\theta^{(s)} - \theta^*\|$. Different inference methods: Gibbs, SGLD, and SGLRD. For SGMCMC methods, solid (—) and dashed (- -) lines indicate buffering and no buffering respectively.

Figure 22: Stochastic gradient error of $Q$ and $R$: (left) varying subsequence size $S$ for no-buffer $B = 0$ and buffer $B = 10$, (right) varying buffer size $B$ for $S = 10$ and $S = 100$. Error bars are SD over $10^4$ randomly drawn subsequences.
D.5.4 SLDS

Figure 23 are plots of additional metrics for the SLDS data.

Figure 23: Additional Metrics vs Runtime on SLDS data: (Top) $|\mathcal{T}| = 10^4$, (Bottom) $|\mathcal{T}| = 10^6$. (Left) NMI between $\hat{z}$ and $z^*$. (Center) root-mean square error (RMSE) between $\hat{x}$ and $x^*$. (Right) estimation error $\|\theta(s) - \theta^*\|$. Inference methods: Gibbs, SGRLD X, SGRLD XZ, and SGLRD Z.
Figure 24: Stochastic gradient error of $Q$ and $R$: (left) varying subsequence size $S$ for no-buffer $B = 0$ and buffer $B = 10$, (right) varying buffer size $B$ for $S = 2$ and $S = 10$.  

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