Adaptive Non-reversible Stochastic Gradient Langevin Dynamics

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Abstract

It is well known that adding any skew symmetric matrix to the gradient of Langevin dynamics algorithm results in a non-reversible diffusion with improved convergence rate. This paper presents a gradient algorithm to adaptively optimize the choice of the skew symmetric matrix. The resulting algorithm involves a non-reversible diffusion algorithm cross coupled with a stochastic gradient algorithm that adapts the skew symmetric matrix. The algorithm uses the same data as the classical Langevin algorithm. A weak convergence proof is given for the optimality of the choice of the skew symmetric matrix. The improved convergence rate of the algorithm is illustrated numerically in Bayesian learning and tracking examples.

Keywords. Langevin dynamics, non reversible dynamics, skew symmetric matrix, stochastic gradient algorithm, weak convergence, adaptive Bayesian learning

I. INTRODUCTION

Langevin dynamics are used for global stochastic optimization (see for example [1], [2]) and also used as a non-parametric method for reconstructing (exploring) cost functions (such as posterior densities) from noisy evaluations of the gradient [3], [4]. The idea is as follows. Suppose \( C(\theta) \) is a continuously differentiable cost function on the interior of a compact set \( \Theta \subset \mathbb{R}^N \). Let \( \hat{\nabla}_\theta C(\theta_k) \) denote a noisy observation of the gradient \( \nabla \theta C(\theta_k) \) evaluated at point \( \theta_k \in \mathbb{R}^N \).

Then the classical stochastic gradient Langevin algorithm and its associated continuous-time Langevin diffusion process are, respectively

\[
\begin{align*}
\text{(Langevin algorithm)} & \quad \theta_{k+1} = \theta_k - \varepsilon \hat{\nabla}_\theta C(\theta_k) + \sqrt{\varepsilon} \frac{1}{\beta} w_k \\
\text{(Langevin diffusion)} & \quad d\theta(t) = -\nabla \theta C(\theta) dt + \frac{1}{\beta} dW(t), \quad t \geq 0,
\end{align*}
\]

In the Langevin algorithm (1), the step size \( \varepsilon \) is a small positive constant, \( \{w_k, k \geq 0\} \) is an i.i.d. sequence of standard \( N \)-variate Gaussian random variables, and \( \beta > 0 \) denotes the inverse temperature parameter. In the continuous-time Langevin diffusion process (2), \( W(t) \) denotes standard \( N \)-variate Brownian motion. The Langevin dynamics algorithm (1) is obtained by an Euler-Maruyama time discretization\(^1\) of the Langevin diffusion process (2).

It is straightforwardly shown that the stationary distribution of the Langevin diffusion (2) is the Gibbs measure

\[
\pi(\theta) \propto \exp(-\beta C(\theta)). \tag{3}
\]

Therefore, Langevin dynamics algorithm (1) leads to the following two immediate applications:

1) Reconstructing costs and Bayesian Learning. For fixed \( \beta \), let \( \hat{\pi}(\theta) \) denote the empirical density function constructed from samples \( \{\theta_k\} \) generated by the Langevin dynamics (1). Then clearly \( \log \hat{\pi}(\theta) \propto C(\theta) \). Thus the Langevin dynamics algorithm serves as a non-parametric method for reconstructing (exploring) \( C(\theta) \) given the gradient estimates \( \{\hat{\nabla}_\theta C(\theta_k)\} \).

Specifically, this is useful in Bayesian learning [3] where \( C(\theta) \) is the expectation of the posterior density; in such cases computing the posterior can be difficult due to the normalization factor; yet it is easy to simulate noisy gradients from the product of the likelihood and the prior.

2) Global Optimization. For sufficiently large \( \beta \), using Laplace asymptotics, it can be shown that the Gibbs distribution \( \pi \) in (3) concentrates around the global minimizers of \( C(\theta) \). So for large \( \beta \), the Langevin dynamics algorithm (1) serves as a global minimization algorithm for non-convex cost \( C(\theta) \).

Motivation. Accelerated Non-reversible Diffusions

The Langevin dynamics (2) is a reversible diffusion process. However, the convergence rate to the stationary distribution \( \pi(\cdot) \) can be slow. It is well known [5], [6], [7] that adding any skew symmetric matrix to the gradient always improves the

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\(^1\)In the opposite direction, it is well known that the interpolated process constructed from (1) converges weakly to (2).
convergence rate of Langevin dynamics to its stationary distribution. That is, for any $N \times N$ skew symmetric matrix\(^2 \) $S$, the non-reversible accelerated diffusion is

\[
\text{(Accelerated Diffusion)} \quad d\theta(t) = -(I + S)\nabla C(\theta)dt + \sqrt{\frac{2}{\beta}} dW(t), \quad t \geq 0,
\]

has a large spectral gap and therefore converges to the same stationary distribution $\pi(\theta)$ faster than (2); see [5], [6], [7] for a formal proof. The accelerated resulting gradient algorithm obtained by a Euler-Maruyama time discretization of (4) is

\[
\text{(Accelerated Algorithm)} \quad \theta_{k+1} = \theta_k - \varepsilon [I + S] \nabla C_k(\theta_k) + \sqrt{\varepsilon} \sqrt{\frac{2}{\beta}} w_k
\]

**Main idea**

The natural question is: How to choose skew symmetric matrix $S$ in the accelerated algorithm (5)? In this context, the main idea of the paper is two fold:

1) Our first result is to construct an adaptive version of the above non-reversible diffusion by adapting the skew symmetric matrix $S$. In simple terms, we adapt skew symmetric matrix $S$ in real time via a stochastic gradient algorithm, so that it converges to a local optimum. Thus the algorithm comprises a non-reversible diffusion (5) cross-coupled with another stochastic gradient algorithm that updates the skew symmetric matrix $S_k$ at each time $k$.

Actually we propose 3 different non-reversible diffusion algorithms in Sec.II; a Hessian based algorithm, and types of finite difference simultaneous perturbation stochastic approximation (SPSA) algorithms (which are computationally more efficient than the Hessian based algorithm). SPSA has been used as finite efficient difference method for evaluating gradient estimates in classical stochastic gradient algorithms [8]. To the best of our knowledge, SPSA has not been used in the context of Lagenvin dynamics. In extensive numerical studies (including real datasets) we show that all 3 algorithms always perform better than the vanilla non-reversible diffusion algorithm (5).

2) Our second result is a tracking analysis for non-stationary global stochastic optimization; we show that the algorithm can track a time-varying global optimum that jump changes according to a slowly varying Markov chain. Specifically, we are interested in tracking the global minimum of a non-convex stochastic optimization problem when the minimum jumps (evolves) over time according to the sample path of an unknown Markov chain. Specifically, we analyze how well does a fixed step size stochastic gradient Langevin algorithm (and generalized Langevin algorithms where the variance of the injected noise is adapted over time) track the time evolving global minima when the algorithm does not have knowledge of the Markovian evolution of the minima.

**Context**

For the case $C(\theta)$ is quadratic in $\theta$, [7] gives an algorithm to choose the optimal skew symmetric $S$ to maximize the spectral gap of the diffusion (4). However, for general costs $C(\cdot)$ there is no obvious way of maximizing the spectral gap. Our idea of adapting the skew symmetric matrix in a non-reversible diffusion, stems from [9], [10] where stochastic gradient algorithms were proposed for adapting the step size of a stochastic gradient algorithm. Indeed, the idea of using a stochastic gradient algorithm to update the step size was proposed originally as an exercise in [10, Exercise 4.4.2] in the context of least squares (LMS) algorithms. Such adaptive step size LMS algorithms have been shown to perform extremely well in wireless communication applications [11], [12]. Of course, the setup in the current paper is different since we are adapting a skew symmetric matrix to accelerate a non-reversible diffusion process (rather than adapting the scalar step size for a classical LMS algorithm).

An important feature of adaptive non-reversible diffusion algorithms (Algorithms 1, 2 and 3 proposed in this paper) is the constant step size $\varepsilon$ (as opposed to a decreasing step size). This facilitates estimating (tracking) parameters that evolve over time. Sec.V gives a formal weak convergence analysis of the asymptotic tracking capability of algorithm (6) when the cost $C(\cdot)$ jump changes over time according to a slow (but unknown) Markov chain. The most interesting case considered in Sec.V is when the reward changes at the same rate as the algorithm. Then stochastic averaging theory yields a Markov switched diffusion limit as the asymptotic behavior of the algorithm. Due to the constant step size, the appropriate notion of convergence is weak convergence [13], [14], [15]. The Markovian hyper-parameter tracking analysis generalizes our earlier work [16], [17] in stochastic gradient algorithms to the current case of Langevin dynamics.

Most existing literature analyzes stochastic approximation algorithms for tracking a parameter that evolves according to a “slowly time-varying” sample path of a continuous-valued process so that the parameter changes by small amounts over small intervals of time. When the rate of change of the underlying parameter is slower than the adaptation rate of the stochastic approximation algorithm (e.g., a slow random walk), the mean square tracking error can be analyzed as in [10], [13], [18], [19]. In comparison, our analysis covers the case where the global optimum evolves with discrete jumps that can be arbitrarily

\(^2\)Recall $S$ is skew symmetric if $S' = -S$. Clearly the diagonal elements of a skew symmetric matrix are zero; also $x'Sx = 0$ for all $x \in \mathbb{R}^N$. 
large in magnitude on short intervals of time. Also, the jumps can occur on the same time scale as the speed of adaptation of the stochastic approximation algorithm. Two-time scale and singularly perturbed jump Markov systems are studied in [20].

Finally, we mention that [21], [22] study convergence of the Langevin dynamics stochastic gradient algorithm in a non-asymptotic setting. Although the setting in our paper is asymptotic, it is interest in future work to study the non-asymptotic setting.

II. ADAPTIVE NON-REVERSIBLE DIFFUSION ALGORITHMS

The key idea behind the adaptive algorithms below is to parametrize $\theta$ by $S$; denote this as $\theta(S)$. Then one can pose a stochastic optimization problem to find the skew symmetric matrix $S^*$ to minimize $C(\theta(S))$. In this section we propose three adaptive algorithms to adapt $S$; a Hessian based algorithm (Algorithm 1), a SPSA algorithm (Algorithm 2), and a two-time scale SPSA algorithm (Algorithm 3). From a practical point of view, the SPSA algorithm is numerically efficient and yields results comparable to the more expensive Hessian based algorithm.

A. Algorithm 1. Hessian Based Adaptive Diffusion

Let $\varepsilon, \alpha$ be small non-negative fixed step sizes with $\alpha = o(\varepsilon)$. Let $e_i$ denote the unit vector with 1 in the $i$-th position. Then the algorithm is as follows:

$$
\begin{align*}
\theta_{k+1} &= \theta_k - \varepsilon (I + S_k) \nabla \theta c_k(\theta_k) + \sqrt{\frac{2}{\beta}} w_k \quad (6a) \\
S_{k+1}(i, j) &= S(k, i) - \alpha \nabla^2 \theta c_k(\theta_k) D_k(i, j) \bigg|_{S^{-}, i > j} \quad (6b) \\
S_{k+1}(i, j) &= -S_{k+1}(j, i), \quad i < j, \quad S_{k+1}(i, i) = 0 \quad (6c) \\
D_{k+1}(i, j) &= D(k, i, j) - \varepsilon (I + S_k) \nabla^2 \theta^2 c_k(\theta_k) D_k(i, j) - \varepsilon (e_j - e_i)' \nabla \theta c_k(\theta_k) \quad (6d)
\end{align*}
$$

Eq.(6a) is simply the non-reversible diffusion (5) with injected noise $w_k$. Recall $\beta > 0$ is the inverse temperature parameter and $S_k$ is a $N \times N$ skew symmetric matrix. In (6b), $S_0$ is initialized to an arbitrary skew symmetric matrix. The notation $[S^{+}]$ indicates that the estimate $S_{k}(i, j)$ is projected onto the closed interval $[S^{-}, S^{+}]$ if the estimate lies outside this region.

The recursion (6b) can be viewed as a stochastic gradient algorithm with step size $\alpha$ to minimize the cost $C(\theta(S))$ wrt $S$. Formally, the gradient

$$
\nabla S_{(i, j)} C = \left[ \nabla \theta C \right]' \frac{d\theta}{dS(i, j)}
$$

so that an estimate of the gradient $\hat{\nabla} S_{(i, j)} C(\theta_k)$ is $\hat{\nabla}^\theta c_k(\theta_k) D_k(i, j)$ where $D_k(i, j) = \frac{\partial}{\partial S(i, j)}$.

The third equation (6c) enforces that $S_k$ is skew symmetric, namely $S_k^t = -S_k$.

The final recursion (6d) is obtained by taking the “derivative” of the first recursion with respect to $S$ by defining the vector $D_k(i, j) = \frac{\partial}{\partial S(i, j)} \in \mathbb{R}^N$ by holding $S$ fixed. Then differentiating (6a) wrt $S(i, j)$ yields

$$
D_{k+1}(i, j) = D(k, i, j) - \varepsilon (I + S_k) \frac{\partial}{\partial S(i, j)} \nabla \theta c_k(\theta_k) - \varepsilon \frac{dS_k}{dS(i, j)} \nabla \theta c_k(\theta_k)
$$

and

$$
\frac{\partial}{\partial S(i, j)} \nabla \theta c_k(\theta_k) = \nabla^2 \theta c_k(\theta_k) \frac{d\theta}{dS(i, j)} \frac{dS_k}{dS(i, j)} = (e_j - e_i)
$$

Note that (6d) involves the Hessian $\nabla^2 \theta c_k(\theta_k)$.

Formally, the process $D_k$ in (6d) is interpreted as the derivative $(d/dS)\theta|\theta=\theta_k$. This derivative process is defined in the mean square sense as in [9, p. 1406]:

$$
\lim_{\Delta \to 0} \mathbb{E} \left| D - \frac{\theta(S + \Delta) - \theta(S)}{\Delta} \right|^2 = 0.
$$

In summary, the adaptive non-reversible diffusion algorithm (6) is given by cross coupling two stochastic gradient algorithms (first and second recursion) along with the derivative update of $\theta$ with respect to the parameter $S$ (final recursion). Note that when $S$ is a fixed constant, $S^+ = S^- = S$, then algorithm (6) reduces to the non reversible diffusion algorithm (5).
Main Convergence Result (Informal)

Since Algorithm 1 uses a constant step size (as opposed to a decreasing step size), the appropriate notion of convergence is weak convergence [13], [14], [15]. Recall that weak convergence is a function space generalization of convergence in distribution of random variables. The assumptions and main result will be stated formally and proved in Sec.IV. Here we give a heuristic statement. We will show that the sequence of estimates \{\theta_k\} generated by the Algorithm 1 converges weakly to a non-reversible accelerated diffusion with the optimal skew symmetric matrix. As is typically done in weak convergence analysis, we first represent the sequence of estimates \{\theta_k\} generated by Algorithm 1 as a continuous-time process. This is done by constructing the continuous-time trajectory via piecewise constant interpolation. Let \( T \) denote a positive real number which denotes the finite time horizon. For \( t \in [0, T] \), define the continuous-time piecewise constant interpolated processes parametrized by the step size \( \varepsilon \) as

\[
\theta^t(t) = \theta_k \quad \text{for} \quad t \in [\varepsilon k, \varepsilon k + \varepsilon)
\]

We can now state our main result

Informal Result 1: Under suitable assumptions (Sec.IV), the interpolated processes \((\theta^t(\cdot), D^t(\cdot), S^t(\cdot))\) converges weakly to \((\theta(\cdot), D(\cdot), S(\cdot))\) such that the limit satisfies the following system of equations

\[
\begin{align*}
\frac{d}{dt} \theta &= (I + S) \nabla C(\theta) + \sqrt{\frac{2}{\beta}} dW \\
\frac{d}{dt} D(i, j) &= (I + S) \nabla^2 C(\theta) D(i, j) - (e_j - e_i)' \nabla C(\theta) \\
\frac{d}{dt} S(i, j) &= \nabla C(\theta) D(i, j)|_{S^+}, \quad i > j
\end{align*}
\]

where \( W(\cdot) \) is \( N \)-dimensional Brownian motion. \( \square \)

The most important takeaway from the above result is that the skew symmetric matrix \( S \) satisfies the projected ordinary differential equation (ODE).

\[
\dot{S}(i, j) = -\frac{d}{dS(i, j)} C(\theta(S)), \quad S \in (S^-, S^+)
\]

Note that (8) implies that the adaptive algorithm for adjusting \( S \) is a gradient decent method. By the weak convergence, \( S_k \) will spend nearly all of the time in an arbitrarily small neighborhood of the local minima of \( \mathbb{E}\{c_k(\theta(S))\} \), which is consistent with our motivation for the adaptive non-reversible diffusion Algorithm 1.

B. Algorithm 2. SPSA based Adaptive Diffusion

An issue with Algorithm 1 is that the computational cost is \( O(N^4) \) which is excessive for large \( N \); this computational cost is due to the update (6d) which is \( O(N^2) \) for each \( i, j \). Also, evaluating the Hessian \( \nabla^2 c_k(\theta) \) can be difficult in some stochastic optimization problems. Examining (6), we see that the Hessian arises as a by-product of evaluating the gradient estimate \( \nabla c_k(\theta_k) \). Below we propose a finite difference evaluation of \( \nabla S c_k(\theta_k) \); this does not involve the Hessian. But a naive evaluation of the finite difference approximation to gradient \( \nabla S c_k(\theta_k) \) would require \( 2N^2 \) evaluations (simulations) of the cost; namely evaluate \( c_k(\theta(S + e_i)) \) and \( c_k(\theta(S - e_i)) \) for each component \((i, j)\) of \( S \). The main idea below is to evaluate this gradient estimate using the SPSA (simultaneous perturbation stochastic approximation) algorithm [8]. The SPSA algorithm picks two random matrices \( S_k + \mu \Delta_k \) and \( S_k - \mu \Delta_k \) to evaluate \( \nabla S c_k(\theta_k) \) and therefore requires only 2 evaluations (simulations) of the cost \( c_k(\cdot) \).

Let \( \varepsilon, \mu, \alpha \) be small non-negative fixed step sizes. We propose the following SPSA based algorithm that does not require computation of the Hessian

\[
\begin{align*}
\theta^+_{k+1} &= \theta^-_k - \varepsilon \left( I + S_k + \mu \Delta_k \right) \nabla \theta c_k(\theta^-_k) + \sqrt{\varepsilon} \sqrt{\frac{2}{\beta}} w_k \\
\theta^-_{k+1} &= \theta^+_k - \varepsilon \left( I + S_k - \mu \Delta_k \right) \nabla \theta c_k(\theta^+_k) + \sqrt{\varepsilon} \sqrt{\frac{2}{\beta}} w_k \\
S_{k+1}(i, j) &= S_k(i, j) - \alpha \frac{c_k(\theta^+_k) - c_k(\theta^-_k)}{2 \mu \Delta_k} \\
\Delta_k(i, j) &= \begin{cases} -1 & \text{w. p. 0.5} \\
1 & \text{w. p. 0.5} \end{cases}, \quad i > j \quad \Delta_k(i, j) = -\Delta_k(j, i), \quad i < j
\end{align*}
\]

Here the elements of the matrix \( \Delta_k \) are simulated as follows: \( \Delta_k(i, i) = 0 \)

\[
\Delta_k(i, j) = \begin{cases} -1 & \text{w. p. 0.5} \\
1 & \text{w. p. 0.5} \end{cases}, \quad i > j, \quad \Delta_k(i, j) = -\Delta_k(j, i), \quad i < j
\]

Note \( S_k + \mu \Delta_k \) and \( S_k - \mu \Delta_k \) are skew symmetric matrices by construction.

Algorithm 2 has computational cost of \( O(N^2) \) at each iteration.
C. Algorithm 3. Two time scale SPSA Adaptive Diffusion

Algorithm 2 discussed above simultaneously evaluates the gradient and updates the estimates in one time step. In comparison, we now construct a two-time scale algorithm that proceeds as follows:

Run the following recursion on the slow time scale \( k = 1, 2, \ldots, \)

\[
\theta_{k+1} = \theta_k - \varepsilon (I + S_k) \nabla \theta c_k(\theta_k) + \sqrt{\frac{2}{\beta}} w_k
\]

(11)

and simulate \( \Delta_k \) according to (10). Then for each \( k \), run multiple steps \( n = 0, \ldots, N \) on the fast time scale to evaluate the estimate \( D_k \) of the gradient of \( c_k(\theta) \) wrt \( S_k \): Initialize \( \theta_0^+ = \theta_0^- = \theta_k \) and

\[
\begin{align*}
\theta_{n+1}^+ &= \theta_n^+ - \varepsilon (I + S_k + \mu \Delta_k) \nabla \theta c_n(\theta_n^+) + \sqrt{\varepsilon} \sqrt{\frac{2}{\beta}} w_n \\
\theta_{n+1}^- &= \theta_n^- - \varepsilon (I + S_k - \mu \Delta_k) \nabla \theta c_n(\theta_n^-) + \sqrt{\varepsilon} \sqrt{\frac{2}{\beta}} w_n \\
D_{n+1}(i,j) &= D_n(i,j) + \frac{c_n(\theta^+) - c_n(\theta^-)}{2 \mu \Delta_n(i,j)}
\end{align*}
\]

(12)

Finally, update \( S \) in (11) on the slow time scale as

\[
S_{k+1}(i,j) = S_k(i,j) - \alpha D_N(i,j)
\]

(13)

Note that in the special case where (11) is omitted and (12) is run for one step, Algorithm 3 specializes to Algorithm 2.

III. Numerical Examples. Adaptive KL Divergence and Bayesian Learning

This section compares the performance of our proposed non-reversible diffusion algorithms (Algorithms 1, 2 and 3) to the classical Langevin algorithm in numerical examples. We present with a low dimensional KL divergence/Bayesian learning problem \((N = 2)\) and then a larger \(N = 10\) dimensional problem. In both cases, we show that Algorithms 1 and 2 converge faster than the accelerated non-reversible diffusion (5); which in turn converges faster than the classical Langevin (1).

A. Estimating KL Divergence

The aim is to use the adaptive algorithms proposed above to explore and reconstruct high value regions of the KL divergence of the posterior. As will be discussed below, a special case of this setup is Bayesian learning discussed in [3], where the algorithms explore high probability regions of the posterior distribution.

Let \( \theta^0 \in \mathbb{R}^N \) denote a true parameter value (which is unknown to the algorithm). Let \( \theta \in \mathbb{R}^N \) denote a random variable with known prior distribution \( p(\theta) \). A sequence of independent observation random variables\(^3\) \( \{Y_k\} \), are generated from a known likelihood \( p(y|\theta^0) \). The KL divergence of a sequence of \( T \) observations is

\[
K(\theta^0, \theta) = -\mathbb{E}_{\theta^0}\{\log \frac{p(\theta|Y_1, \ldots, Y_T)}{p(\theta^0|Y_1, \ldots, Y_T)}\}
\]

(14)

Given the observation sequence \( \{y_k\} \), suppose we use the proposed algorithms on expected cost

\[
C(\theta) = -\mathbb{E}_{\theta^0}\{\log p(\theta, Y_1, \ldots, Y_T)\} = \int \log p(\theta, y_1, \ldots, y_T) p(y_1, \ldots, y_T|\theta^0) dy_1, \ldots dy_T
\]

(15)

A naive implementation of the unbiased gradient estimate is \( \nabla_\theta \log p(\theta, y_1, \ldots, y_T); \) this uses batches of observations of length \( T \) from the sequence \( \{y_k\} \). However, since the observations \( y_k \) are iid, we can instead use a single observation \( y_k \) at each time \( k \) as an unbiased sample path gradient of the cost:

\[
\nabla_\theta c_k(\theta_k) = -\nabla_\theta \log p(\theta_k) - T \nabla_\theta \log p(y_k|\theta_k)
\]

(16)

With this setup, suppose the Langevin dynamics or any of the proposed algorithms above, are run on the observation sequence \( \{y_k\} \), generated from the likelihood \( p(y|\theta^0) \). Then, clearly the algorithms asymptotically generate samples \( \{\theta_k\} \) from the stationary distribution (3), namely

\[
\pi(\theta) \propto \exp(-C(\theta)) \propto \exp(K(\theta^0, \theta))
\]

where the proportionality constant involves terms independent of \( \theta \).

To summarize, the Langevin dynamics algorithm and non-reversible diffusion algorithms (Algorithms 1, 2 and 3) operating on observations \( \{y_k\} \) can be used with gradient estimate \( \nabla_\theta c_k(\theta_k) \) in (16) to estimate the KL divergence. Specifically if the empirical histogram \( \hat{\pi}(\theta) \) is constructed from the samples \( \{\theta_k\} \) generated by the various algorithms, then \( \log \hat{\pi}(\theta) \propto K(\theta^0, \theta) \).

\(^3\)In this section, we use upper case \( Y \) for random variables and lower case \( y \) for their realization.
Remark. Bayesian Learning: Bayesian learning described in [3] is a special case of the above setup. It deals with exploring high probability regions of a posterior density.

To summarize, the Langevin dynamics algorithm and non-reversible diffusion algorithms (Algorithms 1, 2 and 3) operating on algorithms asymptotically generate samples \( \{ \theta_k \} \) from the stationary distribution (3), namely

\[
\pi(\theta) \propto \exp(-\mathcal{C}(\theta)) = p(\theta|y_1, \ldots, y_T)
\]

To summarize, the Langevin dynamics algorithm and any of the adaptive algorithms proposed above, are run on the augmented dataset \( z = y_1, \ldots, y_T, y_1, \ldots, y_T, \ldots \). Note the augmented dataset comprises multiple repetitions of \( y_1, \ldots, y_T \). Then the algorithms asymptotically generate samples \( \{ \theta_k \} \) from the stationary distribution (3), namely

\[
\pi(\theta) \propto \exp(-\bar{\mathcal{C}}(\theta)) = p(\theta|y_1, \ldots, y_T)
\]

Suppose the Langevin dynamics algorithm or any of the adaptive algorithms proposed above, are run on the augmented dataset \( z \) can be used with gradient estimate \( \bar{\nabla}_{\theta}c_k(\theta_k) \) evaluated in (16) for \( k \in 1, \ldots, T \) is a noisy unbiased estimate of \( \bar{\mathcal{C}}(\theta) \).

Example 1. Bayesian Learning

Here we consider the case \( N = 2 \), \( \theta = [\theta(1), \theta(2)]^T \),

\[
y_k \sim \frac{1}{2} \mathcal{N}(\theta(1), \sqrt{2}) + \frac{1}{2} \mathcal{N}(\theta(1) + \theta(2), \sqrt{2})
\]

\[
\theta(1) \sim \mathcal{N}(0, \sqrt{10}), \quad \theta(2) \sim \mathcal{N}(0, 1)
\]

(17)

For true parameter value \( \theta^* = [0, 1] \), it can be verified that the objective \( -\mathcal{C}(\theta) \) is non-concave in \( \theta \) and has two maxima at \( \theta = [0, 1] \) and \( \theta = [1, -1] \).

To illustrate the posterior \( p(\theta|y_1, \ldots, y_T) \) visually, Figure 1 plots the empirical density and contours of \( p(\theta|y_1, \ldots, y_T) \), \( \theta \in \mathbb{R}^2 \), for \( T = 100 \) using the Metropolis Hastings algorithm.

![Fig. 1: Metropolis Hastings simulation of posterior distribution \( p(\theta|y_1, \ldots, y_T) \), \( T = 100 \).](image)

The augmented dataset \( z \) was generated as 1000 repetitions of \( y_1, \ldots, y_{100} \); so \( z \) has \( 10^5 \) points. We ran the Langevin dynamics algorithm, accelerated algorithm and Algorithms 1, 2 and 3 with \( \beta = 1 \) over augmented dataset \( z \) for 30 independent trials each with initial condition \( \theta_0 = [4, 4] \). Each trial has a different sample path of the injected noise \( \{ w_k \} \). The \( 2 \times 2 \) skew symmetric matrix was initialized as \( S_0 = \begin{bmatrix} 0 & -s \\ s & 0 \end{bmatrix} \) where \( s \sim \mathcal{N}(0, 1) \).

Figure 2 displays the estimated posterior means \( \mathbb{E}\{ \theta(i)|y_1, \ldots, y_{100} \} \), \( i = 1, 2 \). As can be seen from Figure 2, Algorithms 1, 2, and 3 converges faster than the accelerated algorithm, which in turn converges faster than the classical Langevin.

In [3] this is termed as running the algorithms on multiple sweeps of \( y_1, \ldots, y_T \). Also [3] uses a decreasing step size algorithm.
Fig. 2: $N = 2$. Comparison of posterior means $\mathbb{E}\{\theta(i)|y_1, \ldots, y_{100}\}, i = 1, 2$ versus iterations for various algorithms.

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C. Example 2. Bayesian Learning $N = 10$

\[
\theta(i) \sim \mathcal{N}(\mu_i, \sigma_i^2), \quad \mu_i \sim \mathcal{U}[-2, 2], \quad \sigma_i^2 \sim \mathcal{U}[1, 10], \quad i \in \{1, \ldots, N\},
\]
\[
y_k \sim \frac{1}{2} \mathcal{N}\left(\sum_{i=1}^{N/2} \theta(i), \sqrt{2}\right) + \frac{1}{2} \mathcal{N}\left(\sum_{j=\frac{N}{2}+1}^{N} \theta(j), \sqrt{2}\right)
\]

As in the previous example the aim is to reconstruct the posterior $p(\theta|y_1, \ldots, y_{100})$.

First, the Metropolis Hastings algorithm was used to generate samples from the posterior. We view the estimates from the Metropolis Hastings as the ground truth.

Next we implemented the classical Langevin algorithm, accelerated algorithm and adaptive algorithms. In the accelerated algorithm and Algorithms 1, 2, the skew symmetric matrix $S_0$ was initialized as a tri-diagonal matrix with elements above the diagonal chosen as $\mathcal{N}(0, 1)$ random variables, and elements below the diagonal chosen as the negative of these. The augmented dataset $z$ was generated as $10^4$ repetitions of $y_1, \ldots, y_{100}$; so $z$ has $10^6$ points. Each algorithm was run for 50 independent trials with step sizes $\varepsilon = 10^{-4}, \alpha = 10^{-4}$.

The posterior $p(\theta|y_1, \ldots, y_{100})$ is a 10-variate distribution. Figure 3 shows the posterior mean estimates of the first two marginals, computed for the various algorithms. Also shown are the $L_1$ distances of these marginals to that of the Metropolis Hastings algorithm. The $L_1$ distance (Wasserstein 1-metric) for the first two marginals is

\[
d(i) = \int |\hat{F}_i(\alpha(i)) - F_i(\alpha(i))| \, d\alpha(i), \quad i = 1, 2
\]

where $F_i$ is the cumulative distribution of marginal $i$ constructed via Metropolis Hastings (ground truth) and $\hat{F}_i$ is the empirical cumulative distribution constructed by the Langevin or adaptive algorithm.

The $L_1$ distance is more appropriate for our purposes than the Kolmogorov-Smirnov distance since typically the constant or proportionality $\beta$ is not known and so the regions of support of the empirical cdfs can vary substantially.

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IV. WEAK CONVERGENCE ANALYSIS

V. NON-STATIONARY GLOBAL OPTIMIZATION AND TRACKING ANALYSIS

Our next main result concerns estimating a time evolving global minimum in a non-stationary global stochastic optimization problem. Alternatively, we use to use non-reversible diffusion based algorithms to explore and track a time evolving expected cost. Since we are estimating (tracking) a time evolving global minimum/cost, we first give a model for the evolution. Below, the Markov chain $\{x_k\}$ will be used as a hyper-parameter to model the evolution of the global minimum. By hyper-parameter we mean that the Markov chain model is not known or used by the algorithms. The Markov chain assumption is used only for our convergence analysis to determine how well does our proposed algorithm estimates (tracks) a global minimum/expected cost that jump changes (evolves) according to an unknown Markov chain.
A. Non-stationary Stochastic Optimization Problem

In this section, we treat the problem minimization of an objective function in which the objective function is randomly changing within a finite set. Effectively, instead of one objective function, we have a finite number of objective functions to deal with. For the reason of mathematical convenience, we assume that the random changing behavior is modeled by a “slow” Markov chain \( \{x_k\} \) on the finite state space \( \mathcal{X} = \{1, \ldots, X\} \) and the one-step transition probability \( I + \alpha Q \). Here \( \alpha > 0 \) is a small parameter and \( Q = (q_{ij}) \) is a generator of a continuous-time Markov chain so that \( q_{ij} \geq 0 \) for \( i \neq j \) and \( \sum_j q_{ij} = 0 \) for each \( i \in \mathcal{X} \). We assume that \( Q \) is irreducible (see [23, p.23]). For notational convenience, we have chosen the states of the Markov chain to take integer values. This is no loss of generality.

With the above setup, we carry out an optimization problem of the form

\[
\theta_{x} \in \arg \min_{\theta \in \Theta \subset \mathbb{R}^N, x \in \mathcal{X}} c(\theta, x)
\]

where \( c(\theta, x) = \mathbb{E}_x \{ c(\theta, x, z) \} = \mathbb{E} \{ c(\theta, x, z) | x_k = x \} \),

where \( z \) is the observation. The above optimization is taken as conditional expectation conditioned on \( x_k = x \). Thus in lieu of one objective function, we have \( X \) objective functions. Thus equivalently, we are treating a time-varying tracking problem of tracking the time-varying minimizer.

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