
Stochastic Approximation with Biased MCMC for Expectation Maximization

Samuel Gruffaz

Centre Borelli, ENS Paris-Saclay

Kyurae Kim

UPenn

Alain Oliviero Durmus

CMAP, CNRS, École Polytechnique

Jacob R. Gardner

UPenn

Abstract

The expectation maximization (EM) algorithm is a widespread method for empirical Bayesian inference, but its expectation step (E-step) is often intractable. Employing a stochastic approximation scheme with Markov chain Monte Carlo (MCMC) can circumvent this issue, resulting in an algorithm known as MCMC-SAEM. While theoretical guarantees for MCMC-SAEM have previously been established, these results are restricted to the case where asymptotically unbiased MCMC algorithms are used. In practice, MCMC-SAEM is often run with asymptotically biased MCMC, for which the consequences are theoretically less understood. In this work, we fill this gap by analyzing the asymptotics and non-asymptotics of SAEM with biased MCMC steps, particularly the effect of bias. We also provide numerical experiments comparing the Metropolis-adjusted Langevin algorithm (MALA), which is asymptotically unbiased, and the unadjusted Langevin algorithm (ULA), which is asymptotically biased, on synthetic and real datasets. Experimental results show that ULA is more stable with respect to the choice of Langevin stepsize and can sometimes result in faster convergence.

1 INTRODUCTION

Probabilistic modeling with latent variables is an essential tool for modeling observational data generated from complex latent structures. While eliciting priors for this class of models is often straight-

forward, *e.g.*, data generated from unobserved groups can be modeled using mixtures (McLachlan et al., 2019), while group-level variabilities can be modeled with mixed effects (Kuhn and Lavielle, 2005), how we should set the hyper-parameters θ is not always self-evident. For this, the empirical Bayes paradigm applies the *maximum likelihood principle* (Robbins, 1956; Efron, 2019). That is, it infers the (hyper-)parameters θ from data by maximizing the marginal log-likelihood $l(\theta) \triangleq \log(p(y|\theta))$,

$$\operatorname{argmax}_{\theta \in \Theta} l(\theta) = \operatorname{argmax}_{\theta \in \Theta} \log \left(\int_{\mathcal{Z}} p(y, z|\theta) dz \right) \quad (1)$$

where $y \in \mathcal{Y} \subset \mathbb{R}^{d_y}$ are the observations, $z \in \mathcal{Z} \subset \mathbb{R}^{d_z}$ are the latent variables, and $\theta \in \Theta \subseteq \mathbb{R}^{d_\theta}$ denote the parameters.

Unfortunately, the marginal log-likelihood is often intractable, making the empirical Bayes problem hard. As a solution, Dempster et al. (1977) have proposed the *expectation-maximization* (EM) algorithm, which has subsequently been immensely successful in practice, and its convergence properties have been studied extensively (McLachlan and Krishnan, 2007). It is now known to converge to stationary points under mild conditions. However, the canonical EM algorithm may not apply immediately in many practical cases. For example, gradient ascent steps must be used when the maximization step (M-step) of EM is not available in closed form (Baey et al., 2023).

This work focuses on the setting where the expectation step (E-step) is intractable. In this case, the integral in Equation (1) needs to be numerically approximated using methods such as Monte Carlo (MC), importance sampling (IS), and Markov chain Monte Carlo (MCMC) (See the book by Robert and Casella (2004) for an overview of these methods). Furthermore, when the model belongs to the exponential family such that the M-step can be computed in closed form, Delyon et al. (1999) show that the EM algorithm can be reduced to approximating sufficient statistics generated from the sampling algorithm. In particular, they leverage stochastic approximation (SA; Rob-

bins and Monro, 1951) for approximating sufficient statistics, resulting in the SAEM algorithm. SAEM has been shown to be particularly efficient in practice, especially since most practical models can be embedded in an exponential family form (Debavelaere and Allasonnière, 2021), and have been widely used through multiple popular software packages such as NONMEM (Bauer, 2019), `saemix` (Comets et al., 2017), `Monolix` (Lavielle, 2014), and many more.

Leveraging SA comes at a price: The performance of SAEM crucially depends on that of the underlying sampling algorithm. However, most popular MCMC algorithms used for SAEM, such as the Metropolis-adjusted Langevin Algorithm (MALA; Roberts and Tweedie, 1996) and Hamiltonian Monte Carlo (HMC; Duane et al., 1987), perform poorly unless carefully tuned, especially in high dimensions. While targeting an “optimal” acceptance rate is an effective way to tune these algorithms (Gilks et al., 1998), this is not straightforward in the SAEM context: the limiting distribution of the Markov Chain is not fixed.

Note that the problem of tuning stems from the fact that we are employing Metropolis-Hastings adjustments. Therefore, not adjusting at all, resulting in approximate MCMC methods such as the unadjusted Langevin algorithm (ULA), would immediately resolve this issue. While these methods are “approximate” in the sense that their limiting stationary distribution is biased, tuning is less critical to their performance (de Bortoli et al., 2021). Furthermore, ULA has theoretically been shown to converge faster than its unbiased counterpart MALA (Durmus and Moulines, 2017). Therefore, this work establishes theoretical guarantees for SAEM with biased MCMC. Also, we compare the performance of MCMC-SAEM with MALA versus ULA on practical examples. The results suggest that, in general, ULA can use larger stepsizes than MALA, resulting in faster convergence.

Contributions Our contributions are two-fold: the asymptotic analysis (Section 3) and non-asymptotic analysis (Section 4) of MCMC-SAEM with biased MCMC. For the asymptotic analysis, we generalize the analysis of Tadić and Doucet (2017) on stochastic gradient optimization to the case of SA. Furthermore, we explicitly control the asymptotic convergence according to the bias of MCMC through the smoothness of the problem. This improves over the almost sure convergence results provided by Dieuleveut et al. (2023, §V). For our non-asymptotic analysis, we extend the framework Karimi et al. (2019) to include asymptotic bias, and the guarantee is in high-probability. This characterizes the effect of Markov chain concentration, unlike the convergence results in expectation provided by Karimi et al. (2019); Dieuleveut et al. (2023).

2 BACKGROUND

2.1 Expectation-Maximization

We assume that the joint distribution of the observations and latent variable belongs to the curved exponential family:

H1. For any $y \in \mathcal{Y}$, $z \in \mathcal{Z}$ and $\theta \in \Theta$,

$$p(y, z|\theta) = h(y, z) \exp(S(y, z)^\top \phi(\theta) - \psi(\theta)) ,$$

where Θ, \mathcal{Z} , are open, $S : \mathcal{Y} \times \mathcal{Z} \rightarrow \mathbb{R}^d$ is continuous, and $\phi : \Theta \rightarrow \mathbb{R}^d$ and $\psi : \Theta \rightarrow \mathbb{R}$ are continuously differentiable.

In this paper, $y \in \mathcal{Y}$ is fixed, and the parameter θ is estimated through maximum marginal log-likelihood $l : \Theta \mapsto \log p(y|\theta)$. In most cases, l cannot be maximized directly and is not even tractable. EM solves this by employing the *majorize-minimize principle*: (See, e.g., Lange, 2016, Chapter 8.) An upper bound of $-l$ is derived using Jensen’s inequality and a density q on \mathcal{Z} , for any $\theta \in \Theta$,

$$\begin{aligned} -\log p(y|\theta) &= \log \left(\int_{\mathcal{Z}} p(y, z|\theta) \times \frac{q(z)}{q(z)} dz \right) \\ &\leq - \int_{\mathcal{Z}} \log \left(\frac{p(y, z|\theta)}{q(z)} \right) q(z) dz = Q(\theta, q) \\ &= -(\mathbb{E}_{z \sim q}(\log(p(y, z|\theta))) dz + \text{Ent}(q) + \text{cst}(y)) . \end{aligned}$$

Denoting $D_{\mathcal{Z}} \triangleq \{f \in L^1(\mathcal{Z}) : f \geq 0, \int_{\mathcal{Z}} f dz = 1\}$, the function $q \in D_{\mathcal{Z}} \mapsto Q(\theta, q)$ is minimized by $q^*(z) \triangleq p(z|y, \theta)$ such that $Q(\theta, q^*) = -l(\theta)$. Thus, by considering $\theta^* = \text{argmin}_{\theta \in \Theta} Q(\theta, q^*)$, we have $l(\theta^*) \leq l(\theta)$. This procedure offers a recipe to construct a maximizing sequence of l . Moreover, under **H1**,

$$\theta^* = \text{argmax}_{\theta \in \Theta} \mathbb{E}_{z \sim p(z|y, \theta)} (S(y, z)^\top \phi(\theta) - \psi(\theta)) .$$

We introduce the following assumption to maximize this last expression:

H2. Denoting $L(s, \theta) \triangleq s \cdot \phi(\theta) - \psi(\theta)$, there exists a function $\hat{\theta} : \mathbb{R}^d \rightarrow \Theta$, such that for any $(s, \theta) \in \mathbb{R}^d \times \Theta$,

$$L(s, \theta) \leq L(s, \hat{\theta}(s)) .$$

If necessary, this assumption can also be met by “exponentializing” as shown by Debavelaere and Allasonnière (2021).

The EM algorithm is defined as follows: Let $(s_k)_{k \geq 0}, (\theta_k)_{k \geq 0}$ be initialized from $\theta_0 \in \Theta$ and follow the recursion for any $k \geq 0$:

- ❶ **Expectation:** Denoting by $\bar{s} : \theta \in \Theta \mapsto \int_{\mathcal{Z}} S(y, z) p(z|\theta, y) dz$, set $s_k = \bar{s}(\theta_k)$.
- ❷ **Maximization:** Set $\theta_{k+1} = \hat{\theta}(s_k)$, which implies $l(\theta_{k+1}) \geq l(\theta_k)$.

This algorithm quickly converges towards a local maximum of l under mild conditions. (See the review by McLachlan and Krishnan (2007).)

2.2 EM as a Root Finding Problem

The EM recursion can be seen as a fixed-point iterative scheme since, for any $k \geq 0$, $\theta_{k+1} = \hat{\theta} \circ \bar{s}(\theta_k)$. If the sequence (s_n) converges towards s^* and $\bar{s} \circ \hat{\theta}$ is continuous, we then have

$$h(s^*) = 0, \text{ where } h \triangleq \bar{s} \circ \hat{\theta}(\cdot) - \text{Id}.$$

Moreover, if s^* is a root of h , then $\hat{\theta}(s^*)$ is a root of $\hat{\theta} \circ \bar{s}(\cdot) - \text{Id}$. And reciprocally, if θ^* is a root of $\hat{\theta} \circ \bar{s}(\cdot) - \text{Id}$, then $\bar{s}(\theta^*)$ is a root of h . This suggests that EM can be reduced to a problem of finding the root h with respect to s .

EM as Stochastic Approximation Finding the root is more general than gradient descent as h may not be the *gradient* of any known function. Instead, it is the *descent direction* for some Lyapunov function $V : s \in \mathbb{R}^d \mapsto -l \circ \hat{\theta}(s)$. As such, the proposed scheme is part of the more general stochastic approximation (SA) framework (Dieuleveut et al., 2023). The most basic form of the SA algorithm is described as follows:

$$s_{k+1} = s_k + \gamma_{k+1} H(s_k, Z_{k+1}), \quad Z_{k+1} \sim p(\cdot | \theta_k, y),$$

where $H(s_k, Z_{k+1}) = S(y, Z_{k+1}) - s_k$ is a random oracle of $h(s_k)$ and $(\gamma_k)_k$ is a deterministic stepsize sequence. Solving the EM problem using these iterates is known as SAEM algorithm (Delyon et al., 1999).

While we have motivated the reduction of optimizing l to finding the root of h , it is not apparent the solutions such that $h = 0$ and $\nabla l = 0$ are equivalent. The following lemma will clarify the relationship between h , l , and the Lyapunov function V given assumptions on the Hessian of L at its maximums:

H 3. *The functions $\hat{\theta}, l(\cdot), \phi(\cdot), \bar{s}(\cdot)$ and $\psi(\cdot)$ are p -continuously differentiable with $p > d$. Moreover, denote*

$$A(s) \triangleq \partial_s \hat{\theta}(s)^\top \partial_\theta^2 L(s, \hat{\theta}(s)) \partial_s \hat{\theta}(s).$$

Then, there exist $\lambda_m, \lambda_M > 0$ such that for any $s \in \mathbb{R}^d$:

$$\lambda_m |v|^2 \leq \langle A(s)v | v \rangle \leq \lambda_M |v|^2, \quad v \in \mathbb{R}^d.$$

Lemma 1. *Under H1, H2 and H3, V is p -continuously differentiable and verifies for any $s \in \mathbb{R}^d$,*

$$\begin{aligned} F(s) &\triangleq \langle \nabla V(s) | h(s) \rangle \leq -\lambda_m |h(s)|^2 \\ |\nabla V(s)| &\leq \lambda_M |h(s)| \\ \mathbb{S} &= \{s \in \mathbb{R}^d : F(s) = 0\} = \{s \in \mathbb{R}^d : \nabla V(s) = 0\} \\ \hat{\theta}(\mathbb{S}) &= \{\theta \in \Theta : l(\theta) = 0\}, \quad \text{int}(V(\mathbb{S})) = \emptyset \end{aligned}$$

Proof. In the proof by Delyon et al. (1999, Lemma 2), they derive that for any $s \in \mathbb{R}^d$, $\nabla V(s) = -A(s)h(s)$, the results are then straightforward with the regularity assumption on A . \square

In other words, $h(s)$ is a proxy of $-\nabla V(s)$ for any $s \in \mathbb{R}^d$. This Lemma makes it clear that converging to \mathbb{S} by working in the sufficient statistics space recovers the solutions of the original problem (1). From now on, we drop the dependence of y in $S(y, z)$ such that $S(z) \triangleq S(y, z)$ since we are interested only in z .

MCMC-SAEM SAEM can be generalized to models with intractable likelihoods by leveraging Markov chain Monte Carlo (MCMC) as proposed by Kuhn and Lavielle (2004). An MCMC algorithm form a Markov kernel Π_θ , such that, for any $z \in \mathcal{Z}$, $\lim_{n \rightarrow \infty} \|\Pi_\theta(z, \cdot)^{(n)} - \pi_\theta\|_{\text{TV}} = 0$, where π_θ is the target distribution related to $p(\cdot | \theta, y)$. It means that asymptotically, sampling from $\Pi_\theta(z, \cdot)$ is nearly equivalent to sampling from π_θ . Then, the Markov chain is said to be asymptotically unbiased, contrary to the case $\lim_{n \rightarrow \infty} \|\Pi_\theta(z, \cdot)^{(n)} - \pi_\theta\|_{\text{TV}} > 0$, where we say that the chain is asymptotically biased.

Note that, in general, the chain is biased in finite time $\|\Pi_\theta(z, \cdot)^{(n)} - \pi_\theta\|_{\text{TV}} > 0$ for any $n \geq 0$. Despite this, MCMC-SAEM, MCMC applied to SAEM, generates a sequence $(\theta_k)_k$ that converges to a local maximum almost surely (Dieuleveut et al., 2023; Kuhn and Lavielle, 2004), where the E -step is replaced by

$$s_{k+1} = s_k + \gamma_{k+1} (S(y, z_{k+1}) - s_k), \quad z_{k+1} \sim \Pi_{\theta_k}(z_k, \cdot),$$

for any $k \geq 0$, starting with $(s_0, z_0) \in \mathbb{R}^d \times \mathcal{Z}$.

2.3 MCMC-SAEM with Approximate MCMC Algorithms

At the core of the practical performance of MCMC-SAEM is the choice of the MCMC algorithm. While MALA is often used, its asymptotically biased counterpart ULA has been shown to mix faster at high dimensions (Durus and Moulines, 2017). This means that, in finite time, the total bias of ULA can be lower compared to the asymptotically unbiased MALA. Therefore, while we consider a general biased Markov chain to study the convergence of MCMC-SAEM in Section 3 and 4, we are interested in studying the difference between ULA and MALA. Our experiments in Section 5 will exclusively focus on this question.

ULA and MALA The ULA Markov chain $(X_k)_{k \geq 0}$ is derived from the Euler–Maruyama discretization scheme associated with the Langevin diffusion related to the force $U \triangleq -\nabla \log(\pi)$ if π is the target distribution, at iteration $k \geq 0$

$$X_{k+1} = X_k - \eta_{k+1} \nabla U(X_k) + \sqrt{2\eta_{k+1}} Z_{k+1}$$

where $(Z_k)_{k \geq 0}$ is an i.i.d sequence of standard Gaussian d -dimensional random vectors and $(\eta_k)_{k \geq 1}$ is a sequence of stepsize, which can be either constant or de-

crease to 0. The MALA Markov chain follows the same recursion by adding an acceptance/rejection step of X_{k+1} , making the chain asymptotically unbiased.

The properties of MALA chains have been studied in depth in (Roberts and Tweedie, 1996), where it is shown that the chain converges geometrically fast (geometric ergodicity) under mild assumptions on the tail of the target distribution. This is key since geometric ergodicity is the main assumption of the MCMC-SAEM convergence theorem (Kuhn and Lavielle, 2004). Despite being geometrically ergodic, the adjustment step of MALA can become a curse in high dimensions. To maintain a sufficient level of acceptance, a smaller stepsize must be used, resulting in a slow mixing chain. (Mixing is a fundamentally non-asymptotic notion, unlike geometric ergodicity.)

On the other hand, for ULA, denoting its limiting distribution as π^η , the mixing rate improves with η (Durmus and Moulines, 2017) at the cost of increasing $\|\pi^\eta - \pi\|_{\text{TV}}$ (de Bortoli et al., 2021). This means one can trade off asymptotic bias for a faster mixing rate. Considering this, we will expand the existing analysis, where η is no longer a stepsize but a “knob” that controls bias, which can vary across the iterations.

2.4 Stochastic Approximation with Biased Dynamics

To incorporate biased MCMC chains into our analysis, we slightly modify the SA formalism (Dieuleveut et al., 2023) to allow some freedom on the bias parameter η .

Let $(\gamma_n)_n$ and $(\eta_n)_n$ be two monotone nonincreasing sequences with $\gamma_0, \eta_0 \in [0, 1]^2$. Define the nonhomogeneous Markov chain $\{Y_n^\gamma = (Z_n, S_n)\}_n$ on $\mathcal{Z} \times \mathbb{R}^d$ as follows: Let $s_0 = \theta \in \mathbb{R}^d$, $z_0 = z \in \mathbb{R}^d$ and for $n \geq 0$,

$$\begin{aligned} Z_{n+1} &\sim \Pi_{s_n}^{\eta_{n+1}}(Z_n, \cdot) \\ s_{n+1} &= s_n + \gamma_{n+1} H(s_n, Z_{n+1}), \end{aligned} \quad (2)$$

where $\{\Pi_s^\eta = \Pi_{\hat{\theta}(s)}^\eta, s, \eta \in \mathbb{R}^d \times (0, \eta_0]\}$ is a family of Markov transition probabilities and $H : s, z \in \mathbb{R}^d \times \mathcal{Z} \mapsto S(z) - s$ is a field which satisfy the following conditions:

H4. For any $s \in \mathbb{R}^d$ and $\eta \in (0, \eta_0]$, the Markov kernel Π_s^η has a single stationary distribution $\pi_{\hat{\theta}(s), \eta}$, also denoted as $\pi_{s, \eta}$, such that $\pi_{s, \eta} \Pi_s^\eta = \pi_{s, \eta}$. In addition, $H : \mathbb{R}^d \times \mathcal{Z} \rightarrow \mathbb{R}^d$ is measurable for all $s \in \mathbb{R}^d$ and $\int_{\mathcal{Z}} |H(s, z)| \pi_{s, \eta}(dz) < \infty$.

By considering the filtration $\{\mathcal{F}_n = \sigma(s_0, Z_i, i \leq n)\}_n$, the following decomposition clarifies the deterministic and stochastic parts of the dynamic:

$$H(s_n, Z_{n+1}) = h(s_n) + \xi_n,$$

$$\begin{aligned} \xi_n &= e_n + \beta_n, \\ e_n &= H(s_n, Z_{n+1}) - \mathbb{E}_{W \sim \pi_{s_n, \eta_{n+1}}} [H(s_n, W)], \\ \beta_n &= \mathbb{E}_{W \sim \pi_{s_n, \eta_{n+1}}} [H(s_n, W)] - h(s_n), \end{aligned}$$

where $h(s_n)$ is the mean field drift, e_n is the Markovian noise and $(\beta_n)_n$ the bias. In the MCMC-SAEM context, this becomes

$$\begin{aligned} e_n &= S(z_{n+1}) - \check{s}_{\eta_{n+1}}(\hat{\theta}(s_n)), \\ \beta_n &= \check{s}_{\eta_{n+1}}(\hat{\theta}(s_n)) - \bar{s}(\hat{\theta}(s_n)), \end{aligned}$$

where, for any $s \in \mathbb{R}^d$ and $\eta \in (0, \eta_0]$,

$$h(s) = \bar{s}(\hat{\theta}(s)) - s,$$

$$\check{s}_\eta(\hat{\theta}(s)) = \int S(z) \pi_{s, \eta}(dz).$$

This way, for any $s \in \mathbb{R}^d$, $\check{s}_\eta(\hat{\theta}(s))$ is the biased approximation of $\bar{s}(\hat{\theta}(s))$. Lastly, we assume that the asymptotic bias is finite:

H5. $\limsup_{n \rightarrow \infty} |\beta_n| = \beta < +\infty$

This assumption is reasonable if the growth of $z \mapsto S(z)$ can be mitigated by the tail decay of $\pi_{\theta, \eta}$ and π_θ .

3 ASYMPTOTIC ANALYSIS

We estimate how the asymptotic bias of MCMC impacts the asymptotic convergence of (s_n) generated by the recursion (2). The analysis takes most of its arguments from (Tadić and Doucet, 2017) where the framework is slightly different, $h = \nabla f$ where f has the same regularity that in **H3**. We extend their results by using Lemma 1, i.e., the mean field is not a gradient but the proxy of a Lyapunov gradient. The results are not specific to the SAEM scheme but can be generalized to other SA schemes as Lemma 1 applies, but this is beyond the scope of this paper.

3.1 Technical Assumptions

All the assumptions presented in this part are also used in (Tadić and Doucet, 2017). We take the following assumptions on (γ_n) , (e_n) :

A1. $\limsup_{n \rightarrow \infty} |\gamma_{n+1}^{-1} - \gamma_n^{-1}| < \infty$, $\lim_{n \rightarrow \infty} \gamma_n = 0$ and $\sum_{n=0}^{\infty} \gamma_n = \infty$.

Denoting by $a(n, t) = \max \left\{ k \geq n : \sum_{i=n}^{k-1} \gamma_i \leq t \right\}$ for $n \geq 0$ and $t \in (0, \infty)$, $a(n, t)$ is well defined thank to **A1**. Furthermore, we assume:

A2. (e_n) and (β_n) are \mathbb{R}^d -valued stochastic processes satisfying,

$$\lim_{n \rightarrow \infty} \max_{n \leq k < a(n, t)} \left| \sum_{i=n}^k \gamma_i e_i \right| = 0$$

almost surely on $\{\sup_n |s_n| < \infty\}$ for any $t \in (0, \infty)$.

A2 can be established from assumptions of geometric ergodicity on the Markov kernels $\{\Pi_\eta^s, s \in \mathbb{R}^d, \eta \in (0, \eta_0]\}$ and by controlling the growth of the sufficient statistics. Due to its technicalities, this development is relegated to Appendix B.1.3.

In numerous cases, we can even make the following assumption,

A3. $V(\cdot)$ is real analytic on \mathbb{R}^d .

This implies that V can be locally represented by a power series.

3.2 Main Result

For any compact $Q \subset \mathbb{R}^d$, Λ_Q denotes the event $\cup_{n=0}^\infty \cap_{k=n}^\infty \{\theta_k \in Q\}$, such that on Λ_Q , $\{\theta_k\}$ is bounded and the bound is controlled by Q . The main result on the asymptotic bias of the recursion (2) can be stated as follows:

Theorem 1. *Suppose that **H1-5**, **A1-2**. Let $Q \subset \mathbb{R}^d$ be any compact set. Then, the following are true:*

(I) *There exists a (deterministic) non-decreasing function $\psi_Q : [0, \infty) \rightarrow [0, \infty)$ (independent of η and depending only on $V(\cdot)$) such that $\lim_{t \rightarrow 0} \psi_Q(t) = \psi_Q(0) = 0$ and*

$$\limsup_{n \rightarrow \infty} d(s_n, \mathbf{S}) \leq \psi_Q(\beta)$$

almost surely on Λ_Q .

(II) *There exists a real number $K_Q \in (0, \infty)$ (independent of β and depending only on $V(\cdot)$) such that*

$$\begin{aligned} \limsup_{n \rightarrow \infty} \|\nabla V(s_n)\| &\leq K_Q \beta^{q/2}, \\ \limsup_{n \rightarrow \infty} V(s_n) - \liminf_{n \rightarrow \infty} V(s_n) &\leq K_Q \beta^q \end{aligned}$$

almost surely on Λ_Q , where $q = (p-d)/(p-1)$.

(III) *If $V(\cdot)$ satisfies **A3** there exist real numbers $r_Q \in (0, 1)$, $L_Q \in (0, \infty)$ (independent of β and depending only on $V(\cdot)$) such that*

$$\begin{aligned} \limsup_{n \rightarrow \infty} \|\nabla V(s_n)\| &\leq L_Q \beta^{1/2} \\ \limsup_{n \rightarrow \infty} d(V(s_n), V(\mathbf{S})) &\leq L_Q \beta \\ \limsup_{n \rightarrow \infty} d(s_n, \mathbf{S}) &\leq L_Q \beta^{r_Q}. \end{aligned}$$

almost surely on Λ_Q .

Proof. See Appendix B.1.2 for the proof. \square

Theorem 1-(I) formalizes the intuition that $\lim_{n \rightarrow \infty} d(s_n, \mathbf{S}) = 0$ if $\beta = \limsup_{n \rightarrow \infty} |\beta_n| \rightarrow 0$. If (η_n) encodes the stepsize of ULA, the last condition can be deduced from $\lim_{n \rightarrow \infty} |\eta_n| = 0$, since a smaller stepsize decreases bias. Even though it is

the case that $\beta > 0$ in practice since $\eta_n = \eta > 0$ is fixed, we can quantify the impact of the bias on V in Theorem 1-(II). Note the impact of the regularity of V according to the dimension encoded in $q = (p-d)/(p-1)$: at the limit when $p \rightarrow \infty$, we recover $q = 1$ as in Theorem 1-(III). Therefore, the impact of the bias β on $\limsup_{n \rightarrow \infty} \|\nabla V(s_n)\|$ is smoothed by the regularity of V . For the case of $\beta = 0$, we recover the convergence of the sequence towards stationary points \mathbf{S} , which has already been established by Kuhn and Lavielle (2004).

Remark that Theorem 1 is local in the sense that it holds on the event Λ_Q and not globally. (*i.e.*, there exists a compact set Q such that Λ_Q holds almost surely.) Previous results have assumed that the sequence (s_n) is bounded to make their result global and have argued that we can bound it by design through “reinitialization” as studied by Kuhn and Lavielle (2004); Andrieu et al. (2005). Here, we did not use the recursion proposed (Andrieu et al., 2005, p.9) to be more aligned with practical implementations.

The constants K_Q, L_Q depend explicitly on the bounds on $|\nabla V|, |\nabla^2 V|$ (the maximal singular value of A to be precise) and the Yomdin and Lojasiewicz constants applied to V . (See, *e.g.* Proposition 8.1 and 8.2 by Tadić and Doucet (2017), which are generalizations of Sard’s Theorem.) The explicit forms of K_Q, L_Q are given at the end of the proof in Appendix B.1.2.

4 NON ASYMPTOTIC ANALYSIS

For the non-asymptotic analysis, we assume the bias parameters are fixed for any $n \geq 0$, $\eta_n \in (0, \eta_0]$. Furthermore, we rely on assumptions typical for non-asymptotic analysis of SA. Our main result is a non-asymptotic high probability convergence guarantee for SAEM with biased MCMC.

4.1 Technical Assumptions

First, we impose assumptions on the MCMC kernel, which are standard in the non-asymptotic analysis of stochastic approximation with state-dependent Markovian noise.

N1. *The update is bounded by a constant $0 < \sigma < \infty$ as*

$$\sup_{(s,z) \in \mathbb{R}^d \times \mathcal{Z}} |H(s, z) - h(s)| \leq \sigma.$$

While this assumption is quite strong, it is necessary to control the properties of the solution to the Poisson equation as in the following assumption:

N2. *For any $s \in \mathbb{R}^d$, there exists a solution $\nu_s^\eta : \mathcal{Z} \rightarrow$*

\mathbb{R}^d to the Poisson equation such that

$$\nu_s^\eta - \Pi_s^\eta \nu_s^\eta = S(\cdot) - \check{s}_\eta(\hat{\theta}(s)),$$

where for any $z \in \mathcal{Z}$, $\Pi_s^\eta \nu_s^\eta(z) = \int_{\mathcal{Z}} \nu_s^\eta(z) \Pi_s^\eta(z, dz)$ and for any $s \in \mathbb{R}^d$, $\check{s}_\eta(\hat{\theta}(s)) = \int_{\mathcal{Z}} S(z) d\pi_{s,\eta}$. Moreover, there exist some bound $L_\nu^{(0)}, L_\nu^{(1)} > 0$ such that

$$\begin{aligned} \sup_{(s,z) \in \mathbb{R}^d \times \mathcal{Z}} \{|\nu_s^\eta(z)|, |\Pi_s^\eta \nu_s^\eta(z)|\} &\leq L_\nu^{(0)}, \\ \sup_{(s,z) \in \mathbb{R}^d \times \mathcal{Z}} |\Pi_s^\eta \nu_s^\eta(z) - \Pi_{s'}^\eta \nu_{s'}^\eta(z)| &\leq L_\nu^{(1)} |s - s'|. \end{aligned}$$

Remark that **N1-2** implies **H4**. Also, under **N2**,

$$e_n = S(Z_{n+1}) - \check{s}_\eta(\hat{\theta}(s_n)) = \nu_{s_n}^\eta(Z_{n+1}) - \Pi_{s_n}^\eta \nu_{s_n}^\eta(Z_{n+1}),$$

which is crucial for the analysis in the Supplementary material Appendix **B.2**. This type of assumption has first been used by Karimi et al. (2019) and has since been standard in the analysis of stochastic approximation with state-dependent Markovian noise. See, e.g. the works of Alacaoglu and Lyu (2023, Assumption 3.7), Roy et al. (2022, Assumption 2.4) for some recent examples. If we assume that **(i)** both Π_s^η , $H(s, z)$ are uniformly Lipschitz with respect to s for any $z \in \mathcal{Z}$, **(ii)** Π is uniformly geometrically ergodically converging, and **(iii)** **N1** holds, Karimi et al. (2019, Lemma 7) establish $L_\nu^{(0)}, L_\nu^{(1)}$ explicitly.

In this work, we are particularly interested in asymptotically biased MCMC algorithms:

N3. *The asymptotic bias of the MCMC kernel is bounded for some $0 \leq \tau_0, \tau_1 < \infty$ as*

$$|\beta_k|^2 \leq \tau_0 + \tau_1 |h(s_k)|^2.$$

Moreover, under **H3**, $C_{b_1} \triangleq \lambda_M (\frac{1}{2}\sqrt{\tau_0} + \sqrt{\tau_1}) < \lambda_m$, where $\lambda_m, \lambda_M > 0$ are defined in **H3**.

This assumption has been used by Dieuleveut et al. (2023), and encompasses both iterate-dependent and -independent bias. It is a refinement of **H5**. The condition about C_{b_1} is specific to the SAEM framework; the bias is bounded by the matrix conditioning of A given in **H3**. This reveals crucial in the high probability bound.

The remaining assumptions are standard in the non-asymptotic analysis of stochastic approximation. (See **H1-2** in the recent review by Dieuleveut et al. (2023).)

N4. *The Lyapunov function V is smooth and bounded below such that*

$$|\nabla V(s) - \nabla V(s')| \leq L_V |s - s'| \quad V(s) \geq V^*$$

for $V^* = \inf_{s \in \mathbb{R}^d} V(s) > -\infty$ and some $0 < L_V < \infty$.

For the EM setting, **N4** is problem-dependent and can not be recovered directly from **H3**.

4.2 Main Result

Theorem 2. *Assume **H1-3**, **N1-3** and **N4**,*

Then, given a stepsize satisfying with $\alpha_1, \alpha_2 > 0$,

$$\begin{aligned} \gamma_{k+1} &\leq \gamma_k, \quad \gamma_k \leq \alpha_1 \gamma_{k+1}, \\ \gamma_k - \gamma_{k+1} &\leq \alpha_2 \gamma_{k+1}^2, \quad \gamma_0 \leq \frac{1}{2} (\lambda_m - C_{b_1}) / C_{n_1}, \end{aligned} \quad (3)$$

with probability at least $1 - \delta$, the MCMC-SAEM algorithm guarantees that

$$\begin{aligned} \min_{k=0, \dots, n} |h(s_k)|^2 &\leq \frac{2}{\lambda_m - C_{b_1}} \times \\ &\left(\frac{V(s_0) - V^* + C_0 + \log \frac{1}{\delta} + C_{n_2} \sum_{k=0}^n \gamma_{k+1}^2 + C_{b_2}}{\sum_{k=0}^n \gamma_{k+1}} + C_{b_2} \right), \end{aligned} \quad (4)$$

where the constants are

$$\begin{aligned} C_0 &= L_\nu^{(0)} (\gamma_0 + 2\lambda_M), \\ C_{b_1} &= \lambda_M \left(\frac{1}{2} \sqrt{\tau_0} + \sqrt{\tau_1} \right), \\ C_{b_2} &= \frac{1}{2} \lambda_M \sqrt{\tau_0}, \\ C_{n_1} &= L_\nu^{(1)} \lambda_M \sigma + L_V L_\nu^{(0)} \lambda_M (1 + \sigma) + L_V \sigma^2, \\ C_{n_2} &= (2\lambda_M L_\nu^{(0)})^2 + L_\nu^{(1)} \lambda_M \left(\frac{1}{2} + \alpha_1 \sigma + \alpha_1 \frac{1}{2} \right) \\ &\quad + L_\nu^{(0)} \lambda_M (L_V + \alpha_2 + 1) + L_V. \end{aligned}$$

Proof. See Appendix **B.2** for the proof. \square

If we set $\gamma_k = (\lambda_m - C_{b_1}) / 2C_{n_1} \sqrt{k}$ for any $k \geq 1$, then the stepsize satisfies (3) with $\alpha_1, \alpha_2 = \sqrt{2}, (\sqrt{2} - 1) / \sqrt{2} \gamma_1$, and thus the right hand in (4) becomes $\mathcal{O}(\log(n)/n + 2C_{b_2} / (\lambda_m - C_{b_1}))$. The results are coherent with Theorem **1-(III)**, the bias is proportional to $\lambda_M \sqrt{\beta}$ as $n \rightarrow \infty$.

The key step in establishing the high-probability bound is to ensure the non-asymptotic transient bias of the Markov chain concentrates. This is done by constructing a Martingale following the strategy of Karimi et al. (2019), while the concentration inequality is by Li and Orabona (2020, Lemma 1). Although this Lemma relied on Gaussian tails, this automatically follows from **N2**. Therefore, with this set of assumptions, SA with MCMC is well-behaved under a concentration perspective.

Overall, as in Section **3**, we conclude that the regularity of the problem determines the limit of biased MCMC within SAEM.

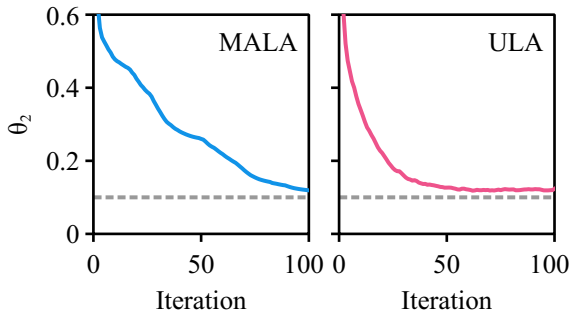


Figure 1: **Trajectory of the MCMC-SAEM iterates for θ_2 with a large MALA/ULA stepsize of $\eta = 5 \times 10^{-3}$.** MALA only makes “occasional” progress due to rejections, while ULA makes progress nonetheless, albeit with some asymptotic bias. The dotted line marks the true value θ_2^* .

5 EXPERIMENTS

We will now empirically compare the performance of MCMC-SAEM with approximate and asymptotically exact MCMC kernels. In particular, we compare ULA and MALA. While the computation cost is comparable—MALA is slightly more expensive as it requires an additional evaluation of the unnormalized target density—their practical behavior can be different, as we will see in the experiments. All experiments were implemented in the Julia language (Bezanson et al., 2017). For the stepsize, we use $\gamma_k = 1/\sqrt{k}$ for all experiments. Furthermore, in the E-step of each SAEM iteration, 4 MCMC steps are performed as burn-in unless stated otherwise. The source code used for the experiments is publically available online¹.

5.1 Logistic Regression on a Synthetic Dataset

To illustrate the difference in the behavior of ULA and MALA, we first consider a toy problem.

Model The model is a typical logistic regression model with a Gaussian prior on the coefficients:

$$\begin{aligned} \beta &\sim \mathcal{N}(\mu \mathbf{1}_d, \sigma^2 \mathbf{I}_d) \\ p_i &= \text{logistic}(\beta^\top x_i) \\ y_i &\sim \text{Bernoulli}(p_i). \end{aligned}$$

We optimize for the hyperparameters $\theta = (\mu, \sigma) \in \mathbb{R} \times \mathbb{R}_{>0}$. The number of datapoints is 1000, while the dimensionality of β is 100. The regression matrix is randomly generated to have a condition number of $\kappa = 1000$. We initially run the respective MCMC algorithm for 10 iterations as burn-in, and then run MCMC-SAEM for 100 iterations. The true parameter is $\theta^* = (1, 0.1)$, while we initialize the algorithm with

¹Link to GITHUB repository: <https://github.com/Red-Portal/MCMCSAEM.jl>

$\theta_0 = (0, 1)$. The MCMC chain is initialized from a standard Gaussian.

Results For a small η (ULA/MALA stepsize), ULA and MALA perform similarly since MALA reduces to ULA. On the other hand, they start to behave differently in the large η regime, as illustrated in Figure 1: MALA starts to reject more proposals, which results in slower convergence. On the other hand, ULA does not reject anything, making constant progress. This illustrates that, in the large- η regime, the asymptotic bias of ULA becomes less critical since MALA suffers from non-asymptotic transient bias from the rejections.

5.2 Pharmacokinetics

A popular application of MCMC-SAEM is nonlinear mixed modeling, which often arises in longitudinal studies with nonlinear models of progression. Here, we will consider modeling the pharmacokinetics of Theophylline, which is a drug for respiratory diseases (Davidian and Giltinan, 1995; Pinheiro and Bates, 1995).

Model Following the formulation of Kuhn and Lavielle (2005), we assume the concentration of the drug on the i th patient at the j th measurement can be modeled as

$$\begin{aligned} \log V_i &\sim \mathcal{N}(\mu_V, \sigma_V^2) \\ \log \text{ka}_i &\sim \mathcal{N}(\mu_{\text{ka}}, \sigma_{\text{ka}}^2) \\ \log \text{Cl}_i &\sim \mathcal{N}(\mu_{\text{Cl}}, \sigma_{\text{Cl}}^2) \\ y_{ij} &\sim \mathcal{N}(h(V_i, \text{Cl}_i, \text{ka}_i, t_{ij}), \sigma^2), \end{aligned}$$

where h is a first-order one-compartment model:

$$h(V_i, \text{Cl}_i, \text{ka}_i, t_{ij}) \triangleq \frac{d_i \text{ka}_i}{V_i (\text{ka}_i - \text{Cl}_i)} \left(e^{-\frac{\text{Cl}_i}{V_i} t_{ij}} - e^{-\text{ka}_i t_{ij}} \right),$$

and for each of the i th patient,

- y_{ij} is the concentration of the drug at t_{ij} (mg/L),
- t_{ij} is the time of the j th measurement (hours),
- d_i is the administered dosage (mg/kg),
- ka_i is the drug absorption rate,
- Cl_i is the drug’s clearance, and
- V_i is the volume of the central compartment.

$z_i = (\log V_i, \log \text{ka}_i, \log \text{Cl}_i) \in \mathbb{R}^3$ for $i = 1, \dots, n$ are the latent variables local to each patient sampled using MCMC, while the hyperparameters $\theta = (\mu_{\text{ka}}, \mu_V, \mu_{\text{Cl}}, \sigma_{\text{ka}}, \sigma_V, \sigma_{\text{Cl}}, \sigma) \in \mathbb{R}^3 \times \mathbb{R}_{>0}^4$ are inferred by maximizing the marginal likelihood.

Dataset We use the Theophylline dataset preprocessed and distributed by the `saemix` package (Comets et al., 2017), which is based on the one originally distributed by NONMEM (Boeckmann et al., 1994). This dataset contains 12 patients who were administered

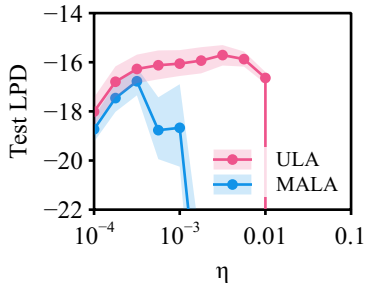


Figure 2: **Test average marginal log-predictive density (LPD) for the pharmacokinetics model versus the MALA/ULA stepsize η .** The colored bands are 80% bootstrap confidence intervals of the mean computed from 32 independent train-test splits of a ratio of 9 : 3.

Table 1: POISSON GLM DATASETS

NAME	# data	dim(z)	dim(θ)
medpar	1495	1495	6
azpro	3589	3589	4

oral doses of the drug, where the concentration was measured 11 times over 25 hours. (The `saemix` version excludes the measurement at $t = 0$, leaving 10 measurements per patient.)

We initialize at $\theta_0 = (-1, 0, 0, 1, 1, 1, 1)$, run MCMC-SAEM for 1000 iterations after 100 initial burn-in MCMC steps. We randomly split the patients into a train and test set of 9 : 3. Then, we estimate the marginal log-predictive density of the test patients resulting from the hyper-parameters found by SAEM. For estimating the test marginal LPD, we use the average of 100 importance weights drawn using annealed importance sampling (Neal, 2001), each using 1000 annealing steps with a quadratic schedule.

Results The results are shown in Figure 2. We can see that ULA converges for the widest range of stepsizes. In this example, MALA struggles the most because the likelihood is highly non-smooth. Misspecifications of the hyper-parameters result in a sudden increase in the rejection rate. Since ULA is immune to this problem, it makes constant progress as long as it doesn’t diverge.

5.3 Robust Poisson Regression

Our first realistic experiment is a generalized linear model (GLM) with a Poisson likelihood. In particular, we consider a robustified, or “localized” (Wang and Blei, 2018), Poisson regression model, also known as the Poisson-log-normal model (Cameron and Trivedi, 2013, §4.2.4). The model is described as follows:

$$\eta_i \sim \mathcal{N}(\beta^\top x_i + \beta_0, \sigma)$$

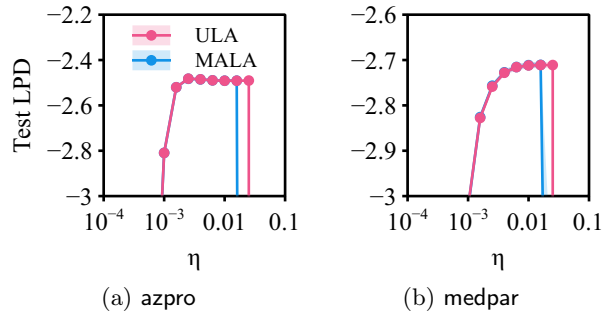


Figure 3: **Test average log-predictive density (LPD) for robust Poisson regression versus the MALA/ULA stepsize η .** ULA is more robust against the choice of stepsize on `azpro`. The colored bands are 80% bootstrap confidence intervals of the mean computed from 32 independent train-test splits of a ratio of 8 : 1.

$$y_i \sim \text{Poisson}(\exp(\eta_i)).$$

The hyper-parameters are $\theta = (\beta, \beta_0, \sigma) \in \mathbb{R}^d \times \mathbb{R} \times \mathbb{R}_{>0}$. Unlike the popular negative-binomial regression model, this model is non-conjugate and intractable. We will apply MCMC-SAEM to perform maximum-likelihood inference of the regression coefficients while marginalizing the local response η_i . We run MCMC-SAEM for 100 iterations after 10 initial burn-in steps. The considered datasets are shown in Table 1 and were obtained from the `COUNT` package in R (Hilbe, 2016).

Results The results are shown in Figure 3. As expected, ULA converges for a wider range of stepsizes. However, in this example, the difference between the two methods is very small. This is because both methods mix quickly for this posterior; it is strongly log-concave and factorizes into univariate posteriors.

5.4 Logistic Regression with Automatic Relevance Determination

Automatic relevance determination (ARD; Neal, 1996; MacKay, 1996) is prior on regression coefficients, where each regressor β_i is assigned its own scale parameter γ_i . When maximizing the marginal likelihood with respect to the relevance parameters γ_i , the ARD prior is known to have a sparsifying effect, where irrelevant features are pruned as $\gamma_i \rightarrow \infty$. This “shrinkage” effect is lost if one does fully Bayesian inference. Therefore the empirical Bayes version of the problem is especially relevant.

Unfortunately, solving the maximum marginal likelihood problem is challenging, even for linear regression models (Tipping, 2001; Wipf and Nagarajan, 2007). Here, we demonstrate that MCMC-SAEM can be used to solve the ARD problem for logistic regression with

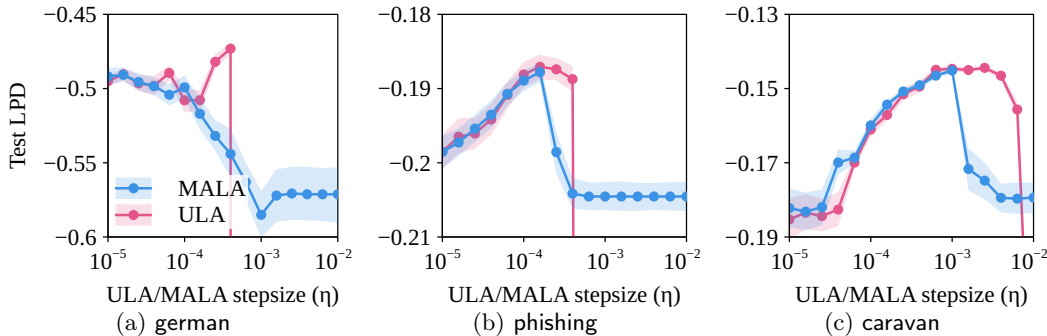


Figure 4: **Test average log-predictive density (LPD) for logistic regression with automatic relevance determination versus MALA/ULA stepsize η .** The colored bands are 80% bootstrap confidence intervals of the mean computed from 32 independent train-test splits of a ratio of 8 : 1.

Table 2: LOGISTIC REGRESSION DATASETS

NAME	# data	dim(z)	dim(θ)
phishing	11054	68	69
german	1000	217	216
caravan	9822	620	619

Bernoulli likelihoods.

The model is described as:

$$\begin{aligned} \beta_0 &\sim \mathcal{N}(0, 10) & \beta &\sim \mathcal{N}(0, \gamma^{-1}) \\ p_i &= \text{logistic}(\beta^\top x_i + \beta_0) \\ y_i &\sim \text{Bernoulli}(p_i), \end{aligned}$$

where $\gamma = (\gamma_1, \gamma_2, \dots, \gamma_d) \in \mathbb{R}_{>0}^d$.

We optimize the hyperparameters $\theta = \gamma$ using MCMC-SAEM for 2000 iterations, after 100 burn-in steps, starting from an initial point of $\theta_0 = (1, \dots, 1)$. On this problem, the result was quite sensitive to the initial point. After running MCMC-SAEM, we test the quality of the hyperparameters by estimating the log-predictive density (LPD) on a held-out test dataset using samples from the posterior. The samples are separately drawn using 2000 steps of MALA after 2000 adaptation/burn-in steps. MALA is automatically tuned to target an acceptance rate of 0.57 (Roberts and Rosenthal, 2001) using Nesterov’s dual averaging procedure (Nesterov, 2009). We replicate this over 32 independent train-test splits. The datasets were obtained from the UCI repository (Dua and Graff, 2017) and are shown in Table 2. The categorical variables were one-hot encoded, while the continuous features were z-standardized.

Furthermore, for this problem, preconditioning MALA and ULA is crucial since the scale of the posterior greatly varies depending on whether a feature is pruned or not. We use a diagonal preconditioner P where the diagonal is set as $P_{ii} = 1/(\gamma_i^2 + 0.01) + \delta$ for β and 1 for β_0 . $\delta = 2 \times 10^{-16} > 0$ is necessary to ensure

that the MCMC chain is not reducible even when a feature is pruned by $\gamma_i \rightarrow \infty$.

Results The results are shown in Figure 4. We can see that ULA converges to a high quality solution for the widest range of stepsizes. On **german**, only ULA achieves the highest level of accuracy. Notably, in the large η regime, the MALA chain tended to reduce to a state with an acceptance rate close to 0. ULA, on the other hand, is immune to this issue since it always makes progress as long as it does not diverge. Furthermore, when η was too large, ULA immediately diverged at the initial SAEM iterations, which is easier to diagnose and correct.

6 DISCUSSIONS

In this work, we theoretically and empirically studied the impact of approximate MCMC algorithms. The theory suggests that they are feasible for SAEM in high dimensions as soon as the marginal log-likelihood is smooth enough. That is, the asymptotic bias will have a minimal effect on the found solution. We empirically confirmed this fact on multiple statistical problems. Furthermore, in our experiments, we observe that ULA versus MALA represents a trade-off between asymptotic bias versus non-asymptotic bias, where the latter can be more significant on high-dimensional and poorly conditioned problems. That is, with large stepsizes, MALA converges slower than ULA due to rejections, incurring a large non-asymptotic transient bias. As a result, ULA converges faster on these problems.

On a different note, this work provides a clear use case of approximate MCMC algorithms in statistics. While recent works (Akyildiz et al., 2023; Kuntz et al., 2023; de Bortoli et al., 2021) in empirical Bayes estimation leveraging approximate MCMC didn’t explore the *benefits* of approximate MCMC methods over exact MCMC, we showed here that being approximate can, in fact, be better.

Acknowledgements

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References

- Ö. Deniz Akyildiz, Francesca Romana Crucinio, Mark Girolami, Tim Johnston, and Sotirios Sabanis. Interacting particle langevin algorithm for maximum marginal likelihood estimation. arXiv Preprint arXiv:2303.13429, arXiv, March 2023.
- Ahmet Alacaoglu and Hanbaek Lyu. Convergence of first-order methods for constrained nonconvex optimization with dependent data. In *Proceedings of the International Conference on Machine Learning*, volume 202 of *PMLR*, pages 458–489. JMLR, July 2023.
- Christophe Andrieu, Éric Moulines, and Pierre Priouret. Stability of stochastic approximation under verifiable conditions. *SIAM Journal on Control and Optimization*, 44(1):283–312, 2005.
- Charlotte Baey, Maud Delattre, Estelle Kuhn, Jean-Benoist Leger, and Sarah Leae. Efficient preconditioned stochastic gradient descent for estimation in latent variable models. In *Proceedings of the International Conference on Machine Learning*, volume 202 of *PMLR*, pages 1430–1453. JMLR, July 2023.
- Robert J. Bauer. Nonmem tutorial part ii: Estimation methods and advanced examples. *CPT: Pharmacometrics & Systems Pharmacology*, 8(8):538–556, 2019.
- Michel Benaïm. Dynamics of stochastic approximation algorithms. In *Seminaire de Probabilites XXXIII*, pages 1–68. Springer, 2006.
- Michel Benaïm, Josef Hofbauer, and Sylvain Sorin. Perturbations of set-valued dynamical systems, with applications to game theory. *Dynamic Games and Applications*, 2:195–205, 2012.
- Jeff Bezanson, Alan Edelman, Stefan Karpinski, and Viral B Shah. Julia: A fresh approach to numerical computing. *SIAM Review*, 59(1):65–98, 2017.
- Alison J. Boeckmann, Lewis B. Sheiner, and Stuart L. Beal. *NONMEM Users Guide: Part V*. NONMEM Project Group, University of California, San Francisco, 1994.
- A. Colin Cameron and Pravin K. Trivedi. *Regression Analysis of Count Data*. Econometric Society Monographs. Cambridge University Press, Cambridge, second edition, 2013.
- Emmanuelle Comets, Audrey Lavenu, and Marc Lavielle. Parameter estimation in nonlinear mixed effect models using saemix, an r implementation of the saem algorithm. *Journal of Statistical Software*, 80(3):1–41, 2017.
- Marie Davidian and David .M Giltinan. *Nonlinear Models for Repeated Measurement Data*, volume 62 of *Monographs on Statistics and Applied Probability*. Routledge, New York, NY, 1995.
- Valentin de Bortoli, Alain Durmus, Marcelo Pereyra, and Ana F Vidal. Efficient stochastic optimisation by unadjusted Langevin monte carlo: Application to maximum marginal likelihood and empirical Bayesian estimation. *Statistics and Computing*, 31, March 2021.
- Vianney Debavelaere and Stéphanie Allasonnière. On the curved exponential family in the stochastic approximation expectation maximization algorithm. *ESAIM: Probability and Statistics*, 25:408–432, 2021.
- Vianney Debavelaere, Stanley Durrleman, and Stéphanie Allasonnière. On the convergence of stochastic approximations under a subgeometric ergodic Markov dynamic. *Electronic Journal of Statistics*, 15(1):1583–1609, 2021.
- Bernard Delyon, Marc Lavielle, and Eric Moulines. Convergence of a stochastic approximation version of the EM algorithm. *Annals of Statistics*, pages 94–128, 1999.
- Arthur P Dempster, Nan M Laird, and Donald B Rubin. Maximum likelihood from incomplete data via the em algorithm. *Journal of the Royal Statistical Society: Series B (Methodological)*, 39(1):1–22, 1977.
- Aymeric Dieuleveut, Gersende Fort, Eric Moulines, and Hoi-To Wai. Stochastic approximation beyond gradient for signal processing and machine learning. *IEEE Transactions on Signal Processing*, 71:3117–3148, 2023.
- Dheeru Dua and Casey Graff. UCI machine learning repository. 2017.
- Simon Duane, Anthony D. Kennedy, Brian J. Pendleton, and Duncan Roweth. Hybrid Monte Carlo. *Physics Letters B*, 195(2):216–222, 1987.

- Alain Durmus and Eric Moulines. Nonasymptotic convergence analysis for the unadjusted Langevin algorithm. *Annals of Applied Probability*, 27(3):1551–1587, 2017.
- Bradley Efron. Bayes, oracle Bayes and empirical Bayes. *Statistical Science*, 34(2):177–201, May 2019.
- Walter R. Gilks, Gareth O. Roberts, and Sujit K. Sahu. Adaptive Markov chain Monte Carlo through regeneration. *Journal of the American Statistical Association*, 93(443):1045–1054, 1998.
- Joseph M Hilbe. *COUNT: Functions, Data and Code for Count Data*, 2016.
- Mike Hurley. Chain recurrence, semiflows, and gradients. *Journal of Dynamics and Differential Equations*, 7:437–456, 1995.
- Belhal Karimi, Blazej Miasojedow, Eric Moulines, and Hoi-To Wai. Non-asymptotic analysis of biased stochastic approximation scheme. In *Proceedings of the Conference on Learning Theory*, volume 99, pages 1944–1974. PMLR, 2019.
- Estelle Kuhn and Marc Lavielle. Coupling a stochastic approximation version of EM with an MCMC procedure. *ESAIM: Probability and Statistics*, 8:115–131, 2004.
- Estelle Kuhn and Marc Lavielle. Maximum likelihood estimation in nonlinear mixed effects models. *Computational Statistics & Data Analysis*, 49(4):1020–1038, 2005.
- Juan Kuntz, Jen Ning Lim, and Adam M. Johansen. Particle algorithms for maximum likelihood training of latent variable models. In *Proceedings of the International Conference on Artificial Intelligence and Statistics*, volume 206 of *PMLR*, pages 5134–5180. JMLR, 25–27 Apr 2023.
- Kenneth Lange. *MM optimization algorithms*. SIAM, 2016.
- Marc Lavielle. *Mixed Effects Models for the Population Approach: Models, Tasks, Methods and Tools*. Biostatistics Series. Chapman and Hall/CRC, New York, NY, 2014.
- Xiaoyu Li and Francesco Orabona. A high probability analysis of adaptive SGD with momentum. In *Workshop on Beyond First Order Methods in ML Systems at ICML’20*, 2020.
- David J. C. MacKay. Bayesian methods for backpropagation networks. In *Models of Neural Networks III: Association, Generalization, and Representation*, Physics of Neural Networks, pages 211–254. Springer, New York, NY, 1996.
- Geoffrey J. McLachlan and Thiriyambakam Krishnan. *The EM Algorithm and Extensions*. Wiley Series in Probability and Statistics. John Wiley & Sons, April 2007.
- Geoffrey J. McLachlan, Sharon X. Lee, and Suren I. Rathnayake. Finite mixture models. *Annual Review of Statistics and its Application*, 6:355–378, 2019.
- Radford M. Neal. *Bayesian Learning for Neural Networks*, volume 118 of *Lecture Notes in Statistics*. Springer New York, New York, NY, 1996.
- Radford M. Neal. Annealed importance sampling. *Statistics and Computing*, 11(2):125–139, 2001.
- Yurii Nesterov. Primal-dual subgradient methods for convex problems. *Mathematical Programming*, 120(1):221–259, August 2009.
- E Nummelin. On the Poisson equation in the potential theory of a single kernel. *Mathematica Scandinavica*, pages 59–82, 1991.
- José C. Pinheiro and Douglas M. Bates. Approximations to the log-likelihood function in the nonlinear mixed-effects model. *Journal of Computational and Graphical Statistics*, 4(1):12–35, 1995.
- Herbert Robbins. An empirical Bayes approach to statistics. In *Proceedings of the 3rd Berkeley Symposium on Mathematical Statistics and Probability, Volume 1: Contributions to the Theory of Statistics*, volume 3.1, pages 157–164. University of California Press, 1956.
- Herbert Robbins and Sutton Monro. A stochastic approximation method. *The Annals of Mathematical Statistics*, 22(3):400–407, 1951.
- Christian P. Robert and George Casella. *Monte Carlo Statistical Methods*. Springer Texts in Statistics. Springer New York, New York, NY, 2004.
- Gareth O. Roberts and Jeffrey S. Rosenthal. Optimal scaling for various Metropolis-Hastings algorithms. *Statistical Science*, 16(4):351–367, 2001.
- Gareth O. Roberts and Richard L. Tweedie. Exponential convergence of Langevin distributions and their discrete approximations. *Bernoulli*, 2(4):341–363, 1996.
- Abhishek Roy, Krishnakumar Balasubramanian, and Saeed Ghadimi. Constrained stochastic nonconvex optimization with state-dependent Markov data. In *Advances in Neural Information Processing Systems*, volume 35, pages 23256–23270, December 2022.
- Vladislav B Tadić and Arnaud Doucet. Asymptotic bias of stochastic gradient search. *Annals of Applied Probability*, 27(6):3255–3304, 2017.
- Michael E. Tipping. Sparse Bayesian learning and the relevance vector machine. *Journal of Machine Learning Research*, 1:211–244, 2001.

Chong Wang and David M. Blei. A general method for robust Bayesian modeling. *Bayesian Analysis*, 13(4):1163–1191, December 2018.

David Wipf and Srikantan Nagarajan. A new view of automatic relevance determination. In *Advances in Neural Information Processing Systems*, volume 20. Curran Associates, Inc., 2007.

Checklist

1. For all models and algorithms presented, check if you include:
 - (a) A clear description of the mathematical setting, assumptions, algorithm, and/or model.
Yes.
 - (b) An analysis of the properties and complexity (time, space, sample size) of any algorithm.
No. But we present a non-asymptotic convergence guarantee.
 - (c) (Optional) Anonymized source code, with specification of all dependencies, including external libraries.
Yes.
2. For any theoretical claim, check if you include:
 - (a) Statements of the full set of assumptions of all theoretical results.
Yes.
 - (b) Complete proofs of all theoretical results.
[Yes/No/Not Applicable]
Yes.
 - (c) Clear explanations of any assumptions.
[Yes/No/Not Applicable]
Yes.
3. For all figures and tables that present empirical results, check if you include:
 - (a) The code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL).
Yes. The link to the repository is disclosed in Section 5.
 - (b) All the training details (e.g., data splits, hyperparameters, how they were chosen).
[Yes/No/Not Applicable]
Yes.
 - (c) A clear definition of the specific measure or statistics and error bars (e.g., with respect to the random seed after running experiments multiple times).
Yes. See the main text.
 - (d) A description of the computing infrastructure used. (e.g., type of GPUs, internal cluster, or cloud provider).
Yes. In Appendix C.
4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets, check if you include:
 - (a) Citations of the creator If your work uses existing assets.
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 - (b) The license information of the assets, if applicable.
Not applicable.
 - (c) New assets either in the supplemental material or as a URL, if applicable.
Not applicable.
 - (d) Information about consent from data providers/curators.
Not applicable.
 - (e) Discussion of sensible content if applicable, e.g., personally identifiable information or offensive content.
Not applicable.
5. If you used crowdsourcing or conducted research with human subjects, check if you include:
 - (a) The full text of instructions given to participants and screenshots.
Not applicable.
 - (b) Descriptions of potential participant risks, with links to Institutional Review Board (IRB) approvals if applicable.
Not applicable.
 - (c) The estimated hourly wage paid to participants and the total amount spent on participant compensation.
Not applicable.

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A TECHNICAL ASSUMPTIONS ON THE MARKOV KERNEL

In this section, we give conditions that imply **A2** in terms of a bound from below of the Markov kernel on a small set and a drift condition toward this small set (see (Nummelin, 1991) for the definitions and main results). It offers some insights regarding what properties are essential for the state-dependent Markov kernels to have convergence guarantees. These conditions are verified for ULA (de Bortoli et al., 2021).

Define, for $\mathcal{V} : \mathcal{Z} \rightarrow [1, \infty)$ and $g : \mathcal{Z} \rightarrow \mathbb{R}^d$ the norm

$$\|g\|_{\mathcal{V}} = \sup_{x \in \mathcal{Z}} \frac{|g(x)|}{\mathcal{V}(x)}$$

Denote, for $\mathcal{V} : \mathcal{Z} \rightarrow [1, \infty)$, $\mathcal{L}_{\mathcal{V}} := \{g : \mathcal{Z} \rightarrow \mathbb{R}^d, \sup_{z \in \mathcal{Z}} \|g\|_{\mathcal{V}} < \infty\}$.

M1. For any $s \in \mathbb{R}^d$, Π_s^η is ψ -irreducible and aperiodic². In addition there exist a function $\mathcal{V} : \mathcal{Z} \rightarrow [1, \infty)$, a constant $l_c \geq 2$ such that for any compact subset $\mathcal{K} \subset \mathbb{R}^d$,

- (DRI1) there exist an integer m , constants $0 < \lambda < 1, b, \kappa, \delta > 0$ and a probability measure ν such that

$$\begin{aligned} \sup_{s \in \mathcal{K}} (\Pi_s^\eta)^m \mathcal{V}^{l_c}(z) &\leq \lambda \mathcal{V}^{l_c}(z) + b \mathbf{1}_{\mathcal{C}}(z), \\ \sup_{s \in \mathcal{K}} \Pi_s^\eta \mathcal{V}^{l_c}(z) &\leq \kappa \mathcal{V}^{l_c}(z) && \forall z \in \mathcal{Z} \\ \inf_{s \in \mathcal{K}} (\Pi_s^\eta)^m(z, A) &\geq \delta \nu(A) && \forall z \in \mathcal{C}, \quad \forall A \in \mathcal{B}(\mathcal{Z}). \end{aligned}$$

- (DRI2) $\|S(\cdot)\|_{\mathcal{V}} < \infty$.

- (DRI3) there exists C such that, for all $((s, \eta), (s', \eta')) \in (\mathcal{K} \times]0, \eta_0])^2$

$$\begin{aligned} \left\| \Pi_s^\eta g - \Pi_{s'}^{\eta'} g \right\|_{\mathcal{V}} &\leq C \|g\|_{\mathcal{V}} |(s, \eta) - (s', \eta')| && \forall g \in \mathcal{L}_{\mathcal{V}}, \\ \left\| \Pi_s^\eta g - \Pi_{s'}^{\eta'} g \right\|_{\mathcal{V}^{l_c}} &\leq C \|g\|_{\mathcal{V}^{l_c}} |(s, \eta) - (s', \eta')|, && \forall g \in \mathcal{L}_{\mathcal{V}^{l_c}} \end{aligned}$$

Assumption (DRI1) is classical in the Markov chain literature; it implies the existence of a stationary distribution $\pi_{s, \eta}$ for all $s, \eta \in \mathbb{R}^d \times]0, \eta_0]$ and \mathcal{V}^{l_c} -uniform ergodicity, i.e. for each $s, \eta \in \mathbb{R}^d \times]0, \eta_0]$ there exist constants $C_{s, \eta} < \infty$ and $\gamma_{s, \eta} \in [0, 1)$, such that for any function $f \in \mathcal{L}_{\mathcal{V}^{l_c}}$ and any integer $k > 0$

$$\|(\Pi_s^\eta)^k f - \pi_{s, \eta}(f)\|_{\mathcal{V}^{l_c}} \leq C_{s, \eta} \gamma_{s, \eta}^k \|f\|_{\mathcal{V}^{l_c}}.$$

Note that the constants $C_{s, \eta}$ and $\gamma_{s, \eta}$ may be bounded over the compact sets of \mathbb{R}^d , i.e. for each $\mathcal{K} \subset \mathbb{R}^d$, there exists $\bar{C} < \infty$ and $\bar{\gamma} \in [0, 1)$, such that $\sup_{s \in \mathcal{K} \times]0, \eta_0]} C_{s, \eta} \leq \bar{C}$ and $\sup_{s, \eta \in \mathcal{K} \times]0, \eta_0]} \gamma_{s, \eta} \leq \bar{\gamma}$. The regularity of the kernels $s, \eta \rightarrow \Pi_s^\eta$ expressed in \mathcal{V} and \mathcal{V}^{l_c} norm is naturally less classical in (DRI3). These conditions can be weakened by considering subgeometric ergodicity conditions (Debavelaere et al., 2021). (DRI2) is just a control on the summary statistic depending on the drift of the Markov kernel.

By **M1**, we can control the solution of the Poisson equation related to the Markov kernels $\{\Pi_s^\eta, s, \eta \in \mathbb{R}^d \times]0, \eta_0]\}$ which are helpful to control the markovian noise (e_n) , these controls are presented in the following assumption.

M2. For any $s \in \mathbb{R}^d$, the Poisson equation $\nu_s^\eta - \Pi_s^\eta \nu_s^\eta = S(\cdot) - \pi_{s, \eta}(S(\cdot))$ $\pi_{s, \eta}(S(\cdot)) = \check{s}_\eta(s)$ has a solution ν_s^η . There exist a function $W : \mathcal{Z} \rightarrow [1, \infty]$ such that $\{x \in \mathcal{Z}, W(x) < \infty\} \neq \emptyset$, constants $\alpha \in (0, 1], l_c \geq 2$ such that for any compact subset $\mathcal{K} \subset \mathbb{R}^d$, by denoting $\mathcal{K}' = \mathcal{K} \times]0, \eta_0]$ the following holds:

$$\begin{aligned} \|S(\cdot)\|_W < \infty, \quad \sup_{(s, \eta) \in \mathcal{K}'} (\|\nu_s^\eta\|_W + \|\Pi_s^\eta \nu_s^\eta\|_W) &< \infty, \\ \sup_{((s, \eta), (s', \eta')) \in \mathcal{K}'} |\theta - \theta'|^{-\alpha} \left\{ \left\| \nu_s^\eta - \nu_{s'}^{\eta'} \right\|_W + \left\| \Pi_s^\eta \nu_s^\eta - \Pi_{s'}^{\eta'} \nu_{s'}^{\eta'} \right\|_W \right\} &< \infty. \end{aligned}$$

We stress here the fact that the function W is global but that the bounds in the previous equations depend on the particular compact \mathcal{K} under consideration.

²We use in this article the standard terminology and the notations introduced in (Nummelin, 1991, Chapter 4.5)

Lemma 2. *Assume **M1**. Then **H4**, **M2** are satisfied.*

It is (Andrieu et al., 2005, Proposition 6.1) adapted to our framework here $\Theta = \mathbb{R}^d \times]0, \eta_0], \beta = 1$. We removed the implications depending on the context of (Andrieu et al., 2005).

Furthermore, if we control the learning steps (γ_n) , the bias paramter (η_n) and momentums of the latent variables (Z_n) , the desired result can be established.

M3. *The sequence (γ_n) and (η_n) are nonincreasing, positive and satisfy $\sum_{k=0}^{\infty} \gamma_k = \infty$, $\lim_{k \rightarrow \infty} \gamma_k = 0$, $\limsup_{k \rightarrow \infty} |\gamma_k^{-1} - \gamma_{k+1}^{-1}| = 0$ and*

$$\sum_{k=1}^{\infty} \{\gamma_k^2 + \gamma_k |\eta_{k+1} - \eta_k|^\alpha + \gamma_k^{1+\alpha}\} < \infty$$

where α is defined in **M2**.

M4. *For any compact $\mathcal{K} \subset \mathbb{R}^d$, there exists a constant $C > 0$ such that for any $z \in \mathcal{Z}$,*

$$\sup_{s \in \mathcal{K}} \sup_{k \geq 0^*} \mathbb{E}_{z,s} [W^{l_c}(Z_k) \mathbf{1}_{\{\sigma(\mathcal{K}) \geq k\}}] \leq CW^{l_c}(z).$$

$$\sigma(\mathcal{K}) = \inf\{k \geq 0 : s_k \notin \mathcal{K}\} \cup \{+\infty\},$$

W is defined in **M2**.

Theorem 3. *Assume **M1**, **M3** and **M4** then **A2** is satisfied.*

The proof is postponed to Appendix **B.1.3**.

The assumption **M4** is essential and cannot be recovery directly from **M1**, if we want this hypothesis, we have to change a little the recursion (2) to ensure that (s_n) stays in a compact by design and that $|s_{n+1} - s_n|$ is controlled by a non increasing sequence (ϵ_n) (Andrieu et al., 2005, p.9). We did not choose this framework because it gives rise to technicalities that are rarely implemented in practice. Even if it offers a guarantee of convergence, there are some drawbacks regarding convergence speed.

B PROOFS

B.1 Asymptotic Convergence

In this section, we will prove Theorem 1 in Section 3 and Theorem 3 in Appendix A.

B.1.1 Auxiliary Lemma

Before to prove the main theorem, we introduce another technical Lemma similar to Lemma 1,

Lemma 3. *Assume **H1-3**, then for any $s \in \mathbb{R}^d$,*

$$\nabla V(s) = -A(s)h(s) \quad \text{and} \quad |\nabla V(s)|^2/\lambda_M \leq \langle \nabla V(s)|h(s) \rangle \leq |\nabla V(s)|^2/\lambda_m . \quad (5)$$

Proof. In the proof of (Delyon et al., 1999, Lemma 2), the authors derive that for any $s \in \mathbb{R}^d$, $\nabla V(s) = -A(s)h(s)$. By **H3**, $A(s)$ is invertible and $A^{-1}(s)$ has respectively for minimal and maximal eigen values $1/\lambda_M$ and $1/\lambda_m$, thus, writing for any $s \in \mathbb{R}^d$, $h(s) = -A^{-1}(s)\nabla V(s)$ yields the inequality (5). \square

B.1.2 Proof of Theorem 1

Except for some inequalities and constants, the proof is nearly the same as in (Tadić and Doucet, 2017). The notations of (Tadić and Doucet, 2017) and ours are not the same: the function V and the sequences $(s_n), (\gamma_i), (\beta_n)$ in this paper are replaced by the function f and the sequences $(\theta_n), (\alpha_i), (\eta_n)$ in their paper. In the following, we detail all the proof modifications in (Tadić and Doucet, 2017) to get the desired theorem. We expose the sketch of proof related to each part of the proof before to details the changes.

Proof of (I) First remark that $S = \{h(s) = 0 : s \in \mathbb{R}^d\}$ by

In (Tadić and Doucet, 2017, p.15), the idea is to consider a perturbed flow equations related to the velocity field $-\nabla f$ with the perturbation size $\beta > 0$, for any $t \geq 0$,

$$\frac{d\theta(t)}{dt} \in F_\beta(\theta(t))^{\text{tadic}}, \quad F_\beta(\theta(t))^{\text{tadic}} = \{-\nabla\theta(s(t)) + v, v \in \mathbb{R}^{d_\theta} : |v| \leq \beta\}. \quad (6)$$

Then, by (Benaïm, 2006, Proposition 4.1, Theorem 5.7), on the event Λ_Q , all limit points of (θ_n) are in a set $R_{Q,2\beta}$ called "recurrent set" which is related to (6)[β]: there is a link between the asymptotics of the discretized and the continuous flow. By (Benaïm et al., 2012, Theorem 3.1), working with (6) instead of the discretization, there exists $\psi_Q : [0, \infty) \rightarrow [0, \infty)$ (depending only on $f(\cdot)$) such that $\lim_{t \rightarrow 0} \psi_Q(t) = \psi_Q(0) = 0$ and $R_{Q,\beta} \subset \{x \in \mathbb{R}^d : d(x, R_{Q,0}) \leq \psi_Q(\beta/2)\}$ for any $\beta \geq 0$. Finally, by (Hurley, 1995, Proposition 4), we can show that $R_{Q,0} = \{x \in \mathbb{R}^d : \nabla f(x) = 0\}$ provided that f is p -continuously differentiable with $p > d$ by using Sard's theorem.

To adapt the reasoning, we take h instead of $-\nabla f$ such that we consider $F_\beta(s(t)) = \{h(s) + v, v \in \mathbb{R}^d : |v| \leq \gamma\}$ for any $t, \beta \geq 0$. (Benaïm et al., 2012, Theorem 3.1) and (Benaïm, 2006, Proposition 4.1, Theorem 5.7) remain usable as long as h is continuous, which is given by **H3**. (Hurley, 1995, Proposition 4) can't be applied directly. This Proposition is for gradient flow, i.e. $dx/dt = -\nabla f(x)$ with f continuously differentiable. However, the proof of (Hurley, 1995, Proposition 4) can still be done by replacing $-\nabla f$ by h and f by V . Indeed, for any $s \in \mathbb{R}^d$ and $K \subset \mathbb{R}^d$ a compact such that $\phi([0, 1], s) \subset K$,

$$\begin{aligned} V(\phi(0, s)) - V(\phi(1, s)) &= - \int_0^1 \frac{dV(\phi(t, s))}{dt} dt = - \int_0^1 \underbrace{\langle \nabla V(\phi(t, s)) | h(\phi(t, s)) \rangle}_{=F(\phi(t, s))} dt \\ &\geq \frac{1}{\lambda_M} \int_0^1 |\nabla V(\phi(t, s))|^2 dt, \end{aligned}$$

where we use (5). This shows that the following flow $dx/dt = h(x)$ decreases an energy V . The others arguments in the proof of (Hurley, 1995, Proposition 4) remains the same as long as we remark that the regular points of V are dense by Sard's theorem and **H3**, and by (5) we have

$$S = \{s \in \mathbb{R}^d : \nabla V(s) = 0\} = \{s \in \mathbb{R}^d : \nabla h(s) = 0\}.$$

The proof of (I) is complete.

Proof of (II)-(III) We work on the event Λ_Q , i.e., the sequence (s_n) is in the compact Q for n large enough.

In (Tadić and Doucet, 2017, Proposition 8.2), the authors show that for any $s \in \mathbb{R}^d$, the distances $d(s, S), d(f(s), S)$ can be bounded from above by a term of the form $a_1 |\nabla f(s)|^{a_2}$ with $a_1, a_2 > 0$ using geometric and regularity arguments. The remaining work is to bound $|\nabla f(s)|$, which is performed in (Tadić and Doucet, 2017, Proposition 8.3) using previous results (Tadić and Doucet, 2017, Lemma 8.1-3) all deriving from a Taylor expansion of $f(s_{a(n,t)}) - f(s_n)$ in s_n given in (Tadić and Doucet, 2017, equation (32) p.17). The idea is to measure the influence of the bias β and the noise e_n compared to the influence of the velocity field ∇f : if ∇f has more influence than the other terms, f will decrease, and its gradient as well till the point when ∇f has less influence than the noise and the bias. They show that the norm of the gradient at the asymptotic is ruled only by the bias since the accumulated noise vanishes by **A2**.

In order to adapt the proof, we should only change the Taylor expansion (Tadić and Doucet, 2017, equation (32) p.17) by replacing $-\nabla f$ by h and then propagating the changes in the analysis related to the norm of the gradient in (Tadić and Doucet, 2017, Lemma 8.1-3) by using (5).

By doing a Taylor expansion, for any $n \geq 0, t \in (0, \infty)$,

$$V(s_{a(n,t)}) - V(s_n) = \sum_{i=n}^{a(n,t)-1} \gamma_i \langle \nabla V(s_n) | h(s_n) \rangle - \left\langle \nabla V(s_n) \middle| \sum_{i=n}^{a(n,t)-1} \gamma_i \xi_i \right\rangle + |\phi_n(t)|$$

where ϕ_n is defined in (Tadić and Doucet, 2017, p.17). Then, by using (5),

$$V(s_{a(n,t)}) - V(s_n) \leq -|\nabla V(s_n)| \left(\frac{1}{\lambda_M} |\nabla V(s_n)| \sum_{i=n}^{a(n,t)-1} \gamma_i - \left| \sum_{i=n}^{a(n,t)-1} \gamma_i \xi_i \right| \right) + |\phi_n(t)|$$

We denote by $\phi = \limsup_{n \rightarrow \infty} |\nabla V(s_n)|$ and $C_{1,Q} = \sup_{s \in Q} |\nabla V(s)|$. The second change are in equations (38),(39) in (Tadić and Doucet, 2017, Lemma 8.1, p.18) which are replaced for any $t \in (0, \infty)$ by

$$\limsup_{n \rightarrow \infty} \max_{n \leq k < a(n,t)} |V(s_k) - V(s_n)| \leq C_{1,Q} t (\phi + \beta) \max \left(\frac{1}{\lambda_m}, 1 \right)$$

$$\limsup_{n \rightarrow \infty} |\phi_n(t)| \leq C_{1,Q} t^2 (\phi + \beta)^2 \max \left(\frac{1}{\lambda_m}, 1 \right)^2$$

since the last equation in (Tadić and Doucet, 2017, p.18) has to be replaced by,

$$|s_k - s_n| \leq \sum_{i=n}^{k-1} \gamma_i |h(s_i)| + \left| \sum_{i=n}^{k_1} \gamma_i \xi_i \right| \leq t(\phi + \epsilon) \max \left(\frac{1}{\lambda_m}, 1 \right) + \max_{n \leq i < a(n,t)} \left| \sum_{i=n}^{k_1} \gamma_i \xi_i \right|$$

where we used again (5) and the fact that $|\nabla V(s_n)| \leq \phi$ for n large enough as in (Tadić and Doucet, 2017).

From these changes, the constants used in the proof are modified. The constant γ is replaced p.20 by $\gamma = 2\lambda_M(\epsilon + \beta)$ and $C_{2,Q} = 4\lambda_M M_Q$. The (Tadić and Doucet, 2017, Lemma 8.3) holds on $(\Lambda_Q \setminus N_0) \cap (\phi > 2\beta\lambda_M)$. It impacts the final constant, we have $K_Q = \lambda_M \max \left(2, \tilde{C}_Q, C_{2,Q} \right)$ instead of $\max \left(2, \tilde{C}_Q, C_{2,Q} \right)$, where M_Q is a constant related to the Yomdin theorem (Tadić and Doucet, 2017, Proposition 8.1, 8.2) and $\tilde{C}_Q = \sup_Q |\nabla V(s)|$.

B.1.3 Proof of Theorem 3

We follow the same scheme of proof of (Andrieu et al., 2005, Proposition 5.2). We will intensely use the conditions **M2** given by Lemma 2 and **M1**. $\mathbb{E}_{s,z}$ denotes the conditionnal expectation given $s_0 = s$ and $Z_0 = z$. Let $\mathcal{K} \subset \mathbb{R}^d$ be a compact set and set the event $\tilde{\Lambda}_{\mathcal{K}} = \cap_{k=0}^{\infty} (s_k \in \mathcal{K})$. Using the existence of solution to the Poisson equation, for any $k \geq 1$, we have,

$$e_{k-1} = S(z_k) - \tilde{s}_{\eta_k}(s_{k-1}) = (I - \Pi_{s_{k-1}}^{\eta_k}) \nu_{s_{k-1}}^{\eta_k}(z_k),$$

and we denote by,

$$T_n = \sum_{k=1}^n \gamma_k e_{k-1} \mathbf{1}_{\sigma(\mathcal{K}, \epsilon) \geq k}.$$

We want to show that T_n converges almost surely on the event $\tilde{\Lambda}_{\mathcal{K}}$. Using for all $k \geq 0$:

$$\mathbf{1}_{\sigma(\mathcal{K}) \geq k} = \mathbf{1}_{\sigma(\mathcal{K}) \geq k+1} + \mathbf{1}_{\sigma(\mathcal{K}) = k},$$

me may write $T_n = \sum_{i=1}^5 T_n^{(i)}$ where,

$$(A.1) \quad T_n^{(1)} = \sum_{k=1}^n \gamma_k \left(\nu_{s_{k-1}}^{\eta_k}(Z_k) - \Pi_{s_{k-1}}^{\eta_k} \nu_{s_{k-1}}^{\eta_k}(Z_{k-1}) \right) \mathbf{1}_{\{\sigma(\mathcal{K}) \geq k\}},$$

$$(A.2) \quad T_n^{(2)} = \sum_{k=1}^{n-1} \gamma_{k+1} \left(\Pi_{s_k}^{\eta_{k+1}} \nu_{s_k}^{\eta_{k+1}}(Z_k) - \Pi_{s_{k-1}}^{\eta_k} \nu_{s_{k-1}}^{\eta_k}(Z_k) \right) \mathbf{1}_{\{\sigma(\mathcal{K}) \geq k+1\}},$$

$$(A.3) \quad T_n^{(3)} = \sum_{k=1}^{n-1} (\gamma_{k+1} - \gamma_k) \Pi_{s_{k-1}}^{\eta_k} \nu_{s_{k-1}}^{\eta_k}(Z_k) \mathbf{1}_{\{\sigma(\mathcal{K}) \geq k+1\}},$$

$$(A.4) \quad T_n^{(4)} = \gamma_1 \Pi_{s_0}^{\eta_1} \nu_{s_0}^{\eta_1}(Z_0) \mathbf{1}_{\{\sigma(\mathcal{K}) \geq 1\}} - \gamma_n \Pi_{s_{n-1}}^{\eta_n} \nu_{s_{n-1}}^{\eta_n}(Z_n) \mathbf{1}_{\{\sigma(\mathcal{K}) \geq n\}},$$

$$(A.5) \quad T_n^{(5)} = - \sum_{k=1}^{n-1} \gamma_k \Pi_{s_{k-1}}^{\eta_k} \nu_{s_{k-1}}^{\eta_k}(Z_k) \mathbf{1}_{\{\sigma(\mathcal{K}) = k\}}$$

We show now the convergence a.e of $T_n^{(i)}$, $i = 1, \dots, 5$ on the event $\tilde{\Lambda}_{\mathcal{K}}$. First remark that $T_n^{(5)} = 0$ on $\tilde{\Lambda}_{\mathcal{K}}$. In the sequel C denotes a constant which depends only upon the compact set \mathcal{K} through the quantities defined in the assumptions and whose value may change upon each appearance. Denoting by

$$D(\gamma, \mathcal{K}, z) = \sup_{s \in \mathcal{K}} \sup_{k \geq 1} \mathbb{E}_{z,s} [W^{l_c}(Z_k) \mathbf{1}_{\{\sigma(\mathcal{K}) \geq k\}}],$$

we have for any $s \in \mathbb{R}^d$ and $z \in \mathcal{Z}$

$$(A.6) \quad \mathbb{E}_{s,z} \left[\sum_{k=1}^{\infty} \gamma_k^2 \left| \nu_{s_{k-1}}^{\eta_k}(Z_k) - \Pi_{s_{k-1}}^{\eta_k} \nu_{s_{k-1}}^{\eta_k}(Z_{k-1}) \right|^2 \mathbf{1}_{\{\sigma(\mathcal{K}) \geq k\}} \right] \\ \leq C \left(\sum_{k=0}^{\infty} \gamma_k^2 \right)^{l_c/2} D(\gamma, \mathcal{K}, z),$$

$$(A.7) \quad \mathbb{E}_{s,z} \left[\sum_{k=1}^{\infty} \gamma_{k+1} \left| \Pi_{s_k}^{\eta_{k+1}} \nu_{s_k}^{\eta_{k+1}}(Z_k) - \Pi_{s_{k-1}}^{\eta_k} \nu_{s_{k-1}}^{\eta_k}(Z_k) \right| \mathbf{1}_{\{\sigma(\mathcal{K}) \geq k+1\}} \right] \leq \\ C \left[\left(\sum_{k=1}^{\infty} |\gamma_k|^{1+\alpha} \right)^{\frac{l_c}{1+\alpha}} + \left(\sum_{k=1}^{\infty} \gamma_k |\eta_{k+1} - \eta_k|^\alpha \right)^{l_c} \right] D(\gamma, \mathcal{K}, z)^{1+\alpha},$$

$$(A.8) \quad \mathbb{E}_{s,z} \left[\sum_{k=1}^{\infty} |\gamma_{k+1} - \gamma_k| \left| \Pi_{s_{k-1}}^{\eta_k} \nu_{s_{k-1}}^{\eta_k}(Z_k) \right| \mathbf{1}_{\{\sigma(\mathcal{K}) \geq k+1\}} \right] \\ \leq C \left(\sum_{k=1}^{\infty} |\gamma_k - \gamma_{k+1}| \right)^{l_c} D(\gamma, \mathcal{K}, z)$$

$$(A.9) \quad \mathbb{E}_{s,z} \left[\gamma_n^{l_c} \left| \Pi_{s_{n-1}}^{\eta_n} \nu_{s_{n-1}}^{\eta_n}(Z_n) \right|^{l_c} \mathbf{1}_{\{\sigma(\mathcal{K}) \geq n\}} \right] \leq C \gamma_k^{l_c} D(\gamma, \mathcal{K}, z).$$

We will show these inequalities at the end of the proof. For any $k \geq 1$,

$$\begin{aligned} \mathbb{E}_{z,s} \left[\left(\nu_{s_k}^{\eta_{k+1}}(Z_{k+1}) - \Pi_{s_k}^{\eta_{k+1}} \nu_{s_k}^{\eta_{k+1}}(Z_k) \right) \mathbf{1}_{\{\sigma(\mathcal{K}) \geq k+1\}} \mid \mathcal{F}_k \right] = \\ \left(\Pi_{s_k}^{\eta_{k+1}} \nu_{s_k}^{\eta_{k+1}}(Z_k) - \Pi_{s_k}^{\eta_{k+1}} \nu_{s_k}^{\eta_{k+1}}(Z_k) \right) \mathbf{1}_{\{\sigma(\mathcal{K}) \geq (k+1)\}} = 0 \end{aligned}$$

$T_n^{(1)}$ is a (\mathbb{R}^d) -valued martingale. Applying Doobs theorem with (A.6), we have the convergence of $(T_n^{(1)})$ almost surely on $\tilde{\Lambda}_{\mathcal{K}}$. Since $T_n^{(5)} \mathbf{1}_{\{\sigma(\mathcal{K}) \geq n\}} = 0$, we have

$$T_n \mathbf{1}_{\{\sigma(\mathcal{K}) \geq n\}} = \sum_{i=1}^4 T_n^{(i)} \mathbf{1}_{\{\sigma(\mathcal{K}) \geq n\}}.$$

Using the inequalities (A.7)-(A.9) with **A1** gives the convergence of $T_n^{(i)}$ for $i = 2, 3, 4$ on the event $\tilde{\Lambda}_{\mathcal{K}}$. On the event $\{\sup_n |s_n| < \infty\}$, we can work in $\tilde{\Lambda}_{\mathcal{K}}$ for some compact set $\mathcal{K} \subset \mathbb{R}^d$, then $\sum_i \gamma_{i+1} e_i$ converges almost surely, which yields the assumption **A2** is given.

Proof of (A.6) Under **M2**, we have for any $k \geq 1$,

$$\left| \nu_{s_{k-1}}^{\eta_k}(Z_k) - \Pi_{s_{k-1}}^{\eta_k} \nu_{s_{k-1}}^{\eta_k}(Z_{k-1}) \right| \mathbf{1}_{\{\sigma(\mathcal{K}) \geq k+1\}} \leq W(Z_k) \mathbf{1}_{\{\sigma(\mathcal{K}) \geq k+1\}} + W(Z_{k-1}) \mathbf{1}_{\{\sigma(\mathcal{K}) \geq k\}}$$

and then,

$$\begin{aligned} \mathbb{E}_{s,z} \left[\sum_{k=1}^{\infty} \gamma_k^2 \left| \nu_{s_{k-1}}^{\eta_k}(Z_k) - \Pi_{s_{k-1}}^{\eta_k} \nu_{s_{k-1}}^{\eta_k}(Z_{k-1}) \right|^2 \mathbf{1}_{\{\sigma(\mathcal{K}) \geq k\}} \right] &\leq \mathbb{E}_{s,z} \left[\sum_{k=1}^{\infty} 4\gamma_k^2 W(Z_k)^2 \mathbf{1}_{\{\sigma(\mathcal{K}) \geq k\}} \right] \\ &\leq C \left(\sum_{k=1}^{\infty} \gamma_k^2 \right)^{\frac{1}{2}} D(\gamma, \mathcal{K}, z), \end{aligned}$$

where we used that $\{\gamma_i\}$ is decreasing and a Minkowski inequality.

Proof of (A.7) Under **M2**, we have For any $k \geq 1$,

$$\gamma_{k+1} \left| \Pi_{s_k}^{\eta_{k+1}} \nu_{s_k}^{\eta_{k+1}}(Z_k) - \Pi_{s_{k-1}}^{\eta_k} \nu_{s_{k-1}}^{\eta_k}(Z_k) \right| \mathbf{1}_{\{\sigma(\mathcal{K}) \geq k+1\}} \leq C \gamma_{k+1} W(Z_k) |(s_k, \eta_{k+1}) - (s_{k-1}, \eta_k)|^\alpha \mathbf{1}_{\{\sigma(\mathcal{K}) \geq k+1\}}$$

then, using the bound on sufficient statistics by **M2** and that s_k is in a compact, for any $k \geq 1$,

$$\begin{aligned} |s_k - s_{k-1}| \mathbf{1}_{\{\sigma(\mathcal{K}) \geq k+1\}} &\leq \gamma_k |S(Z_{k+1}) - s_k| \mathbf{1}_{\{\sigma(\mathcal{K}) \geq k+1\}} \\ &\leq \gamma_k (W(Z_k) + C) \mathbf{1}_{\{\sigma(\mathcal{K}) \geq k+1\}}, \end{aligned}$$

Thus, we have,

$$\begin{aligned} &\sum_{k=1}^{\infty} \gamma_{k+1} \left| \Pi_{s_k}^{\eta_{k+1}} \nu_{s_k}^{\eta_{k+1}}(Z_k) - \Pi_{s_{k-1}}^{\eta_k} \nu_{s_{k-1}}^{\eta_k}(Z_k) \right| \mathbf{1}_{\{\sigma(\mathcal{K}) \geq k+1\}} \\ &\leq C \sum_{k=0}^{\infty} \gamma_{k+1} (|\eta_{k+1} - \eta_k|^\alpha + \gamma_k^\alpha (W(Z_k) + C)^\alpha) W(Z_k) \mathbf{1}_{\{\sigma(\mathcal{K}) \geq k+1\}} \\ &\leq C \sum_{k=0}^{\infty} \gamma_{k+1} |\eta_{k+1} - \eta_k|^\alpha W(Z_k) + \gamma_k^{1+\alpha} (W(Z_k) + W(Z_k)^{\alpha+1}) \mathbf{1}_{\{\sigma(\mathcal{K}) \geq k+1\}}, \end{aligned}$$

in the last inequality, we used that $\{\beta_k\}$ is bounded and that (γ_k) is decreasing. We conclude using the Minkowski's inequality.

Remark that if $\beta > 0$, we have $\epsilon_k = |s_k - s_{k-1}| = \Theta(\gamma_k)$ which makes it impossible to apply the proof of (Delyon et al., 1999) to show that we can have (s_n) in a compact by design. Indeed, it is needed to have $\sum_n (\frac{\gamma_n}{\epsilon_n})^{1/c} < \infty$, but here we have $\epsilon_n \sim \gamma_n$ because of the bias.

Proof of (A.8) Under **M2**,

$$\sum_{k=1}^{n-1} |\gamma_{k+1} - \gamma_k| \left| \Pi_{s_{k-1}}^{\eta_k} \nu_{s_{k-1}}^{\eta_k} (Z_k) \right| \mathbf{1}_{\{\sigma(\mathcal{K}) \geq k+1\}} \leq C \sum_{k=1}^{\infty} |\gamma_k - \gamma_{k+1}| W(Z_k) \mathbf{1}_{\{\sigma(\mathcal{K}) \geq k+1\}},$$

and the proof follows from Minkowski's inequality.

Proof of (A.9) Under **M2**,

$$\mathbb{E}_{s,z} \left[\left| \Pi_{s_{n-1}}^{\eta_{n-1}} \nu_{s_{n-1}}^{\eta_{n-1}} (Z_n) \mathbf{1}_{\{\sigma(\mathcal{K}) \geq n\}} \right|^{l_c} \right] \leq C \mathbb{E}_{s,z} [W^{l_c} (Z_n) \mathbf{1}_{\{\sigma(\mathcal{K}) \geq n\}}]$$

B.2 Non-Asymptotic Convergence

In this section, we will prove Theorem 2 in Section 4.

B.2.1 Auxiliary Lemmas

Before proving the theorem, we need some preliminary results. First, we derive a Robbins-Siegmund Lemma. Then, we control the Markov stochasticity of the process (e_n) by using the Poisson solutions given by N2. It brings out a weighted sum of Martingale difference, which can be bounded by using a concentration inequality given in (Li and Orabona, 2020, Lemma 1). Finally, we conclude by reorganizing the terms. We first state the Robbins-Siegmund Lemma before giving others technical results.

Lemma 4. (*Robbins-Siegmund Lemma*) Assume H1-3, N1, N3, and N4. Then,

$$V(s_{k+1}) \leq V(s_k) + \gamma_{k+1} \langle \nabla V(s_k) | h(s_k) \rangle + \gamma_{k+1} \langle \nabla V(s_k) | e_k \rangle + a_k + b_k |h(s_k)|^2,$$

where the constants are

$$\begin{aligned} a_k &= \frac{1}{2} \lambda_M \sqrt{\tau_0} \gamma_{k+1} + L_V \sigma^2 \gamma_{k+1}^2, \\ b_k &= \left(\frac{1}{2} \lambda_M \sqrt{\tau_0} + \lambda_M \sqrt{\tau_1} \right) \gamma_{k+1} + L_V \gamma_{k+1}^2. \end{aligned}$$

The proof is delayed after the small technical results that followed.

Then, we state the concentration inequality.

Lemma 5 (Adaptation of Lemma 1 by Li and Orabona 2020). Let $(E_n)_{n \geq 1}$ be a martingale difference sequence adapted to the filtration $(\mathcal{F}_{n+1} = \sigma(Z_i, i \leq n+1))_{n \geq 0}$ and a stochastic process $(v_n)_{n \geq 0}$ adapted to the filtration $(\mathcal{F}_n)_{n \geq 0}$, such that for any $k \geq 0$, $\mathbb{E}^{\mathcal{F}^{k+1}} \exp(E_k^2/v_k^2) \leq \exp(1)$. Then, for any fixed $\varrho > 0$ and $\delta \in (0, 1)$, with probability at least $1 - \delta$, it holds that for any $n \geq 1$,

$$n \sum_{k=1}^n E_k \leq \frac{3}{4} \varrho \sum_{k=1}^n v_k^2 + \frac{1}{\varrho} \log \frac{1}{\delta}.$$

This lemma will be used with the following:

Lemma 6. Assume H1-3 and N2. Then, there exists $c \in]0, 2L_\nu^{(0)}]$ such that the MCMC kernel has sub-Gaussian tails for ν_s^η , i.e., for any $s \in \mathbb{R}^d$,

$$\mathbb{E}^{\mathcal{F}^{k+1}} \exp\left(|\nu_s^\eta(Z_{k+1}) - \Pi_s^\eta \nu_s^\eta(Z_k)|^2 / c^2\right) \leq \exp(1). \quad (7)$$

The proof is straightforward: by N2, for any $k \geq 0$ and $s \in \mathbb{R}^d$,

$$|\nu_s^\eta(Z_{k+1}) - \Pi_s^\eta \nu_s^\eta(Z_k)| / 2L_\nu^{(0)} \leq 1,$$

which implies that (7) holds with at least $c = 2L_\nu^{(0)}$.

We introduce the Martingale difference related to Lemma 5. By using the solutions of the Poisson equation by N2, we have for any $k \geq 0$,

$$D_k \triangleq \nu_{s_k}^\eta(Z_{k+1}) - \Pi_{s_k}^\eta \nu_{s_k}^\eta(Z_k), \quad \mathbb{E}(D_k | \mathcal{F}_k) = 0$$

where we use the Markov property related to (Z_k) to remark that $(D_k)_k$ is a sequence of Martingale difference adapted to the filtration $(\mathcal{F}_{k+1})_k$. This yields the following Lemma.

Lemma 7. Assume H1-3 and N2. Then, with probability at least $1 - \delta$, for any $n \geq 1$,

$$-\sum_{k=1}^n \gamma_{k+1} \langle \nabla V(s_k) | D_k \rangle \leq \varrho \lambda_M^2 c^2 \sum_{k=1}^n \gamma_{k+1}^2 |h(s_k)|^2 + \frac{1}{\varrho} \log \frac{1}{\delta},$$

where $\varrho > 0$ is a free variable.

B.2.2 Proof of Lemma 7.

For any $k \geq 1$, denoting by

$$E_k \triangleq -\gamma_{k+1} \langle \nabla V(s_k) | D_k \rangle ,$$

we have,

$$\begin{aligned} |E_k|^2 &= \gamma_{k+1}^2 |\langle \nabla V(s_k) | D_k \rangle|^2 \\ &\leq \gamma_{k+1}^2 |\nabla V(s_k)|^2 |D_k|^2 && \text{(Cauchy-Schwarz)} \\ &\leq \lambda_M^2 \gamma_{k+1}^2 |h(s_k)|^2 |D_k|^2 . && \text{(Lemma 1)} \end{aligned}$$

Since D_k is sub-Gaussian by Lemma 6, (E_k) is also sub-gaussian such that

$$\mathbb{E}^{\mathcal{F}^{k+1}} \exp \left(|E_k|^2 / \left(\lambda_M^2 \gamma_{k+1}^2 |h(s_k)|^2 c^2 \right) \right) \leq \exp(1) .$$

Thus, Lemma 5 applies after setting $v_k \triangleq \lambda_M^2 \gamma_{k+1}^2 |h(s_k)|^2 c^2$, which is adapted to the filtration \mathcal{F}_k . Then, with probability at least $1 - \delta$, for any $n \geq 1$,

$$\begin{aligned} \sum_{k=1}^n E_k &\leq \frac{3}{4} \varrho \sum_{k=1}^n v_k^2 + \frac{1}{\varrho} \log \frac{1}{\delta} \\ &= \frac{3}{4} \varrho \sum_{k=1}^n \lambda_M^2 \gamma_{k+1}^2 |h(s_k)|^2 c^2 + \frac{1}{\varrho} \log \frac{1}{\delta} \\ &\leq \varrho \lambda_M^2 c^2 \sum_{k=1}^n \gamma_{k+1}^2 |h(s_k)|^2 + \frac{1}{\varrho} \log \frac{1}{\delta} , \end{aligned}$$

where we have only organized the constants in the last inequality.

B.2.3 Proof of Lemma 4

We now prove the Robbins-Siegmund Lemma. From the L_V -smoothness of the Lyapunov function by **N4**, we have for any $h \geq 0$,

$$\begin{aligned} V(s_{k+1}) &\leq V(s_k) + \gamma_{k+1} \langle \nabla V(s_k) | H(s_k, Z_{k+1}) \rangle + \frac{L_V \gamma_{k+1}^2}{2} |H(s_k, Z_{k+1})|^2 \\ &= V(s_k) + \gamma_{k+1} \langle \nabla V(s_k) | h(s_k) + \xi_k \rangle + \frac{L_V \gamma_{k+1}^2}{2} |h(s_k) + H(s_k, Z_{k+1}) - h(s_k)|^2, \end{aligned}$$

applying the inequality $|a+b|^2 \leq 2|a|^2 + 2|b|^2$,

$$\leq V(s_k) + \gamma_{k+1} \langle \nabla V(s_k) | h(s_k) + \xi_k \rangle + L_V \gamma_{k+1}^2 \left(|h(s_k)|^2 + |H(s_k, Z_{k+1}) - h(s_k)|^2 \right),$$

and applying **N1**,

$$\begin{aligned} &\leq V(s_k) + \gamma_{k+1} \langle \nabla V(s_k) | h(s_k) \rangle + \gamma_{k+1} \langle \nabla V(s_k) | \xi_k \rangle + L_V \gamma_{k+1}^2 |h(s_k)|^2 + L_V \gamma_{k+1}^2 \sigma^2 \\ &= V(s_k) + \underbrace{\gamma_{k+1} \langle \nabla V(s_k) | h(s_k) \rangle}_{\text{Mean-field dynamics}} + \underbrace{\gamma_{k+1} \langle \nabla V(s_k) | \xi_k \rangle}_{\text{MCMC bias dynamics}} + L_V \gamma_{k+1}^2 \left(|h(s_k)|^2 + \sigma^2 \right). \end{aligned}$$

For the bias dynamics, recall that the bias can be decomposed as

$$\xi_k = \underbrace{e_k}_{\text{non-asymptotic bias}} + \underbrace{\beta_k}_{\text{asymptotic bias}}.$$

Considering this, the bias dynamics can be decomposed as

$$\langle \nabla V(s_k) | \xi_k \rangle = \langle \nabla V(s_k) | e_k + \beta_k \rangle = \langle \nabla V(s_k) | e_k \rangle + \langle \nabla V(s_k) | \beta_k \rangle.$$

For the asymptotic bias, we have

$$\langle \nabla V(s_k) | \beta_k \rangle \leq |\nabla V(s_k)| |\beta_k|,$$

applying Lemma 1 and **N3**,

$$\leq \lambda_M |h(s_k)| \sqrt{\tau_0 + \tau_1} |h(s_k)|,$$

applying the inequality $\sqrt{a+b} \leq \sqrt{a} + \sqrt{b}$,

$$\leq \lambda_M \left(\sqrt{\tau_0} |h(s_k)| + \sqrt{\tau_1} |h(s_k)| \right)^2,$$

and the inequality $a \leq 1/2(1+a^2)$ for $a \geq 0$,

$$\leq \lambda_M \left\{ \frac{1}{2} \sqrt{\tau_0} + \left(\frac{1}{2} \sqrt{\tau_0} + \sqrt{\tau_1} \right) |h(s_k)|^2 \right\}.$$

Combining the results, we have

$$\begin{aligned} V(s_{k+1}) &\leq V(s_k) + \gamma_{k+1} \langle \nabla V(s_k) | h(s_k) \rangle + L_V \gamma_{k+1}^2 \left(|h(s_k)|^2 + \sigma^2 \right) \\ &\quad + \gamma_{k+1} \langle \nabla V(s_k) | e_k \rangle + \lambda_M \gamma_{k+1} \left(\frac{1}{2} \sqrt{\tau_0} + \left(\frac{1}{2} \sqrt{\tau_0} + \sqrt{\tau_1} \right) |h(s_k)|^2 \right) \\ &= V(s_k) + \gamma_{k+1} \langle \nabla V(s_k) | h(s_k) \rangle + \gamma_{k+1} \langle \nabla V(s_k) | e_k \rangle \\ &\quad + \left(\frac{1}{2} \lambda_M \sqrt{\tau_0} \gamma_{k+1} + L_V \sigma^2 \gamma_{k+1}^2 \right) + \left(\frac{1}{2} \lambda_M \sqrt{\tau_0} \gamma_{k+1} + \lambda_M \sqrt{\tau_1} \gamma_{k+1} + L_V \gamma_{k+1}^2 \right) |h(s_k)|^2. \end{aligned}$$

B.2.4 Proof of Theorem 2

From Lemma 4, we have for any $k \geq 0$,

$$-\gamma_{k+1} \langle \nabla V(s_k) | h(s_k) \rangle \leq V(s_k) - V(s_{k+1}) + \gamma_{k+1} \langle \nabla V(s_k) | e_k \rangle + a_k + b_k |h(s_k)|^2 .$$

Applying Lemma 1,

$$\gamma_{k+1} \lambda_m |h(s_k)|_2^2 \leq V(s_k) - V(s_{k+1}) + \gamma_{k+1} \langle \nabla V(s_k) | e_k \rangle + a_k + b_k |h(s_k)|^2 .$$

Summing this bound for $k = 0, \dots, n$ forms a telescoping sum as

$$\begin{aligned} & \lambda_m \sum_{k=0}^n \gamma_{k+1} |h(s_k)|_2^2 \\ & \leq V(s_0) - V(s_{n+1}) + \sum_{k=0}^n \gamma_{k+1} \langle \nabla V(s_k) | e_k \rangle + \sum_{k=0}^n a_k + \sum_{k=0}^n b_k |h(s_k)|^2 \\ & \leq V(s_0) - V^* + \underbrace{\sum_{k=0}^n \gamma_{k+1} \langle \nabla V(s_k) | e_k \rangle}_{\text{non-asymptotic bias dynamics}} + \sum_{k=0}^n a_k + \sum_{k=0}^n b_k |h(s_k)|^2 . \end{aligned}$$

Now, we focus on the non-asymptotic bias dynamics term. Karimi *et al.* (Karimi et al., 2019, Theorem 2) show that the sum of inner products can be decomposed as

$$-\sum_{k=0}^n \gamma_{k+1} \langle \nabla V(s_k) | e_k \rangle = A_1 + A_2 + A_3 + A_4 + A_5 ,$$

where the terms are

$$\begin{aligned} A_1 &= -\sum_{k=1}^n \gamma_{k+1} \langle \nabla V(s_k) | \nu_{s_k}^\eta(Z_{k+1}) - \Pi_{s_k}^\eta \nu_{s_k}^\eta(Z_k) \rangle , \\ A_2 &= -\sum_{k=1}^n \gamma_{k+1} \langle \nabla V(s_k) | \Pi_{s_k}^\eta \nu_{s_k}^\eta(Z_k) - \Pi_{s_{k-1}}^\eta \nu_{s_{k-1}}^\eta(Z_k) \rangle , \\ A_3 &= -\sum_{k=1}^n \gamma_{k+1} \langle \nabla V(s_k) - \nabla V(s_{k-1}) | \Pi_{s_{k-1}}^\eta \nu_{s_{k-1}}^\eta(Z_k) \rangle , \\ A_4 &= -\sum_{k=1}^n (\gamma_{k+1} - \gamma_k) \langle \nabla V(s_{k-1}) | \Pi_{s_{k-1}}^\eta \nu_{s_{k-1}}^\eta(Z_k) \rangle , \\ A_5 &= -\gamma_1 \langle \nabla V(s_0) | \Pi_{s_0}^\eta \nu_{s_{k-1}}^\eta(z_1) \rangle + \gamma_{n-1} \langle \nabla V(s_{n-1}) | \Pi_{s_{n-1}}^\eta \nu_{s_{n-1}}^\eta(z_n) \rangle . \end{aligned}$$

A_1 is given by Lemma 7 where we set $\varrho = 1$ and use that $c \leq 2L_\nu^{(0)}$. On the other hand, for A_2, A_3, A_4, A_5 , we can use the results in the proof of (Karimi et al., 2019, Theorem 2) by setting

$$\begin{aligned} c_0 &= 0, \quad c_1 = \lambda_m, \quad d_0 = 0, \quad d_1 = \lambda_M, \\ L &= L_V, \quad L_{\text{PH}}^{(0)} = L_\nu^{(0)}, \quad L_{\text{PH}}^{(1)} = L_\nu^{(1)}. \end{aligned}$$

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

$$\begin{aligned} A_1 &\leq (2\lambda_M L_\nu^{(0)})^2 \sum_{k=1}^n \gamma_{k+1}^2 |h(s_k)|^2 + \log \frac{1}{\delta} , \\ A_2 &\leq L_\nu^{(1)} \lambda_M \left(\sigma \sum_{k=1}^n \gamma_k^2 + \left(\frac{1}{2} + \alpha_1 \sigma + \alpha_1 \frac{1}{2} \right) \sum_{k=0}^n \gamma_k^2 |h(s_k)|^2 \right) , \end{aligned}$$

$$\begin{aligned}
 A_3 &\leq L_V L_\nu^{(0)} \left((1 + \sigma) \sum_{k=1}^n \gamma_k^2 + \sum_{k=1}^n \gamma_k^2 |h(s_{k-1})|^2 \right) \\
 &\leq L_V L_\nu^{(0)} \left((1 + \sigma) \sum_{k=1}^n \gamma_k^2 + \sum_{k=0}^n \gamma_{k+1}^2 |h(s_k)|^2 \right), \\
 A_4 &\leq L_\nu^{(0)} \left((\gamma_0 - \gamma_n) + \alpha_2 \lambda_M \sum_{k=1}^n \gamma_k^2 |h(s_{k-1})|^2 \right) \\
 &\leq L_\nu^{(0)} \left(\gamma_0 + \alpha_2 \lambda_M \sum_{k=0}^n \gamma_{k+1}^2 |h(s_k)|^2 \right), \\
 A_5 &\leq L_\nu^{(0)} \lambda_M \left(2 + \sum_{k=0}^n \gamma_k^2 |h(s_k)|^2 \right).
 \end{aligned}$$

By reorganizing the terms,

$$\sum_{k=0}^n \gamma_{k+1} (\lambda_m - C_{b_1} - C_{n_1} \gamma_{k+1}) |h(s_k)|^2 \leq V(s_0) - V^* + C_{n_2} \sum_{k=0}^n \gamma_{k+1}^2 + C_0 + \log \frac{1}{\delta} + C_{b_2} \sum_{k=0}^n \gamma_{k+1}.$$

From this, we obtain the condition on the stepsize that $\gamma_{k+1} \leq (\lambda_m - C_{b_1})/C_{n_1}$ for all $k = 0, \dots, n$. Furthermore, constant progress can be guaranteed by further enforcing $\gamma_{k+1} \leq \frac{1}{2}(\lambda_m - C_{b_1})/C_{n_1}$. Then, since $\gamma_{k+1} \leq \gamma_k$, the following inequalities hold:

$$\sum_{k=0}^n \gamma_{k+1} |h(s_k)|^2 \leq \frac{2}{\lambda_m - C_{b_1}} \left(V(s_0) - V^* + C_{n_2} \sum_{k=0}^n \gamma_{k+1}^2 + C_0 + \log \frac{1}{\delta} + C_{b_2} \sum_{k=0}^n \gamma_{k+1} \right).$$

Finally, dividing both sides by $\sum_{k=0}^n \gamma_{k+1}$, we have

$$\frac{1}{\sum_{k=0}^n \gamma_{k+1}} \sum_{k=0}^n \gamma_{k+1} |h(s_k)|^2 \leq \frac{2}{\lambda_m - C_{b_1}} \left(\frac{V(s_0) - V^* + C_{n_2} \sum_{k=0}^n \gamma_{k+1}^2 + C_0 + \log \frac{1}{\delta}}{\sum_{k=0}^n \gamma_{k+1}} + C_{b_2} \right).$$

Since the lower bound forms a weighted average, lower bounding it with the minimum over the iterates yields the result.

C COMPUTATIONAL RESOURCES

Table 3: Computational Resources

Type	Model and Specifications
System Topology	1 socket with 8 physical cores
Processor	1 Intel i9-11900F, 2.5 GHz (maximum 5.2 GHz) per socket
Cache	80 KB L1, 512 KB L2, and 16 MB L3
Memory	64 GiB RAM

All experiments took about 50 hours to complete.