Aggregated Gradient Langevin Dynamics

Chao Zhang\textsuperscript{1,2}, Jiahao Xie\textsuperscript{1}, Zebang Shen\textsuperscript{1,3}, Peilin Zhao\textsuperscript{3}, Tengfei Zhou\textsuperscript{1}, Hui Qian\textsuperscript{1}\textsuperscript{*}

\textsuperscript{1}College of Computer Science and Technology, Zhejiang University
\textsuperscript{2}AI Lab, Tencent
\textsuperscript{3}University of Pennsylvania

zcju@zju.edu.cn, xiejh@zju.edu.cn, shenziebang@zju.edu.cn, zhoutengfei@zju.edu.cn, qianhui@zju.edu.cn, masonzhao@tencent.com

Abstract

In this paper, we explore a general Aggregated Gradient Langevin Dynamics framework (AGLD) for the Markov Chain Monte Carlo (MCMC) sampling. We investigate the nonasymptotic convergence of AGLD with a unified analysis for different data accessing (e.g. random access, cyclic access and random reshuffle) and snapshot updating strategies, under convex and nonconvex settings respectively. It is the first time that bounds for I/O friendly strategies such as cyclic access and random reshuffle have been established in the MCMC literature. The theoretical results also indicate that methods in AGLD possess the merits of both the low per-iteration computational complexity and the short mixture time. Empirical studies demonstrate that our framework allows to derive novel schemes to generate high-quality samples for large-scale Bayesian posterior learning tasks.

1 Introduction

We focus on the Langevin dynamics based Markov Chain Monte Carlo (MCMC) methods for sampling the parameter vector $\theta \in \mathbb{R}^d$ from a target posterior distribution

\begin{equation}
p^* \triangleq p(\theta \mid \{z_i\}_{i=1}^{N}) \propto p(\theta) \prod_{i=1}^{N} p(z_i \mid \theta),
\end{equation}

where $p(\theta)$ is some prior of $\theta$, $z_i$'s are the data points observed, and $p(z_i \mid \theta)$ is the likelihood function. The Langevin dynamics Monte Carlo method (LMC) adopts the gradient of log-posterior in an iterative manner to drive the distribution of samples to the target distribution efficiently (Roberts and Stramer 2002; Roberts et al. 1996). To reduce the computational complexity for large-scale posterior learning tasks, the Stochastic Gradient Langevin Dynamics method (SGLD), which replaces the expensive full gradient with the stochastic gradient, has been proposed (Welling and Teh 2011). While such scheme enjoys a significantly reduced per-iteration cost, the mixture time, i.e., the total number of iterations required to achieve the correction from an out-of-equilibrium configuration to the target posterior distribution, is increased, due to the extra variance introduced by the approximation (Dalalyan and Karagulyan 2017; Dalalyan 2017b).

In recent years, efforts are made to design variance-control strategies to circumvent this slow convergence issue in the SGLD. In particular, borrowing ideas from variance reduction methods in the optimization literature (Johnson and Zhang 2013; Defazio et al. 2014; Lei and Jordan 2017), the variance-reduced SGLD variants exploit the high correlations between consecutive iterates to construct unbiased aggregated gradient approximations with less variance, which leads to better mixture time guarantees (Dubey et al. 2016; Zou et al. 2018b). Among these methods, SAGA-LD and SVRG-LD are proved to be the most effective ones when high-quality samples are required (Chatterji et al. 2018; Zou et al. 2019). While the nonasymptotic convergence guarantees for SVRG-LD and SAGA-LD have been established, it is difficult to seamlessly extend these analyses to cover other Langevin dynamics based MCMC methods with different efficient gradient approximations.

- First of all, different delicate Lyapunov functions are designed for SVRG-LD and SAGA-LD to prove the nonasymptotic convergence to the stationary distribution. Due to the different targets of optimization and MCMC, the mixture-time analysis is not a simple transition of the convergence rate analysis in optimization. The lack of a unified perspective of these variance-reduced SGLD algorithms makes it difficult to effectively explore other variance-reduced estimators used in optimization (e.g., HSAG (Reddi et al. 2015)) for Langevin dynamics based MCMC sampling. In particular, customized Lyapunov functions need to be designed if new variance-reduced estimators are adopted.

- Second, existing theoretical analysis relies heavily on the randomness of the data accessing strategy to construct an unbiased estimator of the true gradient. In practice, the random access strategy entails heavy I/O cost when the dataset is too large to fit into memory, thereby renders existing incremental Langevin dynamics based MCMC algorithms heavily impractical for sampling tasks in the big data scenario. While other data accessing strategies such

\textsuperscript{*}Corresponding Author
as cyclic access and random reshuffle are known to be I/O friendly [Xie et al. 2018], existing analysis can not be directly extended to algorithms with these strategies.

**Contributions** Motivated by such imperatives, we propose a general framework named Aggregated Gradient Langevin Dynamics (AGLD), which maintains a historical snapshot set of the gradient to construct more accurate gradient approximations than that used in SGLD. AGLD possesses a three-step structure: Data-Accessing, Sample-Searching, and Snapshot-Updating. Different Data-Accessing (e.g., random access, cyclic access and random reshuffle) and Snapshot-Updating strategies can be utilized in this framework. By appropriately implementing these two steps, we can obtain several practical gradient approximations, including those used in existing methods like SVRG-LD and SAGA-LD. Under mild assumptions, a unified mixture-time analysis of AGLD is established, which holds as long as each component of the snapshot set is updated at least once in a fixed duration. We list our main contributions as follows.

- **First**, we analyze the mixture time of AGLD under the assumptions that the negative log-posterior $f(x)$ is smooth and strongly convex and then extend the analysis to the general convex case. We also provide theoretical analyses for nonconvex $f(x)$. These results indicate that AGLD has similar mixture time bounds as LMC under similar assumptions, while the per-iteration computation is much less than that of LMC. Moreover, the analysis provides a unified bound for a wide class of algorithms with no need to further design dedicated Lyapunov functions for different Data-Accessing and Snapshot-Updating strategies.

- **Second**, for the first time, mixture time guarantees for cyclic access and random reshuffle Data-Accessing strategies are provided in the Langevin dynamics based MCMC literature. This fills the gap of practical use and theoretical analyses, since cyclic access is I/O friendly and often used as a practical substitute for random access when the dataset is too large to fit into memory.

- **Third**, we develop a novel Snapshot-Updating strategy, named Time-based Mixture Updating (TMU), which enjoys the advantages of both the Snapshot-Updating strategies used in SVRG-LD and SAGA-LD: it always updates components in the snapshot set to newly computed ones as in SAGA-LD and also periodically updates the whole snapshot set to rule out the out-of-date ones as in SVRG-LD. Plugging TMU into AGLD, we derive novel algorithms to generate high-quality samples for Bayesian learning tasks.

Simulated and real-world experiments are conducted to validate our analysis. Numerical results on simulation and Bayesian posterior learning tasks demonstrate the advantages of proposed variants over the state-of-the-art.

**Notation.** We use $[N]$ to denote $\{1, \ldots, N\}$, use $\mathbf{1}_d$ to denote the $d$-dimensional vector with all entries being 1, and use $\mathbf{1}_{d \times d}$ to denote the $d$-dimensional identity matrix. For $a, b \in \mathbb{R}^+$, we use $a = \mathcal{O}(b)$ to denote $a \leq Cb$ for some $C > 0$, and use $a = \tilde{\mathcal{O}}(b)$ to hide some logarithmic terms of $b$. For the brevity of notation, we denote $f(\theta) = \sum_{i=1}^{N} f_i(\theta)$, where each $f_i(\theta) = -\log p(\theta|z_i) - \log p(\theta)/N$, for $i \in [N]$.

## 2 Preliminaries

### 2.1 Wasserstein Distance and Mixture Time

We use the $2$-Wasserstein ($\mathcal{W}_2$) distance to evaluate the effectiveness of our methods. Specifically, the $\mathcal{W}_2$ distance between two probability measures $\rho$ and $\nu$ is defined as

$$
\mathcal{W}_2^2(\rho, \nu) = \inf_{\pi \in \Pi(\rho, \nu)} \left\{ \int \|x - y\|^2 \text{d}\pi(x, y) \right\}.
$$

Here, $(x, y)$ are random variables with distribution density $\pi$ and $\Gamma(\rho, \nu)$ denotes the collection of joint distributions where the first part of the coordinates has $\rho$ as the marginal distribution and the second part has marginal $\nu$.

$\mathcal{W}_2$ distance is widely used in the dynamics based MCMC literature since it is a more suitable measurement of the closeness between two distributions than metrics like the total variation and the Kullback-Leibler divergence (Zou et al. 2018; Dalalyan 2017a). In this paper, we say $K$ is the $\epsilon$-mixture time of a Monte Carlo sampling procedure if for every $k \geq K$, the distribution $\rho(k)$ of the sample generated in the $k$-th iteration is $\epsilon$-close to the target distribution $p^*$ in $\mathcal{W}_2$-Wasserstein distance, i.e., $\mathcal{W}_2(\rho(k), p^*) \leq \epsilon$.

### 2.2 Stochastic Langevin Dynamics

By using the discretization of certain dynamics, dynamics based MCMC methods allow us to efficiently sample from the target distribution. A large portion of such works are based on the Langevin Dynamics (Parisi 1981)

$$
d\theta(t) = -\nabla f(\theta(t))dt + \sqrt{2}\text{d}B(t),
$$

where $\nabla f$ is called the drift term, $B(t)$ is a $d$-dimensional Brownian Motion and $\theta(t) \in \mathbb{R}^d$ is the state variable.

The classic Langevin dynamics Monte Carlo method (LMC) generates samples $\{x^{(k)}\}$ in the following manner:

$$
x^{(k+1)} = x^{(k)} - \eta \nabla f(x^{(k)}) + \sqrt{2}\eta \xi^{(k)},
$$

where $x^{(k)}$ is the time discretization of the continuous time dynamics $\theta(t), \eta$ is the stepsize and $\xi^{(k)} \sim \mathcal{N}(0, I_{d \times d})$ is the $d$-dimensional Gaussian variable. Due to the randomness of $\xi^{(k)}$, $x^{(k)}$ is a random variable and we denote its distribution as $p(k)$. $p(k)$ is shown to converge weakly to the target distribution $p^*$ (Dalalyan 2017a; Raginsky et al. 2017).

To alleviate the expensive full gradient computation in LMC, the Stochastic Gradient Langevin Dynamics (SGLD) replaces $\nabla f(x^{(k)})$ in (3) by the stochastic approximation

$$
g^{(k)} = \frac{N}{n} \sum_{i \in I_k} \nabla f_i(x^{(k)}),
$$

where $I_k$ is the set of $n$ indices independently and uniformly drawn from $[N]$ in iteration $k$. Although the gradient approximation is always an unbiased estimator of the full gradient, the non-diminishing variance results in the inefficiency of sample-space exploration and slows down the convergence to the target distribution.
To overcome such difficulty, SVRG-LD and SAGA-LD (Dubey et al. 2016; Chatterji et al. 2018; Zou et al. 2019) use the two different variance-reduced gradient estimators of $\nabla f(x)$, which utilize the component gradient information of the past samples. While possessing similar low per-iteration component gradient computation as in SGLD, the mixture time bound of SVRG-LD and SAGA-LD are shown to be similar to that of LMC under similar assumptions (Chatterji et al. 2018; Zou et al. 2019).

3 Aggregated Gradient Langevin Dynamics

In this section, we present our general framework named Aggregated Gradient Langevin Dynamics (AGLD). Specifically, AGLD maintains a snapshot set consisting of component gradients evaluated in historical iterates. The information in the snapshot set is used in each iteration to construct a gradient approximation which helps to generate the next iterate. Note that iterates generated during the procedure are samples of random variables, whose distributions converge to the target distribution. At the end of each iteration, the entries in the snapshot set are updated according to some strategy. By customizing the steps in AGLD with different strategies, we can derive different algorithms. Concretely, AGLD is comprised of the following three steps, where the first and third steps can accept different strategies as inputs.

1. **Data-Accessing:** select a subset of indices $S_k$ from $[N]$ according to the input strategy.
2. **Sample-Searching:** construct the aggregated gradient approximation $g^{(k)}$ using the data points indexed by $S_k$ and the historical snapshot set, then generate the next iterate (the new sample) by taking one step along the direction of $g^{(k)}$ with an injected Gaussian noise. Specifically, the $(k+1)$-th sample is obtained in the following manner

$$x^{(k+1)} = x^{(k)} - \eta g^{(k)} + \sqrt{2\eta} \xi^{(k)},$$

where $\xi^{(k)}$ is a Gaussian noise, $\eta$ is the stepsize, and

$$g^{(k)} = \sum_{i \in S_k} \frac{N}{n} (\nabla f_i(x^{(k)}) - \alpha_i^{(k)}) + \sum_{i = 1}^{N} \alpha_i^{(k)}.$$ (6)

3. **Snapshot-Updating:** update historical snapshot set according to the input strategy.

We summarize AGLD in Algorithm 1. While our mixture time analyses hold as long as the input Data-Accessing and Snapshot-Updating strategies meet Requirements 1 and 3, we describe in detail several typical qualified implementations of these two steps below.

3.1 The Data-Accessing Step

We make the following requirement on the Data-Accessing step to ensure the convergence of $\mathcal{W}_2$ distance between the sample distribution $p^{(k)}$ and the target distribution $p^*$.

**Requirement 1.** In every iteration, each point in the dataset has been visited at least once in the past $C$ iterations, where $C$ is some fixed positive constant.

**Algorithm 1 Aggregated Gradient Langevin Dynamics**

**Require:** initial iterate $x^{(0)}$, stepsize $\eta$, Data-Accessing strategy, and Snapshot-Updating strategy.

1. **Initialize** Snapshot set $\mathcal{A}^{(0)} = \{\alpha_i^{(0)}\}_{i=1}^{N}$, where $\alpha_i^{(0)} = \nabla f_i(x^{(0)})$.
2. for $k = 0$ to $K - 1$
3. $S_k = \text{Data-Accessing}(k)$.
4. **Sample-Searching:** find $x^{(k+1)}$ according to (5).
5. $\mathcal{A}^{(k+1)} = \text{Snapshot-Updating}(\mathcal{A}^{(k)}, x^{(k)}, k, S_k)$.
6. end for

We note that Requirement 1 is general and covers three commonly used data accessing strategies: Random Access (RA), Random Reshuffle (RR), and Cyclic Access (CA).

- **RA:** Select uniformly $n$ indices from $[N]$ with replacement;
- **RR:** Select sequentially $n$ indices from $[N]$ with a permutation at the beginning of each data pass;
- **CA:** Select $n$ indices from $[N]$ in a cyclic way.

RA is widely used to construct unbiased gradient approximations in gradient-based Langevin dynamics methods, which is amenable to theoretical analysis. However, in big data scenarios when the dataset does not fit into the memory, RA is not memory-friendly, since it entails heavy data exchange between memory and disks. On the contrary, CA strategy promotes the spatial locality property significantly and therefore reduces the page fault rate when handling huge datasets using limited memory (Xie et al. 2018). RR can be considered as a trade-off between RA and CA. However, methods with either CA or RR are difficult to analyze in that the gradient approximation is commonly not an unbiased estimator of the true gradient (Shamir 2016).

It can be verified that these strategies satisfy Requirement 1. For RR, in the $k$-th iteration, all the data points have been accessed in the past $2N/n$ iterations. For CA, all the data points are accessed in the past $N/n$ iterations. Note that, RA satisfies the Requirement 1 with $C = O(N \log N)$ w.h.p., according to the Coupon Collector Theorem (Dawkins 1991).

3.2 The Snapshot-Updating Step

The Snapshot-Updating step maintains a snapshot set $\mathcal{A}^{(k)}$ such that in the $k$-th iteration, $\mathcal{A}^{(k)}$ contains $N$ records $\alpha_i^{(k)}$ for $\nabla f_i(y_i^{(k)})$ where $y_i^{(k)}$ is some historic iterate $y_i^{(k)} = x^{(j)}$ with $j \leq k$. Additionally, for our analyses to hold, the input strategy should satisfy the following requirement.

**Requirement 2.** The gradient snapshot set $\mathcal{A}^{(k)}$ should satisfy $\alpha_i^{(k)} \in \{\nabla f_i(x^{(j)})\}^{k}_{j=k-D}$, where $D$ is a fixed constant.

This requirement guarantees that $\alpha_i^{(k)}$‘s are not far from the $\nabla f_i(x^{(k)})$‘s and thus can be used to construct a proper approximation of $\nabla f(x^{(k)})$. The Snapshot-Updating step tries to strike a balance between the approximation accuracy
and the computation cost. Specifically, in each iteration, updating a larger portion of the \( N \) entries in the snapshot set would lead to a more accurate gradient approximation at the cost of a higher computation burden. In the following, we list three feasible Snapshot-Updating strategies considered in this paper: Per-iteration Partial Update (PPU), Periodically Total Update (PTU), and Time-based Mixture Update (TMU).

**PTU**: This strategy operates in an epoch-wise manner: at the beginning of each epoch all the entries in the snapshot set are updated to the current component gradient \( \alpha_i^{(k)} = \nabla f_i(x^{(k)}) \), and in following \( D - 1 \) iterations the snapshot set remains unchanged (see Strategy 2). Such synchronous update to the snapshot set allows us to implement PTU in a memory efficient manner. In the \( k \)-th iteration, PTU only needs to store the iterate \( \hat{x} \) and its gradient \( \nabla f(\hat{x}) \) where \( \hat{x} = x^{k-\text{mod}(k,D)} \), as we can obtain the snapshot entry \( \alpha_i^{(k)} \) via a simple evaluation of the corresponding component gradient at \( \hat{x} \) in the calculation of \( g^{(k)} \). Therefore the PTU strategy is preferable when storage is limited.

**PPU**: This strategy substitutes \( \alpha_i^{(k)} \) by \( \nabla f_i(x^{(k)}) \) for \( i \in S_k \) in the \( k \)-th iteration (see Strategy 3). This partial substitution strategy together with Requirement 1 can ensure the Requirement 3. The downside of PPU is the extra \( O(dN) \) memory used to keep the snapshot set \( A^{(k)} \). Fortunately, in many applications of interest, \( \nabla f_i(x) \) is actually the product of a scalar and the data point \( z_i \), which implies that only \( O(N) \) extra storage is needed to store \( N \) scalars.

**TMU**: This strategy updates the whole \( A \) once every \( D \) iterations and substitutes \( \alpha_i^{(k)} \) by \( \nabla f_i(x^{(k)}) \) in the \( k \)-th iteration (see Strategy 4). TMU possesses the merits of both PPU and PTU: it updates components of gradient snapshot set in \( S_k \) to newly computed one in each iteration as PPU, and also periodically updates the whole snapshot set as PTU in case that there exist indices unselected for a long time. Note that both PTU and TMU need one extra access to the whole dataset every \( D \) iterations. Practically, we usually choose \( D = cN \), which makes PTU and TMU have an extra \( 1/c \) averaged data point access in each iteration.

**Remark 1.** PPU is the Snapshot-Updating strategy used in SAGA-LD and PTU is the strategy used in SVRG-LD (Dubač et al. 2017). To the best of our knowledge, TMU has never been proposed in the MCMC literature before. Note that the HSAG Snapshot-Updating strategy proposed by Reddi et al. (2015) also satisfies our requirement, and we omit the discussion of it due to the limit of space.

### 3.3 Derived Algorithms

By plugging the aforementioned Data-Accessing and Snapshot-Updating strategies into AGLD, we derive several practical algorithms. We name the algorithms by “Snapshot-updating - Data-Accessing”, e.g. TMU-RA uses TMU as the Snapshot-Updating strategy and RA as the Data-Accessing strategy. Note that we recover SAGA-LD and SVRG-LD when we use PPU-RA and PTU-RA, respectively. In the following section, we will provide unified analyses for all derived algorithms under different regularity conditions. We emphasize that, in the absence of the unbiasedness of the gradient approximation, our mixture time analyses are the first to cover algorithms with the I/O friendly cyclic data accessing scheme.

### 4 Theoretical Analysis

In this section, we provide the mixture time analysis for AGLD. The detailed proofs of the theorems are postponed to the Appendix due to the limit of space.

#### 4.1 Analysis for AGLD with strongly convex \( f(x) \)

We first investigate the \( \mathcal{W}_2 \) distance between the sample distribution \( p^{(k)} \) of the iterate \( x^{(k)} \) and the target distribution \( p^* \) under the smoothness and strong convexity assumptions.

**Assumption 1** (Smoothness). Each individual \( f_i \) is \( \tilde{M} \)-smooth. That is, \( f_i \) is twice differentiable and there exists a constant \( \tilde{M} > 0 \) such that for all \( x, y \in \mathbb{R}^d \),

\[
    f_i(y) \leq f_i(x) + \langle \nabla f_i(x), y - x \rangle + \frac{\tilde{M}}{2} \| y - x \|^2. \quad (7)
\]

Accordingly, we can verify that the summation \( f \) of \( f_i \)'s is \( M \)-smooth with \( M = \tilde{M}N \).

**Assumption 2** (Strong Convexity). The sum \( f \) is \( \mu \)-strongly convex. That is, there exists a constant \( \mu > 0 \) such that for all \( x, y \in \mathbb{R}^d \),

\[
    f(y) \geq f(x) + \langle \nabla f(x), y - x \rangle + \frac{\mu}{2} \| y - x \|^2. \quad (8)
\]
Note that these assumptions are satisfied by many Bayesian sampling models such as Bayesian ridge regression, Bayesian logistic regression and Bayesian Independent Component Analysis, and they are used in many existing analyses of Langevin dynamics based MCMC methods.\cite{Dalalyan2017b, Baker2017, Zou2018b, Chatterji2018}.

Theorem 1. Under Assumption\cite{Dalalyan2017b} and Requirement\cite{Dalalyan2017b} AGLD outputs sample $x^{(k)}$ with its distribution $p^{(k)}$ satisfying $W_2(p^{(k)}, p^*) \leq \epsilon$ for any $k \geq K = \tilde{O}(\epsilon^2)$ with $\eta = O(\epsilon^2)$.

Remark 2. Under this assumption, the $\epsilon$-mixture time $K$ of AGLD has the same dependency on $\epsilon$ as that of LMC\cite{Dalalyan2017b}. Note that we hide the dependency of other regularity parameters such as $\mu$, $L$ and $N$ in the $O(\cdot)$ for simplicity. Actually, AGLD methods with CA/RR have a worse dependency on these parameters than algorithms with RA. However, when the dataset does not fit into the memory, the sequential data accessing nature of CA enjoys less I/O cost than random data accessing, which makes CA based AGLD methods have a better time efficiency than the RA based ones.

The bound of the mixture time for AGLD with RA can be improved under the Lipschitz-continuous Hessian condition.

Assumption 3. [Lipschitz-continuous Hessian] There exists a constant $L > 0$ such that for all $x, y \in \mathbb{R}^d$

$$\|\nabla^2 f(x) - \nabla^2 f(y)\| \leq L\|x - y\|_2.$$

Theorem 2. Under Assumption\cite{Dalalyan2017b} and Requirement\cite{Dalalyan2017b} AGLD methods with RA output sample $x^{(k)}$ with its distribution $p^{(k)}$ satisfying $W_2(p^{(k)}, p^*) \leq \epsilon$ for any $k \geq K = O(\log(1/\epsilon)/\epsilon)$ by setting $\eta = O(\epsilon)$.

Additionally, when we adopt the random data accessing scheme, the mixture time of the proposed TMU-RA method can be written in a more concrete form, which is established in the following theorem.

Theorem 3. Under Assumption\cite{Dalalyan2017b} and denote $\kappa = M/\mu$. TMU-RA outputs sample $x^{(k)}$ with its distribution $p^{(k)}$ satisfying $W_2(p^{(k)}, p^*) \leq \epsilon$ for any $k \geq K = O(\kappa^{3/2}/d(\epsilon))$ if we set $\eta < \epsilon n^{3/2}/(\sqrt{M}dN)$, $n \geq 9$, and $D = N$.

Remark 3. Note that the component gradient complexity to achieve $W_2(p^{(k)}, p^*) \leq \epsilon$ in TMU-RA is $T_g = O(N + \kappa^{3/2}/\sqrt{d}/\epsilon)$, which is the same as those of SAGA-LD\cite{Chatterji2018} and SVRG-LD\cite{Zou2018b}.

Practically, in our experiments, TMU based methods always have a better empirically performance than the PPU based and PTU based counterparts as the entries in the snapshot set maintained by TMU is more up-to-date.

4.2 Extension to general function $f(x)$

Following a similar idea from\cite{Zou2018b}, we can extend AGLD to drawing samples from densities with general convex $f(x)$. Firstly, we construct the following strongly convex approximation $\hat{f}(x)$ of $f(x)$,

$$\hat{f}(x) = f(x) + \lambda\|x\|^2/2.$$

Then, we run AGLD to generate samples with $\hat{f}(x)$ until the sample distribution $p^{(K)}$ satisfies $W_2(p^{(K)}, \hat{p}^*) \leq \epsilon/2$ where $\hat{p}^* \propto e^{-\hat{f}(x)}$ denotes stationary distribution of Langevin Dynamics with the drift term $\nabla \hat{f}$ (check\cite{Dalalyan2017b} for definition). If we choose a proper $\lambda$ to make $W_2(\hat{p}^*, p^*) \leq \epsilon/2$, then by the triangle inequality of the $W_2$ distance, we have $W_2(p^{(K)}, p^*) \leq W_2(p^{(K)}, \hat{p}^*) + W_2(\hat{p}^*, p^*) \leq \epsilon/2$. Thus, we have the following theorem.

Theorem 4. Suppose the assumptions in Theorem 1 hold and further assume the target distribution $p^* \propto e^{-f}$ has bounded forth order moment, i.e. $E_p[\|x\|^4] \leq U\bar{d}^2$. If we choose $\lambda = 4\epsilon^2/(U\bar{d}^2)$ and run the AGLD algorithm with $\hat{f}(x) = f(x) + \lambda\|x\|^2/2$, we have $W_2(p^{(K)}, p^*) \leq \epsilon$ for any $k \geq K = O(\epsilon^{-8})$. If we further assume that $f$ has Lipschitz-continuous Hessian, then SVRG-LD, SAGA-LD, and TMU-RA can achieve $W_2(p^{(K)}, p^*) \leq \epsilon$ in $K = \tilde{O}(\epsilon^{-3})$ iterations.

4.3 Theoretical results for nonconvex function $f(x)$

In this subsection, we characterize the $\epsilon$-mixture time of AGLD for sampling from densities with nonconvex $f(x)$. The following assumption is necessary for our theory.

Assumption 4. [Dissipative] There exists constants $a, b > 0$ such that for all $x \in \mathbb{R}^d$, the sum $f$ satisfies

$$\langle \nabla f(x), x \rangle \geq b\|x\|^2_2 - a.$$

This assumption is typical for the ergodicity analysis of stochastic differential equations and diffusion approximations. It indicates that, starting from a position that is sufficiently far from the origin, the Langevin dynamics\cite{Roberts1996} moves towards the origin on average. With this assumption, we establish the following theorem on the nonasymptotic convergence of AGLD for nonconvex $f(x)$.

Theorem 5. Under Assumption\cite{Dalalyan2017b} and Requirement\cite{Dalalyan2017b} AGLD outputs sample $x^{(k)}$ with distribution $p^{(k)}$ satisfying $W_2(p^{(k)}, p^*) \leq \epsilon$ for any $k \geq K = O(\epsilon^{-4})$ with $\eta = O(\epsilon^3)$.

Remark 4. This $\tilde{O}(\epsilon^{-4})$ result is similar to the bound for LMC sampling from nonconvex $f(x)$\cite{Raginsky2017}. Note that, as pointed out by\cite{Raginsky2017}, vanilla SGLD fails to converge in this setting.

5 Related Work

In this section, we briefly review the literature of Langevin dynamics based MCMC algorithms.

By directly discretizing the Langevin dynamics\cite{Roberts1996},\cite{Durmus2017},\cite{Durrmus2017},\cite{Durrmus2017},\cite{Durrmus2017} proposed to use LMC\cite{Dalalyan2017b} to generate samples of the target distribution. The first nonasymptotic analysis of LMC was established by\cite{Dalalyan2017b}, which analyzed the error of approximating the target distribution with strongly convex $f(x)$ in the total variational distance. This result was soon improved by\cite{Durmus2017}. Later,\cite{Durrmus2017} and Cheng and Bartlett\cite{Cheng2018} established the convergence of LMC in the 2-Wasserstein distance and KL-divergence, respectively. While the former works focus on sampling from distribution with (strongly-)convex $f(x)$,
Algorithm (MALA) (Roberts and Rosenthal 1998), which gives rise to Metropolis Adjusted Langevin Algorithm (MALA) (Roberts and Rosenthal 1998), Eberle (2014) and Dwivedi et al. (2018) proved the nonasymptotic convergence of MALA for sampling from distribution with general convex and strongly convex $f(x)$, respectively. Typically, MALA has better mixture bounds than LMC under the same assumption due to the extra correction step. However, the MH correction step needs extra full data access, and is not suitable for large-scale Bayesian learning tasks.

With the increasing amount of data size in modern machine learning tasks, SGLD method (Welling and Teh 2011), which replaces the full gradient in LMC with a stochastic gradient (Robbins and Monro 1951), has received much attention, Vollmer et al. (2015) analyzed the nonasymptotic bias and variance of SGLD using Poisson equations, and Dalalyan and Karagulyan (2017) proved the convergence of SGLD in the 2-Wasserstein distance when the target distribution is strongly log-concave. Despite the great success of SGLD, the large variance of stochastic gradients may lead to unavoidable bias. Baker et al. (2017) and Betancourt (2015) proposed to decrease the step size to alleviate the bias and proved the asymptotic rate of SGLD in terms of Mean Square Error (MSE). Dang et al. (2019) utilized an approximate MH correction step, which only uses part of the whole data set, to decrease the influence of variance.

Another way to reduce the variance of stochastic gradients and save gradient computation is to apply variance-reduction techniques. Dubey et al. (2016) used two different variance-reduced gradient estimators of $\nabla f(x)$, which utilize the component gradient information of the past samples, and devised SVRG-LD and SAGA-LD algorithms. They proved that these two algorithms improve the MSE upon SGLD. Chatterji et al. (2018) and Zou et al. (2019) studied the nonasymptotic convergence of these methods in the 2-Wasserstein distance when sampling from densities with strongly convex and nonconvex $f(x)$, respectively. Their results show that SVRG-LD and SAGA-LD can achieve similar $\epsilon$-mixture time bound as LMC w.r.t. $\epsilon$, while the per-iteration computational cost is similar to that of SGLD. There is another research line which uses the mode of the log-posterior to construct control-variate estimates of full gradients (Baker et al. 2017; Bierkens et al. 2016; Nagapetyan et al. 2017).

6 Experiments
We follow the experiment settings in the literature (Zou et al. 2018b; Dubey et al. 2016; Chatterji et al. 2018; Welling and Teh 2011; Zou et al. 2019) and conduct empirical studies on two simulated experiments (sampling from distribution with convex and nonconvex $f$, respectively) and two real-world applications (Bayesian Logistic Regression and Bayesian Ridge Regression). Nine instances of AGLD are considered, including SVRG-LD (PTU-RA), PTU-RR, PTU-CA, SAGA-LD (PPU-RA), PPU-RR, PPU-CA, TMU-RA, TMU-RR, and TMU-CA. We also include LMC, SGLD, SVGR-LD+ (Zou et al. 2018b), SVRG-RR+ and SVRG-CA+ as baselines. Due to the limit of space, we put the experiment sampling from distribution with convex $f$ into the Appendix. The statistics of datasets are listed in Table 1.

6.1 Sampling for Gaussian Mixture Distribution
In this simulated experiment, we consider sampling from distribution $p^\star \propto \exp(-f(x)) = \exp(-\sum_{i=1}^{N} f_i(x)/N)$, where each component $\exp(-f_i(x)) = e^{\frac{-\|x-a_i\|^2}{2}} + e^{\frac{\|x+a_i\|^2}{2}}$, $a_i \in \mathbb{R}^d$. It can be verified that $\exp(-f_i(x))$ is proportional to the PDF of a Gaussian mixture distribution. According to (Dalalyan 2017b), when the parameter $a_i$ is chosen such that $\|a_i\|^2 \geq 1$, $f_i(x)$ is nonconvex. We set the sample size $N = 500$ and dimension $d = 10$, and randomly generate parameters $a_i \sim N(\mu, \Sigma)$ with $\mu = (2, \cdots, 2)^T$ and $\Sigma = I_{d \times d}$.

In this experiment, we fix the Data-Accessing strategy to RA in AGLD and compare the performance of LMC, SGLD,

![Figure 1: Gaussian Mixture Model. The red line denotes the projection of the target distribution $p^\star$.](image)

Table 1: Statistics of datasets used in our experiments.

| DATASET         | DIMENSION | DATASIZE  |
|-----------------|-----------|-----------|
| YearPredictionMSD | 90        | 515,345   |
| SliceLocation   | 384       | 53500     |
| CRM              | 999,999   | 45,840,617|
| TD               | 54,686,45 | 149,639,105|
Bayesian ridge regression aims to predict the response $y$ according to the covariate $x$, given the dataset $Z = \{x_i, y_i\}_{i=1}^N$. The response $y$ is modeled as a random variable sampled from a conditional Gaussian distribution $p(y|x, w) = \mathcal{N}(w^T x, \lambda)$, where $w$ denotes the weight variable and has a Gaussian prior $p(w) = \mathcal{N}(0, \lambda I_{d \times d})$. By the Bayesian rule, one can infer $w$ from the posterior $p(w|Z)$ and use it to make the prediction. Two publicly available benchmark datasets are used for evaluation: YearPredictionMSD and SliceLocation. All these datasets are small and can be loaded to the memory.

In this task, we fix the Data-Accessing strategy to RA and compare the performance of different Snapshot-Updating strategies. To have a better understanding of the newly-proposed TMU Snapshot-Updating strategy, we also investigate the performance of TMU type methods with different Data-Accessing strategies.

By randomly partitioning the dataset into training (4/5) and testing (1/5) sets, we report the test Mean Square Error (MSE) of the compared methods on YearPredictionMSD in Fig. 5. The results for SliceLocation are similar to that of YearPredictionMSD, and are postponed to the Appendix due to the limit of space. We use the number of effective passes (epoch) of the dataset as the x-axis, which is proportional to the CPU time. From the first three columns of the figure, we can see that (i) TMU-type methods have the best performance among all the methods with the same Data-Accessing strategy, (ii) SVRG+ and PPU type methods constantly outperform LMC, SGLD, and PTU type methods. These results validate the advantage of TMU strategy over PPU and PTU. The last column of Figure 5 shows that TMU-RA outperforms TMU-CA/TMU-RR, when the dataset is fitted to the memory. These results imply that the TMU-RA is the best choice if we have enough memory.

6.3 Bayesian Logistic Regression

Bayesian Logistic Regression is a robust binary classification task. Let $Z = \{x_i, y_i\}_{i=1}^N$ be a dataset with $y_i \in \{-1, 1\}$ denoting the sample label and $x_i \in \mathbb{R}^d$ denoting the sample covariate vector. The conditional distribution of label $y$ is modeled by $p(y|x, w) = \phi(y,w^T x_i)$, where $\phi(\cdot)$ is the sigmoid function and the prior of $w$ is $p(w) = \mathcal{N}(0, \lambda I_{d \times d})$.

We focus on the big data setting, where the physical memory is insufficient to load the entire dataset. Specifically, two large-scale datasets criteo (27.32GB) and kdd12 (26.76GB) are used \footnote{https://archive.ics.uci.edu/ml/index.php} and we manually restrict the available physical memory to 16 GB and 8 GB for simulation.

We demonstrate that CA strategy is advantageous in such setting by comparing 6 AGLD methods with either CA or RA in the experiment, namely, SVRG-LD, PTU-CA, SAGA-LD, PPU-CA, TMU-RA, and TMU-CA. We also include LMC, SGLD, SVRG-LD+, and SVRG-CA+ as baseline. Methods with the RR strategy have almost identical performance as their RA counterparts and are hence omitted. The average test log-likelihood versus execution time are reported in Fig. 5. The empirical results show that methods with CA outperform their RA counterparts. As the amount of physical memory gets smaller (from 16 GB to 8 GB),
the time efficiency of CA becomes more apparent. The results also show that TMU has better performance than other Snapshot-Updating strategies with the same Data-Accessing strategy.

7 Conclusion and Future Work
In this paper, we proposed a general framework called Aggregated Gradient Langevin Dynamics (AGLD) for Bayesian posterior sampling. A unified analysis for AGLD is provided without the need to design different Lyapunov functions for different methods individually. In particular, we establish the first theoretical guarantees for cyclic access and random reshuffle based methods. By introducing the new Snapshot-Updating strategy TMU, we derive some new methods under AGLD. Empirical results validate the efficiency and effectiveness of the proposed TMU in both simulated and real-world tasks. The theoretical analysis and empirical results indicate that TMU-RA would be the best choice if the memory is sufficient and TMU-CA would be used, otherwise.

References
[Baker et al. 2017] Jack Baker, Paul Fearnhead, Emily B Fox, and Christopher Nemeth. Control variates for stochastic gradient mcmc. arXiv preprint arXiv:1706.05439, 2017.
[Betancourt 2015] Michael Betancourt. The fundamental incompatibility of scalable hamiltonian monte carlo and naive data subsampling. In International Conference on Machine Learning, pages 533–540, 2015.
[Bierkens et al. 2016] Joris Bierkens, Paul Fearnhead, and Gareth Roberts. The zig-zag process and super-efficient sampling for bayesian analysis of big data. arXiv preprint arXiv:1607.03188, 2016.
[Brosse et al. 2018] Nicolas Brosse, Alain Durmus, and Eric Moulines. The promises and pitfalls of stochastic gradient langevin dynamics. In Advances in Neural Information Processing Systems, pages 8268–8278, 2018.
[Chatterji et al. 2018] Niladri Chatterji, Nicolas Flammarion, Yi-An Ma, Peter L Bartlett, and Michael I Jordan. On the theory of variance reduction for stochastic gradient monte carlo. arXiv preprint arXiv:1802.05431, 2018.
[Cheng and Bartlett 2018] Xiang Cheng and Peter L Bartlett. Convergence of langevin mcmc in kl-divergence. PMLR 83, (83):186–211, 2018.
[Dalalyan and Karagulyan 2017] Arnak S Dalalyan and Avetik G Karagulyan. User-friendly guarantees for the langevin monte carlo with inaccurate gradient. arXiv preprint arXiv:1710.00095, 2017.
[Dalalyan 2017a] Arnak S Dalalyan. Further and stronger analogy between sampling and optimization: Langevin monte carlo and gradient descent. arXiv preprint arXiv:1704.04752, 2017.
[Dalalyan 2017b] Arnak S Dalalyan. Theoretical guarantees for approximate sampling from smooth and log-concave densities. Journal of the Royal Statistical Society: Series B (Statistical Methodology), 79(3):651–676, 2017.
[Dang et al. 2019] Khue-Dung Dang, Matias Quiroz, Robert Kohn, Minh-Ngoc Tran, and Mattias Villani. Hamiltonian monte carlo with energy conserving subsampling. Journal of machine learning research, 20(100):1–31, 2019.
[Dawkins 1991] Brian Dawkins. Siobhan’s problem: the coupon collector revisited. The American Statistician, 45(1):76–82, 1991.
[Defazio et al. 2014] Aaron Defazio, Francis Bach, and Simon Lacoste-Julien. Saga: A fast incremental gradient method with support for non-strongly convex composite objectives. In Advances in neural information processing systems, pages 1646–1654, 2014.
[Dubey et al. 2016] Kumar Avinava Dubey, Sashank J Reddi, Sinead A Williamson, Barnabas Poczos, Alexander J Smola, and Eric P Xing. Variance reduction in stochastic gradient langevin dynamics. In Advances in Neural Information Processing Systems, pages 1154–1162, 2016.
[Durmus and Moulines 2016] Alain Durmus and Eric Moulines. High-dimensional bayesian inference via the unadjusted langevin algorithm. arXiv preprint arXiv:1605.01559, 2016.
[Durmus et al. 2017] Alain Durmus, Eric Moulines, et al. Nonasymptotic convergence analysis for the unadjusted langevin algorithm. The Annals of Applied Probability, 27(3):1551–1587, 2017.
[Dwivedi et al. 2018] Raaz Dwivedi, Yuansi Chen, Martin J Wainwright, and Bin Yu. Log-concave sampling: Metropolis-hastings algorithms are fast! arXiv preprint arXiv:1801.02309, 2018.
[Eberle 2014] Andreas Eberle. Error bounds for metropolis–hastings algorithms applied to perturbations of gaussian measures in high dimensions. The Annals of Applied Probability, 24(1):337–377, 2014.
[Hastings 1970] W Keith Hastings. Monte carlo sampling methods using markov chains and their applications. 1970.
[Johnson and Zhang 2013] Rie Johnson and Tong Zhang. Accelerating stochastic gradient descent using predictive variance reduction. In Advances in neural information processing systems, pages 315–323, 2013.
[Lei and Jordan 2017] Lihua Lei and Michael Jordan. Less variance: More frequent updates for accelerated optimization. arXiv preprint arXiv:1706.05439, 2017.
[Moulines et al. 2020] Eric Moulines, Alain Durmus, and Yurii Nesterov. Variance reduction for markov chain monte carlo: from fast mixing to heavy tail. arXiv preprint arXiv:2002.02379, 2020.
[Mattingly et al. 2004] Jonathan C Mattingly, Andrew M Stuart, and Desmond J Higham. Ergodicity for sdes and approximations: locally lipschitz vector fields and degenerate noise. Stochastic processes and their applications, 101(2):185–232, 2002.
[Nagapetyan et al. 2017] Tigran Nagapetyan, Andrew B Duncan, Leonard Hasenclever, Sebastian J Vollmer, Lukasz Szpruch, and Konstantinos Zygalakis. The true cost of stochastic gradient langevin dynamics. arXiv preprint arXiv:1706.02692, 2017.
[Parisi 1981] G Parisi. Correlation functions and computer simulations. Nuclear Physics B, 180(3):378–384, 1981.
[Raginsky et al. 2017] Maxim Raginsky, Alexander Rakhlin, and Matus Telgarsky. Non-convex learning via stochastic gradient langevin dynamics: a nonasymptotic analysis. arXiv preprint arXiv:1702.03849, 2017.

[Reddi et al. 2015] Sashank J Reddi, Ahmed Hefny, Suvrit Sra, Barnabas Poczos, and Alexander J Smola. On variance reduction in stochastic gradient descent and its asynchronous variants. In Advances in Neural Information Processing Systems, pages 2647–2655, 2015.

[Robbins and Monro 1951] Herbert Robbins and Sutton Monro. A stochastic approximation method. The annals of mathematical statistics, pages 400–407, 1951.

[Roberts and Rosenthal 1998] Gareth O Roberts and Jeffrey S Rosenthal. Optimal scaling of discrete approximations to langevin diffusions. Journal of the Royal Statistical Society: Series B (Statistical Methodology), 60(1):255–268, 1998.

[Roberts and Stramer 2002] Gareth O Roberts and Osnat Stramer. Langevin diffusions and metropolis-hastings algorithms. Methodology and computing in applied probability, 4(4):337–357, 2002.

[Roberts et al. 1996] Gareth O Roberts, Richard L Tweedie, et al. Exponential convergence of langevin distributions and their discrete approximations. Bernoulli, 2(4):341–363, 1996.

[Shamir 2016] Ohad Shamir. Without-replacement sampling for stochastic gradient methods. In NeurIPS, pages 46–54, 2016.

[Teh et al. 2016] Yee Whye Teh, Alexandre H Thiery, and Sebastian J Vollmer. Consistency and fluctuations for stochastic gradient langevin dynamics. Journal of Machine Learning Research, 17:1–33, 2016.

[Vollmer et al. 2015] Sebastian J Vollmer, Konstantinos C Zygalakis, et al. (non-) asymptotic properties of stochastic gradient langevin dynamics. arXiv preprint arXiv:1501.00438, 2015.

[Welling and Teh 2011] Max Welling and Yee W Teh. Bayesian learning via stochastic gradient langevin dynamics. In Proceedings of the 28th International Conference on Machine Learning (ICML-11), pages 681–688, 2011.

[Xie et al. 2018] Jiahao Xie, Hui Qian, Zebang Shen, and Chao Zhang. Towards memory-friendly deterministic incremental gradient method. In International Conference on Artificial Intelligence and Statistics, pages 1147–1156, 2018.

[Zou et al. 2018a] Difan Zou, Pan Xu, and Quanquan Gu. Stochastic variance-reduced hamilton monte carlo methods. arXiv preprint arXiv:1802.04791, 2018.

[Zou et al. 2018b] Difan Zou, Pan Xu, and Quanquan Gu. Subsampled stochastic variance-reduced gradient langevin dynamics. conference on uncertainty in artificial intelligence, 2018.

[Zou et al. 2019] Difan Zou, Pan Xu, and Quanquan Gu. Sampling from non-log-concave distributions via variance-reduced gradient langevin dynamics. In AISTATS, pages 2936–2945, 2019.
8 Appendix

8.1 Theoretical results under strongly convex and smooth assumption

We first list the requirement for AGLD and the assumptions on $f$.

**Requirement 3.** For the gradient snapshot $\mathcal{A}^{(k)}$, we have $\alpha_i^{(k)} \in \{\nabla f_i(x^{(j)})\}_{j=k-D+1}^{(k)}$, where $D$ is a fixed constant.

**Assumption 5 (Smoothness).** Each individual $f_i$ is $M$ smooth. That is, $f_i$ is twice differentiable and there exists a constant $M > 0$ such that for all $x, y \in \mathbb{R}^d$

$$f_i(y) \leq f_i(x) + \langle \nabla f_i(x), y - x \rangle + \frac{M}{2} \|x - y\|_2^2.$$ \tag{9}

Accordingly, we can verify that the summation $f$ of $f_i$'s is $M = MN$ smooth.

**Assumption 6 (Strongly Convexity).** The sum $f$ is $\mu$ strongly convex. That is, there exists a constant $\mu > 0$ such that for all $x, y \in \mathbb{R}^d$,

$$f(y) \geq f(x) + \langle \nabla f(x), y - x \rangle + \frac{\mu}{2} \|x - y\|_2^2.$$ \tag{10}

According to (Dalalyan and Karagulyan 2017), we have the following bound for the $\mathcal{W}_2$ distance

$$\mathcal{W}_2^2(p, q) \leq \mathbb{E} \|x - y\|^2,$$ \tag{11}

for arbitrary $x \sim p, y \sim q$. Thus, in order to bound the $\mathcal{W}_2$ distance of $p^{(k+1)}$ and $p^*$, we construct a auxiliary sequence $y^{(k)}$ with $y^{(k)} \sim p^*$ for all $k \geq 0$ and bound $\mathbb{E} \|x^{(k+1)} - y^{(k+1)}\|^2$. Specifically, we make $y^{(k)} = y(\eta k)$, where $y(t)$ is the following auxiliary dynamics

$$dy(t) = -\nabla f(y(t))dt + \sqrt{2}dB(t)$$ \tag{12}

with $y(0) \sim p^*$. According to the Fokker-Planck theorem (2), $y(t) \sim p^*$ for all $t \geq 0$. It can be verified that $y^{(k+1)}$ satisfies the following iteration relation.

$$y^{(k+1)} = y^{(k)} - \int_{k\eta}^{(k+1)\eta} \nabla f(y(s))ds + \sqrt{2}\eta \xi^{(k)},$$ \tag{13}

where $y^{(0)} = y(0)$ and $\xi^{(k)}$ is the same Gaussian variable used in $(x^{(k+1)})$.

For the simplicity of notation, we denote $\Delta^{(k+1)} = y^{(k+1)} - x^{(k+1)}$ and decompose it as

$$\Delta^{(k+1)} = \Delta^{(k)} - V^{(k)} - \eta U^{(k)} + \eta \Phi^{(k)},$$ \tag{14}

where

$$\begin{align*}
V^{(k)} &= \int_{k\eta}^{(k+1)\eta} \nabla f(y(s))ds, \\
U^{(k)} &= \nabla f(y^{(k)}) - \nabla f(x^{(k)}), \\
\Phi^{(k)} &= g^{(k)} - \nabla f(x^{(k)}).
\end{align*}$$

Here, $\Phi^{(k)}$ is the difference between the gradient approximation $g^{(k)}$ and the full gradient $\nabla f(x^{(k)})$. It can be further decomposed into an unbiased part $\Psi^{(k)}$ and the remainder $\Gamma^{(k)}$. If the Data-Accessing strategy is RA, then $\Psi^{(k)} = \Phi^{(k)}$ and $\Gamma^{(k)} = 0$. For other strategies, we make

$$\begin{align*}
\Psi^{(k)} &= \frac{1}{n} \sum_{i \in I_k} \nabla f_i(x^{(k)}) - \alpha_i^{(k)} + \frac{1}{n} \sum_{i=1}^{N} \alpha_i^{(k)} - \nabla f(x^{(k)}), \\
\Gamma^{(k)} &= \frac{1}{n} \sum_{i \in S_k} \nabla f_i(x^{(k)}) - \alpha_i^{(k)} - \frac{1}{n} \sum_{i \in I_k} \nabla f_i(x^{(k)}) - \alpha_i^{(k)},
\end{align*}$$ \tag{15-16}

where $I_k$ is a set with $n$ indexes uniformly sampled from $\{1, \ldots, N\}$. It can be verified that $\mathbb{E}[\Psi^{(k)}|x^{(k)}] = 0$ in both setting.

By bounding $\mathbb{E}||\Delta^{(k)} - \eta U^{(k)}||^2, \mathbb{E}||V^{(k)}||^2, \mathbb{E}||\Psi^{(k)}||$ and $\mathbb{E}||\Gamma^{(k)}||$ from above properly, we can establish a per-iteration decreasing result of $\mathbb{E}||\Delta^{(k)}||$.

**Bound for $\mathbb{E}||\Delta^{(k)} - \eta U^{(k)}||^2$ and $\mathbb{E}||V^{(k)}||^2$:** By Lemma 1 and Lemma 3 in (Dalalyan 2017a), this two terms can be bounded from above as follows.

**Lemma 1 (Lemma 1 & 3 in Dalalyan 2017a).** Assuming that $f$ is $M$-smooth and $\mu$-strongly convex, and $\eta \leq \frac{2}{M+\mu}$, we have

$$\begin{align*}
\mathbb{E}||V^{(k)}||^2 &\leq (\sqrt{\eta^2 M^2 d/3} + \sqrt{h^3 M^2 d})^2 \leq \frac{2}{3} \eta^4 M^2 d + 2h^3 M^2 d, \\
\mathbb{E}||\Delta^{(k)} - \eta U^{(k)}||^2 &\leq (1 - \eta \mu)^2 \mathbb{E}||\Delta^{(k)}||^2.
\end{align*}$$ \tag{17-18}
Bound for $E\|\Psi^{(k)}\|$ and $E\|\Gamma^{(k)}\|$: These two terms can be bounded from above in the following lemma, the proof of which is postponed to the appendix.

Lemma 2. Assuming that $f$ is $M$-smooth and $\mu$-strongly convex, and Requirement $[3]$ is satisfied, we have the following upper bound on $E\|\Psi^{(k)}\|^2$ and $E\|\Gamma^{(k)}\|^2$

$$E\|\Psi^{(k)}\|^2 \leq \frac{N}{n} \sum_{i=1}^{N} E\|\nabla f_i(x^{(k)}) - \alpha_i^{(k)}\|^2,$$

$$E\|\Gamma^{(k)}\|^2 \leq \frac{2N(N+n)}{n} \sum_{i=1}^{N} E\|\nabla f_i(x^{(k)}) - \alpha_i^{(k)}\|^2,$$

and

$$\sum_{i=1}^{N} E\|\nabla f_i(x^{(k)}) - \alpha_i^{(k)}\|^2 \leq 32\eta^2D^2M^2E\|\Delta^{(k-2D)}\|_{2,\infty} + 4\eta Dd + 48\eta^3M^2D^3(d\eta DM + 1) + 8\eta^2 MN D^2d, \quad (19)$$

where $\Delta^{(k-2D)} := [\Delta^{(k)}, \Delta^{(k-1)}, \cdots, \Delta^{(|k-2D|+)}]$. If Data-Accessing strategy is RA, then $E\|\Gamma^{(k)}\|^2 = 0$.

Proof.

$$E\|\Psi^{(k)}\|^2 = E\|\sum_{i \in I_k} \frac{N}{n} (\nabla f_i(x^{(k)}) - \alpha_i^{(k)}) + \sum_{i=1}^{N} \alpha_i^{(k)} - \nabla f(x^{(k)})\|^2$$

$$= E\left\| \frac{1}{n} \sum_{i \in I_k} \left( N(\nabla f_i(x^{(k)}) - \alpha_i^{(k)}) - (\nabla f(x^{(k)}) - \sum_{i=1}^{N} \alpha_i^{(k)}) \right) \right\|^2$$

$$= E\left\| \frac{1}{n} N(\nabla f_i(x^{(k)}) - \alpha_i^{(k)}) - (\nabla f(x^{(k)}) - \sum_{i=1}^{N} \alpha_i^{(k)}) \right\|^2$$

$$\leq \frac{N^2}{n} E\|\nabla f_i(x^{(k)}) - \alpha_i^{(k)}\|^2 = \frac{N}{n} \sum_{i=1}^{N} E\|\nabla f_i(x^{(k)}) - \alpha_i^{(k)}\|^2.$$

The third equality follows from the fact that $I_k$ are chosen uniformly and independently. The first inequality is due to the fact that $E\|X - EX\|^2 \leq E\|X\|^2$ for any random variable $X$. Here in the last equality, we use that $i$ is chosen uniformly from $\{1, \cdots, N\}$ and $i$ here is no longer a random variable.

$$E\|E^{(k)}\|^2 = E\left\| \frac{N}{n} \sum_{i \in S_k} (\nabla f_i(x^{(k)}) - \alpha_i^{(k)}) - \frac{N}{n} \sum_{i \in I_k} (\nabla f_i(x^{(k)}) - \alpha_i^{(k)}) \right\|^2$$

$$\leq \frac{2N^2}{n^2} E\left( \left\| \sum_{i \in S_k} (\nabla f_i(x^{(k)}) - \alpha_i^{(k)}) \right\|^2 + \left\| \sum_{i \in I_k} (\nabla f_i(x^{(k)}) - \alpha_i^{(k)}) \right\|^2 \right)$$

$$\leq \frac{2N^2}{n^2} E(n \sum_{i \in S_k} \|\nabla f_i(x^{(k)}) - \alpha_i^{(k)}\|^2 + n \sum_{i \in I_k} \|\nabla f_i(x^{(k)}) - \alpha_i^{(k)}\|^2)$$

$$\leq \frac{2N^2}{n^2} E(n \sum_{i=1}^{N} \|\nabla f_i(x^{(k)}) - \alpha_i^{(k)}\|^2 + \frac{n^2}{N} \sum_{i=1}^{N} \|\nabla f_i(x^{(k)}) - \alpha_i^{(k)}\|^2)$$

$$= \frac{2N(N+n)}{n} \sum_{i=1}^{N} E\|\nabla f_i(x^{(k)}) - \alpha_i^{(k)}\|^2.$$

In the first two inequality, we use that $\| \sum_{i=1}^{n} a_i \|^2 \leq n \sum_{i=1}^{n} |a_i|^2$. The third inequality follows from the fact that $\{S_k\}$ are subset of $\{1, \cdots, N\}$ in CA and RS and $I_k$ are chosen uniformly and independently from $\{1, \cdots, N\}$. When we use RA, $S_k$ just equals to $I_k$ and $E\|E^{(k)}\|^2 = 0$.

Suppose that in the $k$-th iteration, snapshot $\alpha_i^{(k)}$ are taken at $x^{(k_i)}$, where $k_i \in \{(k-1) \lor 0, (k-2) \lor 0, \cdots, (k-D) \lor 0\}$. By the $M$ smoothness of $f_i$, we have

$$\sum_{i=1}^{N} E\|\nabla f_i(x^{(k)}) - \alpha_i^{(k)}\|^2 \leq \sum_{i=1}^{N} M^2 E\|x^{(k)} - x^{(k_i)}\|^2 = \sum_{i=1}^{N} \frac{M^2}{N^2} E\|x^{(k)} - x^{(k_i)}\|^2.$$
According to the update rule of \( x^{(k)} \), we have
\[
\mathbb{E}\|x^{(k)} - x^{(k_i)}\|^2 = \mathbb{E}\| - \sum_{j=k_i}^{k-1} g^{(j)} + \sqrt{2} \sum_{j=k_i}^{k-1} \xi^{(j)}\|^2 \leq 2D\eta^2 \sum_{j=k-D}^{k-1} \mathbb{E}\|g^{(j)}\|^2 + 4Dd\eta,
\]
where the inequality follows from \( \|a + b\|^2 \leq 2(\|a\|^2 + \|b\|^2) \), \( \xi^{(j)} \) are independent Gaussian variables and \( k_i \geq k - D \).

By expanding \( g^{(j)} \), we have
\[
\mathbb{E}\|g^{(j)}\|^2 = \mathbb{E}\| \sum_{p \in S_j} \frac{N}{n} (\nabla f_p(x^{(j)}) - \alpha_p^{(j)}) + \sum_{p=1}^{N} \alpha_p^{(j)}\|^2
\leq 2\mathbb{E}\| \sum_{p \in S_j} \frac{N}{n} (\nabla f_p(x^{(j)}) - \alpha_p^{(j)})\|^2 + 2\mathbb{E}\| \sum_{p=1}^{N} \alpha_p^{(j)}\|^2.
\]

For \( A \), we have
\[
A \leq 2n \sum_{p \in S_j} \frac{N^2}{n^2} \mathbb{E}\| (\nabla f_p(x^{(j)}) - \nabla f_p(y^{(j)})) + (\nabla f_p(y^{(j)}) - \nabla f_p(y^{(j_p)})) + (\nabla f_p(y^{(j_p)}) - \alpha_p^{(j)})\|^2
\leq \frac{6N^2}{n} \sum_{p \in S_j} (\mathbb{E}\| \nabla f_p(x^{(j)}) - \nabla f_p(y^{(j)})\|^2 + E\| \nabla f_p(y^{(j)}) - \nabla f_p(y^{(j_p)})\|^2 + E\| \nabla f_p(y^{(j_p)}) - \alpha_p^{(j)}\|^2)
\leq \frac{6M^2}{n} \sum_{p \in S_j} (\mathbb{E}\|x^{(j)} - y^{(j)}\|^2 + E\|y^{(j)} - y^{(j_p)}\|^2 + E\|y^{(j_p)} - x^{(j_p)}\|^2).
\]

where the last inequality follows from the smoothness of \( f_p \).

But further expanding \( y^{(j)} \) and \( y^{(j_p)} \), we have
\[
\mathbb{E}\|y^{(j)} - y^{(j_p)}\|^2 = \mathbb{E}\| \int_{j_p \eta}^{j \eta} \nabla f(y(s))ds - \sqrt{2} \sum_{q=j_p}^{j} \xi^{(q)}\|^2
\leq 2(j - j_p)\eta \int_{j_p \eta}^{j \eta} \mathbb{E}\|\nabla f(y(s))\|^2 ds + 4\eta Dd \leq 2D\eta \cdot D\eta M d + 4\eta Dd \leq 2D^2 \eta^2 M d + 4\eta Dd,
\]

where, the first inequality is due to the Jensen’s inequality and the second inequality follows by Lemma 3 in (Dalalyan and Karagulyan 2017) to bound \( \mathbb{E}\|\nabla f(y(s))\|^2 ds \leq M d \).

Then we can bound \( A \) above by
\[
A \leq \frac{6M^2}{n} \sum_{p \in S_j} (\mathbb{E}\|\Delta^j\|^2 + 2D^2 \eta^2 M d + 4\eta D d + \mathbb{E}\|\Delta^{j_p}\|^2)
\leq \frac{6M^2}{n} (\mathbb{E}\|\Delta^j\|^2 + 2D^2 \eta^2 M d + 4\eta D d + \mathbb{E}\|\Delta^{j_p}\|^2).
\]

Now we can bound \( B \) with similar technique
\[
B = 2\mathbb{E}\sum_{p=1}^{N} (\alpha_p^{(j)} - \nabla f_p(y^{(j_p)})) + \sum_{p=1}^{N} \nabla f_p(y^{(j_p)})\|^2
\leq 4N \mathbb{E}\| \nabla f_p(x^{(j_p)}) - \nabla f_p(y^{(j_p)})\|^2 + 4N \mathbb{E}\| \nabla f_p(y^{(j_p)})\|^2
\leq \frac{4M^2}{N} \sum_{p=1}^{N} \mathbb{E}\|\Delta^{j_p}\|^2 + 4N M D \leq 4M^2 \mathbb{E}\|\Delta^{j_p}\|^2 + 4N D M.
\]
By substituting all these back, then we have
\[
\sum_{i=1}^{N} \mathbb{E}\|\nabla f_i(x^{(k)}) - \alpha^{(k)}_i\|^2 \leq \sum_{i=1}^{N} \frac{M^2}{N^2} \mathbb{E}\|x^{(k)} - x^{(k,i)}\|^2 \leq \frac{M^2}{N^2} \sum_{i=1}^{N} (2D\eta^2 \sum_{j=k-D}^{k-1} \mathbb{E}\|g^{(j)}\|^2 + 4D\eta n)
\]
\[
\leq \frac{M^2}{N} \sum_{i=1}^{N} (2D\eta^2 \sum_{j=k-D}^{k-1} (6M^2 \mathbb{E}\|\Delta_j\|^2 + 2D^2\eta^2 M d + 4\eta D d + \mathbb{E}\|\Delta^{(j+D-D)}\|_\infty^2 + 4M^2 \mathbb{E}\|\Delta_j\|^D + 4NMD + 4D\eta n))
\]
\[
\leq \frac{M^2}{N} (4D\eta^2 + 2D^2\eta^2 (16\mathbb{E}\|\Delta^{(k:k-2D)}\|_\infty^2 + 24M^2 D\eta (\eta DM + 1) + 4NMD)).
\]

Then we can conclude this lemma.

Based on the above lemmas, we establish the following theorem for \(\mathbb{E}\|\Delta^{(k)}\|_2\):**

**Proposition 1.** Assuming that \(f\) is \(M\)-smooth and \(\mu\)-strongly convex, and Requirement 2 is satisfied, if \(\eta \leq \min\{\frac{\mu \sqrt{\pi}}{8\sqrt{10}DMN}, \frac{2}{m+M}\}\), we have for all \(k \geq 0\)
\[
\mathbb{E}\|\Delta^{(k+1)}\|_2^2 \leq (1 - \frac{\mu \eta}{2}) \mathbb{E}\|\Delta^{(k:k-2D)}\|_\infty^2 + C_1 \eta^3 + C_2 \eta^2,
\]
where both \(C_1\) and \(C_2\) are constants that only depend on \(M, N, D, \mu\).

**Proof.** Since \(E[\Psi^{(k)}|x^{(k)}] = 0\), we have
\[
\mathbb{E}\|\Delta^{(k+1)}\|_2^2 = \mathbb{E}\|\Delta^{(k)} - \eta U^{(k)} - V^{(k)} + \eta E^{(k)}\|_2^2 + \eta^2 \mathbb{E}\|\Psi^{(k)}\|^2
\]
\[
\leq (1 + \alpha) \mathbb{E}\|\Delta^{(k)} - \eta U^{(k)}\|_2^2 + (1 - \frac{\mu}{1 + \alpha}) \mathbb{E}\|\Delta^{(k)} - \eta E^{(k)}\|_2^2 + \eta^2 \mathbb{E}\|\Psi^{(k)}\|^2
\]
\[
\leq (1 + \alpha) \mathbb{E}\|\Delta^{(k)} - \eta U^{(k)}\|_2^2 + 2(1 + \frac{\mu}{1 + \alpha}) \mathbb{E}\|\Delta^{(k)} - \eta E^{(k)}\|_2^2 + \eta^2 \mathbb{E}\|\Psi^{(k)}\|^2,
\]
where the first and the second inequalities are due to the Young’s inequality.

By substituting the bound in Lemma 1 and Lemma 2, we can get a one step result for \(\mathbb{E}\|\Delta^{(k+1)}\|_2^2\).

\[
\mathbb{E}\|\Delta^{(k+1)}\|_2^2 \leq (1 + \alpha)(1 - \mu \eta)^2 \mathbb{E}\|\Delta^{(k)}\|_2^2 + 2(1 + \frac{\mu}{1 + \alpha}) \mathbb{E}\|\Delta^{(k)} - \eta U^{(k)}\|_2^2 + \frac{N\eta^2}{n} \sum_{i=1}^{N} \mathbb{E}\|\nabla f_i(x^{(k)}) - \alpha^{(k)}_i\|^2
\]
\[
\leq (1 + \alpha)(1 - \mu \eta)^2 \mathbb{E}\|\Delta^{(k)}\|_2^2 + 2(1 + \frac{\mu}{1 + \alpha}) \mathbb{E}\|\Delta^{(k)} - \eta E^{(k)}\|_2^2 + \frac{N\eta^2}{n} \sum_{i=1}^{N} \mathbb{E}\|\nabla f_i(x^{(k)}) - \alpha^{(k)}_i\|^2
\]
\[
\leq (1 + \alpha)(1 - \mu \eta)^2 + \frac{2N\eta^2}{n} \sum_{i=1}^{N} \mathbb{E}\|\nabla f_i(x^{(k)}) - \alpha^{(k)}_i\|^2
\]
\[
\leq (1 + \alpha)(1 - \mu \eta)^2 + \frac{160\eta^2 M^4 (N + n) \eta^4}{n} (1 + \frac{1}{\alpha}) \mathbb{E}\|\Delta^{(k:k-2D)}\|_\infty^2 + C,
\]
where \(C = 2(1 + \frac{1}{\alpha}) \mathbb{E}\|\Delta^{(k:k-2D)}\|_\infty^2 + \frac{5M^2 (N + n) \eta^2}{n} (4\eta D d + 32\eta^2 M^2 d) + 48\eta^3 M^2 D^3 d (\eta DM + 1) + 8\eta^2 M N D^2 d).

By choosing \(\alpha = \mu \eta < 1\) and \(\eta \leq \frac{\mu \nu \sqrt{n}}{8\sqrt{10}(N + n) DM^2}\), we have \((1 + \alpha)(1 - \mu \eta)^2 + \frac{160\eta^2 M^4 (N + n) \eta^4}{n} (1 + \frac{1}{\alpha}) \leq 1 - \frac{\mu}{\alpha}\) and

\[
C \leq 2(1 + \frac{1}{\alpha}) \mathbb{E}\|\Delta^{(k:k-2D)}\|_\infty^2 + \frac{5M^2 (N + n) \eta^2}{n} (4\eta D d + 32\eta^2 M^2 D^3 d (\eta DM + 1) + 8\eta^2 M N D^2 d)
\]
\[
\leq \eta^3 \left( \frac{4M^3 d}{\mu} + \frac{10m^2 (N + n)}{n\mu} \left( \frac{3\mu^2 D^2 n d}{40(N + n) M} + \frac{6D^2 d \mu \sqrt{n}}{\sqrt{10(M + n)}} + 8M N D^2 d \right) \right) + \frac{4M^2 d}{\mu} + \frac{40M^2 (N + n) D d}{n\mu}.
\]

Then we can simplify the one iteration relation into
\[
\mathbb{E}\|\Delta^{(k+1)}\|_2^2 \leq (1 - \frac{\mu \eta}{2}) \mathbb{E}\|\Delta^{(k:k-2D)}\|_\infty^2 + C_1 \eta^3 + C_2 \eta^2.
\]
Theorem 6. Assume that $f$ is $M$-smooth and $\mu$-strongly convex, and Requirement 3 is satisfied. AGLD output sample $x^{(k)}$ with its distribution $p^{(k)}$ satisfies $W_2(p^{(k)}, p^*) \leq \epsilon$ for any $k \geq K = O(\log(1/\epsilon)/\epsilon^2)$ by setting $\eta = O(\epsilon^2)$.

Proof. Now we try to get a $\epsilon$-accuracy 2-Wasserstein distance approximation. In order to use Lemma 3, we can assume that $E\|\Delta^{(k)}\|^2 > \frac{\epsilon^2}{16}$ (for otherwise, we already have $\epsilon / 2$-accuracy) and $\frac{\exp(a\sqrt{\mu})}{\sqrt{\mu}} \leq \frac{\epsilon}{4}$ and $\frac{\exp(b\sqrt{\mu})}{\sqrt{\mu}} \leq \frac{\epsilon}{4}$. Then by using Lemma 3 and the fact that $|a|^2 + |b|^2 + |c|^2 \leq (|a| + |b| + |c|)^2$, the Wasserstein distance between $p^{(k)}$ and $p^*$ is bounded by

$$W_2(p^{(k)}, p^*) \leq \exp(-\frac{\eta\|k/(2D)\|}{4})W_0 + \frac{C_1\eta}{\sqrt{\mu}} + \frac{C_2\eta}{\sqrt{\mu}}.$$ 

Then by requiring that $\exp(-\frac{\eta\|k/(2D)\|}{4})W_0 \leq \frac{\epsilon}{8}$, $\frac{C_1\eta}{\sqrt{\mu}} \leq \frac{\epsilon}{8}$, $\frac{C_2\eta}{\sqrt{\mu}} \leq \frac{\epsilon}{8}$, we have $W_2(p^{(k)}, p^*) \leq \epsilon$. That is $\eta = O(\epsilon^2)$ and $k = O(\frac{1}{\epsilon^2} \log \frac{1}{\epsilon^2})$.

Lemma 3. Given a positive sequence $\{a_i\}_{i=0}^N$ and $\rho \in (0, 1)$, if we have $\frac{C}{\rho} < a_i$ for all $i \in \{1, 2, \cdots, N\}$ and $a_k \leq (1 - \rho) \max(a_{k-1} + a_{k-2} + \cdots + a_{k-D} + C)$, we can conclude

$$a_k \leq (1 - \rho)^{[k/D]} a_0 + \sum_{i=1}^{[k/D]} (1 - \rho)^{i-1}C \leq \exp(-\rho [k/D]) a_0 + \frac{C}{\rho}.$$

Proof. For all $i \in \{1, 2, \cdots, D\}$, we have $a_i \leq (1 - \rho)a_0 + C < a_0$.

Then $a_{D+1} \leq (1 - \rho) \max(a_1, a_{D-1}, \cdots, a_1) + C \leq (1 - \rho)^2 a_0 + \sum_{i=1}^2 (1 - \rho)^{i-1}C < (1 - \rho)a_0 + C$.

And $a_{D+2} \leq (1 - \rho) \max(a_{D+1}, a_D, \cdots, a_2) + C \leq (1 - \rho)^2 a_0 + \sum_{i=1}^3 (1 - \rho)^{i-1}C < (1 - \rho)a_0 + C$.

By repeating this argument, we can conclude $a_k \leq (1 - \rho)^{[k/D]} a_0 + \sum_{i=1}^{[k/D]} (1 - \rho)^{i-1}C$ by induction.

Since $1 - x \leq \exp(-x)$ and $\sum_{i=1}^\infty (1 - \rho)^{i-1}C \leq \frac{C}{\rho}$, we conclude this lemma.

8.2 B. Improved results under additional smoothness assumptions

Under the Hessian Lipschitz-continuous condition, we can improve the convergence rate of AGLD with random access.

Hessian Lipschitz: There exists a constant $L > 0$ such that for all $x, y \in \mathbb{R}^d$

$$\|\nabla^2 f(x) - \nabla^2 f(y)\| \leq L\|x - y\|_2^2.$$

(21)

We first give a technical lemma

Lemma 4. [Dalalyan and Karagulyan 2017] Assuming the $M$-smoothness $\mu$-strongly convex and $L$ Hessian Lipschitz smoothness of $f$, we have

$$\mathbb{E}\|S^{(k)}\|^2 \leq \frac{\eta^3 M^2d}{3},$$

(22)

$$\mathbb{E}\|V^{(k)} - S^{(k)}\|^2 \leq \frac{\eta^4 (L^2d^2 + M^3d)}{2},$$

(23)

where $S^{(k)} = \sqrt{\frac{\eta}{2}} \int_{k_0}^{(k+1)\eta} \int_{k_0}^{s} \nabla^2 f(y(r))dW(r)ds$.

Theorem 7. Assume that $f$ is $M$-smooth, $\mu$-strongly convex, and has Lipschitz-continuous Hessian, then AGLD variants with RA output sample $x^{(k)}$ with its distribution $p^{(k)}$ satisfies $W_2(p^{(k)}, p^*) \leq \epsilon$ for any $k \geq K = O(\log(1/\epsilon)/\epsilon^2)$ by setting $\eta = O(\epsilon)$. 

Proof. The proof is similar to the proof in Theorem 6 but there are some key differences. First, we also give the one-iteration result here. Since $E[\Psi^{(k)}|x^{(k)}] = 0$, we have

$$\mathbb{E}\|\Delta^{(k+1)}\|^2 = \mathbb{E}\|\Delta^{(k)} - \eta U^{(k)} - (V^{(k)} - S^{(k)}) - S_k + \eta E^{(k)}\|^2 + \eta^2 E\|\Psi^{(k)}\|^2$$

$$\leq (1 + \alpha)\mathbb{E}\|\Delta^{(k)} - \eta U^{(k)} - S^{(k)}\|^2 + (1 + \frac{1}{\alpha})\mathbb{E}\|V^{(k)} - S^{(k)} + \eta E^{(k)}\|^2 + \eta^2 E\|\Psi^{(k)}\|^2$$

$$\leq (1 + \alpha)\mathbb{E}\|\Delta^{(k)} - \eta U^{(k)}\|^2 + \mathbb{E}\|S^{(k)}\|^2 \leq \frac{\eta^2 E\|\Psi^{(k)}\|^2}{2(1 + 1/\alpha)(\mathbb{E}\|V^{(k)} - S^{(k)}\|^2 + \eta^2 E\|E^{(k)}\|^2)},$$

where $\alpha = \frac{\sqrt{\eta^2 + \eta^4 M^2d^2 + \eta^3 L^2d^3}}{\eta^2 M^2d}$.
where in the second inequality, we use the fact that $\mathbb{E}(S^{(k)}|\Delta^{(k)}, u^{(k)}) = 0$. By substituting the bound in Lemma 1, Lemma 2 and Lemma 3 we can get a one step result for $\mathbb{E}\|\Delta^{(k+1)}\|^2$ in the same way as in Proposition 1.

$$\mathbb{E}\|\Delta^{(k+1)}\|^2 \leq (1 - \eta_k \mu) \mathbb{E}\|\Delta\|^2_{k} + C_1 \eta^3 + C_2 \eta^2 \left(1 - T_{(RA)}\right).$$

Here, we can see that for RA, the $\eta^2$ term has now disappeared and that is the reason why we can get a better result. Then following similar argument as the proof of Theorem 8 it can be verified that AGLD with RA procedure can achieve $\epsilon$-accuracy after $k = \tilde{O}(\kappa^{3/2}/(\mu \epsilon))$ if we set $\eta < c_0 \sqrt{n}/(M \sqrt{dN})$, $n \geq 9$, and $D = N$. Moreover, the total number of component gradient evaluations is $T_g = \tilde{O}(N + \kappa^{3/2}/\sqrt{d}/\epsilon)$.

\[\Box\]

8.3 A deeper analysis for TMU-RA

Here, we probe into the TMU-RA algorithm to have a better understanding of the newly proposed Snapshot-Updating strategy. We first give the proof of the Theorem 3 in the main paper, and then extend the results to the general convex $f$.

**Theorem 8.** Assume $f$ is $M$-smooth, $\mu$-strongly convex and the has $L$-lipschitz Hessian and denote $\kappa = M/\mu$. TMU-RA output sample $x^{(k)}$ with its distribution $p^{(k)}$ satisfies $W_2(p^{(k)}, p^*) \leq \epsilon$ for any $k \geq K = \tilde{O}(\kappa^{3/2}/\sqrt{d}/(n\epsilon))$ if we set $\eta < c_0 \sqrt{n}/(M \sqrt{dN})$, $n \geq 9$, and $D = N$. Moreover, the total number of component gradient evaluations is $T_g = \tilde{O}(N + \kappa^{3/2}/\sqrt{d}/\epsilon)$.

**Proof of Theorem 8** Follow similar procedure as "B.2 SAGA Proof" of [Chatterji et al. 2018], we can establish the result for TMU-RA. The only difference is that snapshot are now totally updated every $D = N$ iterations, and we need to adjust the Step 5 and Step 9 in the original proof for SAGA-LD.

In Step 5, we need to bound $\mathbb{E}\|h_i^{(k)} - \nabla f_i(y^{(k)})\|^2$ where $\{h_i^{(k)}\}$ denotes the snapshot for $\{y_i^{(k)}\}$ updated at the same time with $\{\alpha_i^{(k)}\}$. Let $p = 1 - (1 - 1/N)^n$ denotes the probability that a index is chosen in RA and $N_k = [(k-1)/N] \cdot N$ denotes the nearest multiple of $N$ that is smaller than $k$, then for TMU-RA, we have

$$\mathbb{E}\|h_i^{(k)} - \nabla f_i(y^{(k)})\|^2 = \sum_{j=N_k}^{k-1} \mathbb{E}\|h_i^{(k)} - \nabla f_i(y^{(k)})\|^2 h_i^{(k)} = \nabla f_i(y^{(j)})\cdot \mathbb{P}[h_i^{(k)} = \nabla f_i(y^{(j)})]$$

$$\leq \tilde{M}^2 \sum_{j=N_k}^{k-1} \mathbb{E}\|y^{(j)} - y^{(k)}\|^2 \cdot (1 - p)^{k-1-j} + \mathbb{E}\|y^{(N_k)} - y^{(k)}\|^2 \cdot (1 - p)^{k-1-N_k}$$

$$\leq \tilde{M}^2 \sum_{j=N_k+1}^{k-1} \left[2\delta^2 (k-j)^2 M d + 4\delta j (k-j)\right]^2 \cdot (1 - p)^{k-1-j} + \left[2\delta^2 (k-N_k)^2 M d + 4\delta j (k-N_k)\right] \cdot (1 - p)^{k-1-N_k}$$

$$\leq \tilde{M}^2 \sum_{j=N_k+1}^{k-1} \left[2\eta^2 (k-j)^2 M d + 4\eta j (k-j)\right]^2 \cdot (1 - p)^{k-1-j} + \left[2\eta^2 (k-N_k)^2 M d + 4\eta j (k-N_k)\right] \cdot (1 - p)^{k-1-N_k}$$

$$\leq \tilde{M}^2 \sum_{j=1}^{\infty} \left[2\eta^2 j^2 M d + 4\eta j\right]^2 \cdot (1 - p)^j \cdot \left(1 - p \right)^{k-1-N_k}$$

$$\leq \tilde{M}^2 \sum_{j=1}^{\infty} \left[2\eta^2 j^2 M d + 4\eta j\right]^2 \cdot (1 - p)^j \leq \frac{2\eta^2 \tilde{M}^2 M d}{p^2} + \frac{4\eta \tilde{M}^2}{p},$$

where the second inequality is due to the update rule of TMU, the third inequality follows from [20] and the rest are just basic calculation. Inequality [23] is just the same as Step 5 in the proof of SAGA-LD in [Chatterji et al. 2018].

In Step 9, the authors establish following iterative relation for the Lyapunov function $T_k = \sum_i \|x_i^{(k)} - h_i^{(k)}\|^2 + \|x^{(k)} - y^{(k)}\|^2$.

$$\mathbb{E}[T_{k+1}] \leq (1 - \rho)T_k + 2\eta^3 \Delta + \frac{2\eta^3 \Delta}{\mu},$$

(25)
where $\rho = \min\{\frac{L}{\mu}, \frac{\mu}{L}\}$, $\Box = 2M^2d + \frac{72N^2M^2}{\eta MN} + 1$ and $\triangle = \frac{1}{2}(L^2d^2 + M^3d)$. For TMU-RA, we can just follow the same way to get (28) if $k \mod N \neq 0$. If $k \mod N = 0$, since we update the whole snapshot set, the result in Step 7 of their analysis no longer holds and we cannot conclude (25) following their analysis.

Actually, if $k \mod N = 0$, then $g^{(k)} = \nabla f(x^{(k)})$. Follow [13] we have

$$E\|y^{(k+1)} - x^{(k+1)}\|_2^2$$

$$= E\|y^{(k)} - x^{(k)}\|_2^2 - E\|\nabla f(y^{(k)}) - \nabla f(x^{(k)})\|_2^2 - \sqrt{2} \int_{k\eta}^{(k+1)\eta} \int_{k\eta}^{s} \nabla^2 f(y(t))dB(t)ds$$

$$- \frac{\eta}{\Delta^{(k)}} \{ \nabla f(y(s)) - \nabla f(y^{(k)}) - \sqrt{2} \int_{k\eta}^{s} \nabla^2 f(y(t))dB(t) \} ds^2$$

$$\leq (1 + a)E\|\Delta^{(k)} - \eta U^{(k)} - \nabla f(x^{(k)})\|_2^2 + (1 + a)E\|\Delta^{(k)}\|_2^2 + \|\Delta^{(k)} - \eta U^{(k)} - \nabla f(x^{(k)})\|_2^2$$

$$\leq (1 + a)E\|\Delta^{(k)} - \eta U^{(k)}\|_2^2 + (1 + a)\|\nabla f(x^{(k)})\|_2^2$$

(26)

where the first inequality is due to Cauchy-Schwartz inequality and the second inequality follows from the fact that $E\|\nabla f(x^{(k)}) - y^{(k)}\|_2 = 0$ and $\Delta^{(k)} = \nabla f(x^{(k)}) - \eta U^{(k)}$.

By lemma [13] and lemma [3] we have

$$\begin{align*}
E\|\nabla f(x^{(k)})\|_2^2 &\leq \frac{1}{2}n^4(M^3d + M^2d^2), \\
E\|\Delta^{(k)} - \eta U^{(k)}\|_2^2 &\leq (1 - \eta \mu)^2 E\|\Delta^{(k)}\|_2^2, \\
E\|\nabla f(x^{(k)})\|_2^2 &\leq 2M^2\frac{n^3d}{\eta}. \\
\end{align*}$$

By substituting the above inequality back to (28) we have

$$E\|y^{(k+1)} - x^{(k+1)}\|_2^2 \leq (1 + a)(1 - \eta \mu)^2 E\|\Delta^{(k)}\|_2^2 + \frac{2(1 + a)M^2\eta^3d}{3} + \frac{1}{2}\eta^4(1 + a)(M^3d + L^2d^2).$$

Since all the snapshot $a_i^{(k)}$ are now updated at $x^{(k)}$, we have

$$\sum_{i=1}^{N} \|a_i^{(k)} - h_i^{(k)}\|_2^2 = \sum_{i=1}^{N} \|\nabla f_i(x^{(k)}) - \nabla f_i(y^{(k)})\|_2^2 \leq \frac{M^2\|x^{(k)} - y^{(k)}\|_2^2}{\eta},$$

where the inequality follows from the smoothness of $f_i$.

Thus we have

$$E[T_{k+1}] = E\|x^{(k)} - y^{(k)}\|_2^2 + c \sum_{i=1}^{N} E\|a_i^{(k)} - h_i^{(k)}\|_2^2$$

$$\leq (1 + a)(1 - \eta \mu)^2 E\|\Delta^{(k)}\|_2^2 + \frac{2(1 + a)M^2\eta^3d}{3} + \frac{1}{2}\eta^4(1 + a)(M^3d + L^2d^2) + \frac{cM^2}{N} E\|\Delta^{(k)}\|_2^2.$$

By choosing $a = \eta \mu \leq 1/6$ and $c \leq \frac{\eta \mu}{2}$, we can conclude

$$E[T_{k+1}] \leq (1 - \rho)T_k + 2\eta^3\Box + \frac{2\eta^3\triangle}{\mu}.\quad (27)$$

Note that in Step 9 of [Chatterji et al. 2018], they require $c \leq \frac{24\eta^2N^2}{\eta^2}$. If we choose $\eta \leq \frac{\mu}{48\sqrt{N}}$, then $\frac{24\eta^2N^2}{\eta^2} \leq \frac{\mu}{2}$.

With all these in hand, we can follow the proof of SAGA-LD and obtain similar result for TMU-RA as Theorem 4.1. in [Chatterji et al. 2018].

$$\mathcal{W}_2(p^{(k)}, p^*) \leq 5 \exp\left(-\frac{\mu}{T}\right)\mathcal{W}_2(p^{(0)}, p^*) + \frac{2\eta Ld}{\mu} + \frac{2\eta M^3/2\sqrt{d}}{\mu} + \frac{24\eta M\sqrt{dN}}{\sqrt{mn}}.\quad (28)$$

Then by making each part in the right hand of (28) less than $\epsilon/4$, and treating $M, \mu$ and $L$ as constants of order $O(N)$ if they appear alone, we complete the proof of Theorem 8 and conclude that the component gradient evaluations is $T_g = \tilde{O}(N + \kappa^{3/2}\sqrt{d}/\epsilon)$. □
8.4 Extension to general convex \( f \)

By inequality (A.17) in supplementary in [Zou et al. 2018a], we have the following lemma.

**Lemma 5.** Assuming the target distribution \( p^* \propto e^{-f} \) has bounded forth order moment, i.e., \( \mathbb{E}_p[||x||^4] \leq \tilde{U}d^2 \), and \( \hat{f} = f(x) + \lambda ||x||^2/2 \), then for \( \hat{p}^* \propto e^{-\hat{f}} \), we have \( \mathbb{E}(\hat{p}^*, p^*) \leq \sqrt{\lambda \tilde{U}d^2}/2 \).

As we have figure out the dependency on the condition number \( \kappa \) for TMU-RA in Theorem 3. Combining Theorem 8 and Lemma 5, we have the following result.

**Theorem 9.** Suppose the assumptions in Theorem 6 hold and further assume the target distribution \( x \sim \text{AGLD} \). By integrating \( \tilde{x} \), where \( h_{\xi} \) is dissipative. There exists constants \( a, b > 0 \).

8.5 Theoretical results for nonconvex \( f(x) \)

In this section, we characterize the convergence rates of AGLD for sampling from non-log-concave distributions. We first lay out the assumptions that are necessary for our theory.

**Assumption 7.** [Dissipative] There exists constants \( a, b > 0 \) such that the sum \( f \) satisfies

\[
\langle \nabla f(x), x \rangle \geq b ||x||^2 - a,
\]

for all \( x \in \mathbb{R}^d \).

This assumption is typical for the ergodicity analysis of stochastic differential equations and diffusion approximations. It indicates that, starting from a position that is sufficiently far from the origin, the Langevin dynamics \( \text{[12]} \) moves towards the origin on average.

In order to analyze the long-term behavior of the error between the discrete time AGLD algorithm and the continuous Langevin dynamics, we follow [Raginsky et al. 2017] and construct the following continuous time Markov process \( \{x(t)\}_{t \geq 0} \) to describe the approximation sequence \( x^{(k)} \):

\[
dx(t) = -h(x(t))dt + \sqrt{2}dB(t),
\]

where \( h(x(t)) = \sum_{k=0}^{\infty} g^{(k)} \mathbb{1}_{[\eta k, \eta (k+1)]} \) and \( g^{(k)} \) are the aggregated gradient approximation constructed in the \( k \)-th step of AGLD. By integrating \( x(t) \) on interval \([\eta k, \eta (k+1)]\), we have

\[
x(\eta (k+1)) = x(\eta k) - \eta g^{(k)} + \sqrt{2}\xi^{(k)},
\]

where \( \xi^{(k)} \) is a standard Gaussian variable. This implies that the distribution of \( \{x(0), \ldots, x(\eta k), \ldots\} \) is equivalent to \( \{x^{(0)}, \ldots, x^{(k)}, \ldots\} \), i.e., the iterates in AGLD. Note that \( x(t) \) is not a time-homogeneous Markov chain since the drift term \( h(x(t)) \) also depends on some historical iterates. However, (8.20) showed that one can construct an alternative Markov chain which enjoys the same one-time marginal distribution as that of \( x(t) \) and is formulated as follows,

\[
d\tilde{x}(t) = -\tilde{h}(\tilde{x}(t))dt + \sqrt{2}dB(t),
\]

where \( \tilde{h}(\tilde{x}(t)) = \mathbb{E}[h(x(t))|x(t) = \tilde{x}(t)] \). We denote the distribution of \( \tilde{x}(t) \) as \( \mathbb{P}_t \), which is identical to that of \( x(t) \). Recall the Langevin dynamics starting from \( y(0) = x(0) \), i.e.,

\[
dy(t) = -\nabla f(y(t))dt + \sqrt{2}dB(t),
\]

and define the distribution of \( y(t) \) as \( \mathbb{Q}_t \). According to the Girsanov formula, the Radon-Nykodim derivative of \( \mathbb{P}_t \) with respect to \( \mathbb{Q}_t \) is

\[
\frac{d\mathbb{P}_t}{d\mathbb{Q}_t}(\tilde{x}(s)) = \exp\left\{ -\int_0^t (\tilde{h}(\tilde{x}(s)) - \nabla f(\tilde{x}(s)))^T dB(s) - \frac{1}{4} \int_0^t \mathbb{E}[h(\tilde{x}(s)) - \nabla f(\tilde{x}(s))]^2 ds \right\},
\]

where \( \tilde{h}(\tilde{x}(t)) = \mathbb{E}[h(x(t))|x(t) = \tilde{x}(t)] \).
which in turn indicates that the KL-divergence between $\mathbb{P}_t$ and $\mathbb{Q}_t$ is

$$KL(\mathbb{Q}_t \| \mathbb{P}_t) = -\mathbb{E}[\log(\frac{d\mathbb{P}_t}{d\mathbb{Q}_t}(\tilde{x}(s)))] = \frac{1}{4} \int_0^t \mathbb{E}[\|b(\tilde{x}(s)) - \nabla f(\tilde{x}(s))\|_2^2] ds. \quad (33)$$

According to the following lemma, we can upper bound the $\mathcal{W}_2$ distance $\mathcal{W}_2(P(x^{(k)}), x(\eta k))$ with the KL-divergence $KL(\mathbb{Q}_{\eta k} \| \mathbb{P}_{\eta k})$.

**Lemma 6 (\S) .** For any two probability measures $P$ and $Q$, if they have finite second moments, we have

$$\mathcal{W}_2(Q, P) \leq \Lambda(\sqrt{KL(Q \| P)} + \sqrt{KL(P \| Q)})$$

where $\Lambda = 2 \inf_{\lambda>0} \sqrt{1/\lambda (3/2 + \log E_{x \sim P} [\exp(\lambda \|x\|_2^2)])}$

**Lemma 7 (Lemma 3.3 in (Raginsky et al. 2017)).** Under Assumption 6 and 7, if $b \geq 2$, we have

$$\log E[exp(||x(t)||_2^2)] \leq \|x(0)\|_2^2 + 2 \beta d + \eta t.$$

Note that if $b$ is less than 2, we can divide $f$ by $b/2$ and consider the dynamic $dx(t) = 2\nabla f(x(t))/b + \sqrt{b}d(t)$, whose stationary distribution is still the target distribution $p^* \propto \exp(-f(x))$. It can be verified that the smoothness of $2f(x)/b$ is the same as $f(x)$ and the analysis we derive here is still suitable for this dynamic. From now on, we assume that $b \geq 2$ holds for $f(x)$, and we do not make this transformation in order to keep the notation similar to that in the convex setting.

First, we establish some lemmas will be useful in the proof of the main results.

**Lemma 8 (Lemma A.2 in (Zou et al. 2019)).** Under Assumption 9 and 7, the continuous-time Markov chain $y(t)$ generated by Langevin dynamics converges exponentially to the stationary distribution $p^*$, i.e.,

$$\mathcal{W}_2(P(y(t)), p^*) \leq D_4 \exp(-t/D_5),$$

where both $D_4$ and $D_5$ are in order of $\exp(\tilde{O}(d))$ if we use $a = \tilde{O}(b)$ to hide some logarithmic terms of $b$.

**Lemma 9.** Under Assumption 9 for all $x \in \mathbb{R}^d$ and $i \in \{1, \ldots, N\}$, we have

$$\|\nabla f_i(x)\| \leq \tilde{M} \|x\| + G \quad \text{and} \quad \|\nabla f_i(x)\|^2 \leq \tilde{M}^2 \|x\|^2 + 2G^2,$$

where $G = \max_{i=1, \ldots, N} \|f_i(0)\|$. \qedhere

**Proof.** According to the $\tilde{M}$-smoothness of $f_i$, we have

$$\|f_i(x)\| = \|f_i(x) - f_i(0) + f_i(0)\| \leq \|f_i(x) - f_i(0)\| + \|f_i(0)\| \leq \tilde{M} \|x\| + G.$$ Follow the Cauchy-Schwartz inequality, we can conclude the second part of the lemma.

**Lemma 10.** Under Assumption 9 and 7 for sufficiently small stepsizes $\eta$, if the initial point $x^{(0)} = 0$, the expectation of the $l^2$ norm of iterates and aggregated gradient generated in AGLD is bounded by

$$\mathbb{E}\|x^{(k)}\|_2^2 \leq 4(1 + 1/b)(a + G^2 + d) := D_B \quad \text{and} \quad \mathbb{E}\|g^{(k)}\|_2^2 \leq 4N^2(2\tilde{M}^2D_B + G^2),$$

where $G = \max_{i=1, \ldots, N} \|f_i(0)\|$. \qedhere

**Proof.** We prove the bound of $\mathbb{E}\|x^{(k)}\|_2$ by induction.

When $k = 1$, we have

$$\mathbb{E}\|x^{(1)}\|_2^2 = \mathbb{E}\|x^{(0)}\|_2^2 - \eta \nabla f(x^{(0)})_2^2 + \sqrt{2\eta} \xi^{(0)}_2^2 = \eta^2 \mathbb{E}\|\nabla f(0)\|_2^2 + \mathbb{E}\|\sqrt{2\eta} \xi^{(0)}\|_2^2 \leq \eta^2 G^2 + 2\eta d,$$

where the second equality holds since $x^{(0)} = 0$, $g^{(0)} = \nabla f(0)$, and $\xi^{(0)}$ is independent of $\nabla f(0)$. Thus, for sufficiently small $\eta$, it is easy to make the conclusion hold for $\mathbb{E}\|x^{(1)}\|_2^2$.

Now assume that the result holds for all iterates from 1 to $k$, then for the $(k+1)$-th iteration, we have

$$\mathbb{E}\|x^{(k+1)}\|_2^2 = \mathbb{E}\|x^{(k)}\|_2^2 - \eta \nabla f(x^{(k)})_2^2 + \sqrt{2\eta} \xi^{(k)}_2^2 \leq \mathbb{E}\|x^{(k)}\|_2^2 - \eta g^{(k)}_2 + 2\eta d. \quad (34)$$

For the first part of the last inequality, we have

$$\mathbb{E}\|x^{(k)} - \eta g^{(k)}\|_2^2 = \mathbb{E}\|x^{(k)} - \eta \nabla f(x^{(k)}) + \eta \nabla f(x^{(k)}) - \eta g^{(k)}\|$$

$$\leq (1 + \alpha)\mathbb{E}\|x^{(k)} - \eta \nabla f(x^{(k)})\|_2^2 + \frac{2\eta^2 N\tilde{M}^2}{n}(N + n)(2 + \frac{1}{\alpha^2}) + \frac{1}{\alpha^2} \sum_{i=1}^{N} \mathbb{E}\|x^{(k)} - x^{(k_i)}\|_2^2, \quad (35)$$
where the second equality follows from the definition of $\Psi^{(k)}$ (35) and $\Gamma^{(k)}$ (36), the third equality is due to that $\mathbb{E}[\Gamma^{(k)}] = 0$ and the conditional independence of $\Gamma^{(k)}$ and $x^{(k)} - \eta \nabla f(x^{(k)})$, the first inequality follows from that $\mathbb{E}\|X + Y\|^2 \leq (1 + \alpha)\mathbb{E}\|X\|^2 + (1 + \frac{1}{2})\mathbb{E}\|Y\|^2$ and $2\mathbb{E}(X, Y) \leq \mathbb{E}\|X\|^2 + \mathbb{E}\|Y\|^2$ for $\forall \alpha > 0$ and any random variable $X$ and $Y$, and the last inequality is due to Lemma 2 and the $M$-smoothness of $f_k$.

For the first term in (35), we have

$$\mathbb{E}\|x^{(k)} - \eta \nabla f(x^{(k)})\|^2 = \mathbb{E}\|x^{(k)}\|^2 + \eta^2 \mathbb{E}\sum_{i=1}^{N} \nabla f_i(x^{(k)}) - 2\eta \mathbb{E}(x^{(k)}, \nabla f(x^{(k)}))$$

$$\leq \mathbb{E}\|x^{(k)}\|^2 + 2\eta^2 N(\tilde{M}^2 \mathbb{E}\|x^{(k)}\|^2 + G^2) + 2\eta(a - b\mathbb{E}\|x^{(k)}\|^2)$$

$$= (1 - 2b\eta + 2\eta^2 \tilde{M}^2)\mathbb{E}\|x^{(k)}\|^2 + 2\eta^2 G^2 + 2\eta a,$$  

(36)

where in the first inequality, we use $\|\sum_{i=1}^{N}a_i\|^2 \leq N\sum_{i=1}^{N}a_i^2$, Lemma 9 and the dissipative assumption of $f_k$.

For the second term of (35), we have

$$\mathbb{E}\|x^{(k)} - x^{(k,i)}\|^2 = \mathbb{E}\|\sum_{j=k-i}^{k-1} g^{(j)} + \sqrt{2\eta} \xi^{(j)}\|^2 \leq 2\eta^2 \mathbb{E}\sum_{j=k-i}^{k-1} g^{(j)} + 2\mathbb{E}\sum_{j=k-i}^{k-1} \sqrt{2\eta} \xi^{(j)}$$

$$\leq 2D\eta^2 \sum_{j=k-D}^{k-1} \mathbb{E}\|g^{(j)}\|^2 + 2 \sum_{j=k-D}^{k-1} \mathbb{E}\|\sqrt{2\eta} \xi^{(j)}\|^2 \leq 2D\eta^2 \sum_{j=k-D}^{k-1} \mathbb{E}\|g^{(j)}\|^2 + 4Ddn,$$  

(37)

where in the second inequality, we use $k_i \geq k - D$ and $\|\sum_{j=1}^{D}a_j\|^2 \leq D\sum_{j=1}^{D}a_j$, and the independence of $\xi^{(j)}$s. Moreover, we have

$$\mathbb{E}\|g^{(j)}\|^2 = \mathbb{E}\|\sum_{p \in S_j} \frac{N}{n} (\nabla f_p(x^{(j)})) - \alpha^{(j)}_p\|^2 + \sum_{p=1}^{N} \alpha^{(j)}_p$$

$$\leq 2\mathbb{E}\sum_{p \in S_j} \frac{N}{n} (\nabla f_p(x^{(j)})) - \alpha^{(j)}_p\|^2 + 2\mathbb{E}\sum_{p=1}^{N} \alpha^{(j)}_p$$

$$\leq \frac{N^2}{n} \sum_{p \in S_j} \mathbb{E}\|\nabla f_p(x^{(j)})) - \alpha^{(j)}_p\|^2 + 2N \sum_{p=1}^{N} \mathbb{E}\|\alpha^{(j)}_p\|^2$$

$$\leq \frac{2N^2}{n} \sum_{p \in S_j} \mathbb{E}\|x^{(j)} - x^{(j,p)}\|^2 + 4N \sum_{p=1}^{N} (\tilde{M}^2 \mathbb{E}\|x^{(j,p)}\|^2 + G^2)$$

$$\leq 8N^2 \tilde{M}^2 (\Delta^{(k)}_D)^+ + 4N^2 G^2$$  

(38)

where we denote $[\Delta^{(k)}_D]^+ := \max\{\mathbb{E}\|x^{(j-D)}\|^2, \mathbb{E}\|x^{(j-D+1)}\|^2, \cdots, \mathbb{E}\|x^{(j)}\|^2\}$, and the third inequality follows from the definition of $\alpha^{(j)}_p$ and Lemma 9.

Combining (35), (36), (37), and (38) and choosing $\alpha = b\eta/2$, we have

$$\mathbb{E}\|x^{(k+1)}\|^2 \leq \mathbb{E}\|x^{(k)} - \eta g^{(k)}\|^2 + 2\eta d$$

$$\leq (1 + b\eta/2)((1 - 2b\eta + 2\eta^2 \tilde{M}^2)\mathbb{E}\|x^{(k)}\|^2 + 2\eta^2 G^2 + 2\eta a)$$

$$+ \frac{2\eta^2 N \tilde{M}^2}{n} ((N + n)(2 + \frac{2}{b\eta}) + 1)N(2D^2 \eta^2 (8N^2 \tilde{M}^2 (\Delta^{(k)}_D)^+ + 4N^2 G^2) + 4Ddn) + 2\eta d$$

$$\leq (1 - 3b\eta/2 - b^2 \eta^2 + 2N\eta^2 \tilde{M}^2 + bN\eta^3 \tilde{M}^2 + \frac{64N^4 \tilde{M}^4 D^2 \eta^4}{n} (N + n)(2\eta + 2/b))\|\Delta^{(k)}_D\|^+$$

$$+ (1 + b\eta/2)(2N\eta^2 G^2 + 2\eta a) + \frac{4N^2 \tilde{M}^2 \eta^4}{n} (N + n)(2\eta + 2/b)(8N^2 G^2 D^2 \eta^2 + 4Ddn) + 2\eta d,$$  

(39)

By selecting small enough $\eta$, we can make $A \leq b\eta/2, B \leq 2\eta d, b\eta/2 \leq 1$ and $N\eta \leq 1$ and thus have

$$\mathbb{E}\|x^{(k+1)}\|^2 \leq 4(1 - b\eta)(1 + 1/b)(a + G^2 + d) + 4\eta(a + G^2 + d) \leq 4(1 + 1/b)(a + G^2 + d),$$
where we use the induction condition $|\Delta_D^{(k)}|^+ \leq 4(1 + 1/b)(a + G^2 + d)$.

According to (38), we can establish
\[
\mathbb{E}\|g^{(k)}\|^2 \leq 4N^2(2\hat{M}^2D_B + G^2).
\]

Based on these lemmas, we now give our main theorem on the convergence of sample distribution.

**Theorem 10.** Under Assumption 2 and AGLD output sample $x^{(k)}$ with its distribution $p^{(k)}$ satisfies $W_2(p^{(k)}, p^*) \leq \epsilon$ for any $k \geq O(\log(1/\epsilon)/\epsilon^4)$ by setting $n = O(\epsilon^4)$.

**Proof.** Denote the distribution of $x^{(k)}$ and $x(\eta k)$ as $p^{(k)}$ and $Q_k$ respectively. By Lemma 6, we have
\[
W(Q_k, p^{(k)}) \leq \Lambda(\sqrt{KL(Q_k || p^{(k)})} + \sqrt{KL(Q_k || p^{(k)})}).
\]

By data-processing theorem in terms of KL-divergence, we have
\[
KL(Q_k || p^{(k)}) \leq KL(Q_{\eta k} || p_{\eta k}) = \frac{1}{4} \int_0^{k\eta} \mathbb{E}||h(\tilde{x}(s)) - \nabla f(\tilde{x}(s))||^2 ds = \frac{1}{4} \int_0^t \mathbb{E}||h(x(s)) - \nabla f(x(s))||^2 ds,
\]
where the last equality holds since $x(s)$ and $\tilde{x}(s)$ have the same one-time distribution.

Since $h(x(s))$ is a step function and remains constant when $s \in [v\eta, (v + 1)\eta]$ for any $v$, we have
\[
\int_0^t \mathbb{E}||h(x(s)) - \nabla f(x(s))||^2 ds = \sum_{v=0}^{k-1} \int_{v\eta}^{(v+1)\eta} \mathbb{E}||g^{(v)} - \nabla f(x(s))||^2 ds
\]
\[
\leq 2 \sum_{v=0}^{k-1} \int_{v\eta}^{(v+1)\eta} \mathbb{E}||g^{(v)} - \nabla f(x^{(v)})||^2 ds + 2 \sum_{v=0}^{k-1} \mathbb{E}||\nabla f(x(v\eta)) - \nabla f(x(s))||^2 ds
\]
where we use the Young’s inequality and the fact that $x^{(v)} = x(v\eta)$ in the inequality.

According to Lemma 2, we have
\[
\mathbb{E}||g^{(v)} - \nabla f(x^{(v)})||^2 \leq 2\mathbb{E}||\Psi^{(v)}||^2 + 2\mathbb{E}||\Gamma^{(v)}||^2 \leq \frac{2N(2(N + n) + 1)}{n} \sum_{i=1}^N \mathbb{E}||\nabla f_i(x^{(v)}) - \alpha_i^{(v)}||^2
\]
\[
\leq \frac{2N\hat{M}^2(2(N + n) + 1)}{n} \sum_{i=1}^N \mathbb{E}||x^{(v)} - x^{(v)}||^2 = \frac{2M^2(2(N + n) + 1)}{n} \sum_{i=1}^N \mathbb{E}||x^{(v)} - x^{(v)}||^2
\]
\[
= \frac{2M^2(2(N + n) + 1)}{n} \sum_{i=1}^N \mathbb{E}||x^{(v)} - x^{(v)}||^2 \eta^{(j)} + \sum_{j=v}^N \sqrt{2}\eta_j ||^2 \leq \frac{2M^2(2(N + n) + 1)}{n} \sum_{j=v}^N (2\eta^2 ||g^{(j)}||^2 + 2\mathbb{E}||\sqrt{2}\eta_j ||^2)
\]
\[
\leq \frac{16M^2(2(N + n) + 1)}{n} (\eta^2 N^2D^2(2\hat{M}^2D_B + G^2) + D\eta d),
\]
where we use the $\hat{M}$ smoothness of $f_i$’s and $M = N\hat{M}$ in the second line, Requirement 3 and Jensen’s inequality in the third line and Lemma 10 in the last line.

For the second term of (41), we have
\[
\sum_{v=0}^{k-1} \int_{v\eta}^{(v+1)\eta} \mathbb{E}||\nabla f(x(v\eta)) - \nabla f(x(s))||^2 ds \leq \sum_{v=0}^{k-1} \int_{v\eta}^{(v+1)\eta} M^2||\nabla f(x(v\eta)) - x(s)||^2 ds
\]
\[
= \sum_{v=0}^{k-1} \int_{v\eta}^{(v+1)\eta} M^2((s - v\eta)^2||g^{(k)}||^2 + 2(s - v\eta))ds \leq \sum_{v=0}^{k-1} \left( \frac{M^2\eta^3}{3} ||g^{(k)}||^2 + 2M^2\eta^2d \right)
\]
\[
\leq \frac{4kN^2M^2\eta^3(2\hat{M}^2D_B + G^2)}{3} + 2kM^2\eta^2d,
\]
where the first inequality follows from the $M$-smoothness assumption of $f(x)$, the first equality follows from the definition of $x(s)$, and the last inequality is due to Lemma 10.
Combining (40), (41), (42) and (43), we have

\[
KL(Q_k\|p^{(k)}) \leq \frac{8kM^2(2(N + n) + 1)\eta^2}{n}(\eta N^2 D^2(2M^2DB + G^2) + Dd) + \frac{4kN^2M\eta^3(2M^2DB + G^2)}{3} + 2kM^2\eta^2d
\]

(44)

Applying Lemma6, Lemma7 and Lemma8, and choosing \(\lambda = 1\) and \(x(0) = 0\) in Lemma6 we obtain

\[
W_2(P(x^{(k)}), \mu) \leq W_2(P(x^{(k)}), P(x(\eta k))) + W_2(P(x(\eta k)), \mu^*)
\]

\[
\leq D_A \frac{8kM^2(2(N + n) + 1)\eta^2}{n}(\eta N^2 D^2(2M^2DB + G^2) + Dd) + \frac{4kN^2M\eta^3(2M^2DB + G^2)}{3} + 2kM^2\eta^2d^{1/4} + D_A e^{-k\eta/D_3},
\]

where we assume \(\sqrt{KL(Q_k\|p^{(k)})} \leq 1\) since our target is to obtain high equality samples, and we denote \(D_A = 4\sqrt{3}/2 + (2b + d)\eta k\). If we denote \(T = k\eta\) and hide the constants, we have

\[
W_2(p^{(k)}, \mu^*) \leq O((T\eta + T^2\eta^2)^{1/4} + e^{-T/D_3}).
\]

By letting \(T = O(D_5 \log(\frac{1}{\epsilon}))\), \(\eta = \tilde{O}(\epsilon^4)\) and \(k = T/\eta = \tilde{O}(\frac{1}{\epsilon^4})\), we have \(W_2(P(x^{(k)}), \mu^*) \leq \epsilon\). 

8.6 Extra experiments

In this section, we present the simulation experiment of sampling from distribution with convex \(f(x)\) and the Bayesian ridge regression experiment on SliceLocation dataset.

**Sampling from distribution with convex \(f(x)\)** In this simulated experiment, each component function \(f_i(x)\) is convex and constructed in the following way: first a \(d\)-dimensional Gaussian variable \(a_i\) is sampled from \(N(21d, 4I_{d \times d})\), then \(f_i(x)\) is set to \(f_i(x) = (x - a_i)^T \Sigma (x - a_i)/2\), where \(\Sigma\) is a positive definite symmetric matrix with maximum eigenvalue \(M = 40\) and minimum eigenvalue \(\mu = 1/2\). It can be verified that \(f(x)\) is \(M\) smooth, \(\mu\) strongly convex and \(0\) Hessian Lipschitz. The target density \(p^*\) is a multivariate Gaussian distribution with mean \(\tilde{a} = \sum_{i=1}^n a_i\) and covariance matrix \(\Sigma\). In order to compare the performance of different Data-Accessing and Snapshot-Updating strategies, we show the results for PPU/PTU/TMU with RA and TMU with RA/CA/RR.

We report the \(W_2\) distance between the distribution \(p^{(k)}\) of each iterate and the target distribution \(p^*\) for different algorithms with respect to the number of data passes (evaluation of \(n \nabla f_i\)’s) in Figure 4. In order to estimate \(W_2(p^{(k)}, p^*)\), we repeat all algorithms for 20,000 times and obtain 20,000 random samples for each algorithm in each iteration. From the left sub-figure of Figure 4 we can see that TMU-RA outperforms SVRG-LD (PTU-RA) and SAGA-LD (PPU-RA). The right sub-figure of Figure 4 shows that RA Data-Accessing strategy outperforms CA/RR when using the same Snapshot-Updating strategy.

![Figure 4: \(W_2\) distance on simulated data.](image)

**Bayesian ridge regression on SliceLocation dataset** Here, we present the results of Bayesian ridge regression on SliceLocation dataset. Similar results as that on YearPredictionMSD dataset can be observed, i.e. (i) TMU type methods have the best performance among all the methods with the same Data-Accessing strategy, (ii) SVRG+ and PPU type methods constantly outperform LMC, SGLD, and PTU type methods. (iii) TMU-RA outperforms TMU-CA/TMU-RR, when the dataset is fitted to the memory.
Figure 5: Bayesian Ridge Regression on SliceLocation dataset.