Stochastic Gradient Hamiltonian Monte Carlo for Non-Convex Learning *

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Abstract
Stochastic Gradient Hamiltonian Monte Carlo (SGHMC) is a momentum version of stochastic gradient descent with properly injected Gaussian noise to find a global minimum. In this paper, non-asymptotic convergence analysis of SGHMC is given in the context of non-convex optimization, where subsampling techniques are used over an i.i.d dataset for gradient updates. Our results complement those of [RRT17] and improve on those of [GGZ18].

1 Introduction
Let \((\Omega, \mathcal{F}, P)\) be a probability space where all the random objects of this paper will be defined. The expectation of a random variable \(X\) with values in a Euclidean space will be denoted by \(E[X]\).

We consider the following optimization problem

\[
F^* := \min_{x \in \mathbb{R}^d} F(x), \quad F(x) := E[f(x, Z)] = \int_Z f(x, z) \mu(dz), \quad x \in \mathbb{R}^d
\]

and \(Z\) is a random element in some measurable space \(Z\) with an unknown probability law \(\mu\). The function \(x \mapsto f(x, z)\) is assumed continuously differentiable (for each \(z\)) but it can possibly be non-convex. Suppose that one has access to i.i.d samples \(Z = (Z_1, ..., Z_n)\) drawn from \(\mu\), where \(n \in \mathbb{N}\) is fixed. Our goal is to compute an approximate minimizer \(X^\dagger\) such that the population risk

\[
E[F(X^\dagger)] - F^*
\]

is minimized, where the expectation is taken with respect to the training data \(Z\) and additional randomness generating \(X^\dagger\).

Since the distribution of \(Z_i, i \in \mathbb{N}\) is unknown, we consider the empirical risk minimization problem

\[
\min_{x \in \mathbb{R}^d} F^\sharp(x), \quad F^\sharp(x) := \frac{1}{n} \sum_{i=1}^n f(x, z_i)
\]

using the dataset \(Z := \{z_1, ..., z_n\}\).

Stochastic gradient algorithms based on Langevin Monte Carlo have gained more attention in recent years. Two popular algorithms are Stochastic Gradient Langevin Dynamics (SGLD) and Stochastic Gradient Hamiltonian Monte Carlo (SGHMC). First, we summarize the use of SGLD in optimization, as presented in [RRT17]. Consider the overdamped Langevin stochastic differential equation

\[
dX_t = - \nabla F^\sharp(X_t) dt + \sqrt{2\beta^{-1}} dB_t,
\]

where \((B_t)_{t \geq 0}\) is the standard Brownian motion in \(\mathbb{R}^d\) and \(\beta > 0\) is the inverse temperature parameter. Under suitable assumptions on \(f\), the SDE (3) admits the Gibbs measure \(\pi^\sharp(dx) \propto \exp(-\beta F^\sharp(x))\) as its unique invariant distribution. In addition, it is known that for sufficiently big \(\beta\), the Gibbs distribution concentrates around global minimizers of \(F^\sharp\). Therefore, one can use the value of \(X_t\) from (3), (or from its discretized counterpart SGLD), as an approximate solution to the empirical risk problem, provided that \(t\) is large and temperature is low.

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In this paper, we consider the underdamped (second-order) Langevin diffusion
\[ dV_t = -\gamma V_t dt - \nabla F(x, \mu) dt + \sqrt{2\gamma \beta^{-1}} dB_t, \]
\[ dX_t = V_t dt, \]
where \((X_t)_{t \geq 0}, (V_t)_{t \geq 0}\) model the position and the momentum of a particle moving in a field of force \(F_x\) with random force given by Gaussian noise. It is shown that under some suitable conditions for \(F_x\), the Markov process \((X, V)\) is ergodic and has a unique stationary distribution
\[ \pi_x(dx, dv) = \frac{1}{\Gamma_x} \exp \left( -\beta \left( \frac{1}{2} \|v\|^2 + F_x(x) \right) \right) \, dx dv \]
where \(\Gamma_x\) is the normalizing constant
\[ \Gamma_x = \left( \frac{2\pi}{\beta} \right)^{d/2} \int_{\mathbb{R}^d} e^{-\beta F(x)} \, dx. \]

It is easy to observe that the \(x\)-marginal distribution of \(\pi_x(dx, dv)\) is the invariant distribution \(\pi_x(dx)\) of (3).

We consider the first order Euler discretization of (4), (5), also called Stochastic Gradient Hamiltonian Monte Carlo (SGHMC), given as follows
\[ \hat{V}_{k+1} = \hat{V}_k - \lambda \gamma \hat{V}_k + \nabla F_k(X_k) + \sqrt{2\gamma \beta^{-1}} \xi_{k+1}, \quad \hat{V}_0 = v_0, \]
\[ \hat{X}_{k+1} = \hat{X}_k + \lambda \hat{V}_k, \quad \hat{X}_0 = x_0, \]
where \(\lambda > 0\) is a step size parameter and \((\xi_k)_{k \in \mathbb{N}}\) is a sequence of i.i.d standard Gaussian random vectors in \(\mathbb{R}^d\). The initial condition \(v_0, x_0\) may be random, but independent of \((\xi_k)_{k \in \mathbb{N}}\).

In certain contexts, the full knowledge of the gradient \(F_x\) is not available, however, using the dataset \(z\), one can construct its unbiased estimates. In what follows, we adopt the general setting given by [RRT17]. Let \(U\) be a measurable space, and \(g : \mathbb{R}^d \times U \to \mathbb{R}^d\) such that for any \(z \in \mathbb{N}^n\),
\[ E[g(x, U)] = \nabla F_k(x), \forall x \in \mathbb{R}^d, \]
where \(U_z\) is a random element in \(U\) with probability law \(Q_z\). Conditionally on \(Z = z\), the SGHMC algorithm is defined by
\[ V_{k+1} = V_k - \lambda \gamma V_k + g(X_k, U_z), \quad V_0 = v_0, \]
\[ X_{k+1} = X_k + \lambda V_k, \quad X_0 = x_0, \]
where \((U_{z,k})_{k \in \mathbb{N}}\) is a sequence of i.i.d. random elements in \(U\) with law \(Q_z\). We also assume from now on that \(v_0, x_0, (U_{z,k})_{k \in \mathbb{N}}, (\xi_k)_{k \in \mathbb{N}}\) are independent.

Our ultimate goal is to find approximate global minimizers to the problem (1). Let \(X^+ := X_{k}^+\) be the output of the algorithm (9), (10) after \(k \in \mathbb{N}\) iterations, and \((\hat{X}_z, \hat{V}_z)\) be such that \(\mathcal{L}(\hat{X}_z, \hat{V}_z) = \pi_x\). The excess risk is decomposed as follows, see also [RRT17],
\[ E[F(X^+)] - F^* = \frac{E[F(X^+)] - E[F(\hat{X}_z^+)\]]}{\tau_1} \]
\[ + \frac{E[F(\hat{X}_z^+) - F(\hat{X}_z)\]]}{\tau_2} \]
\[ + \frac{E[F(\hat{X}_z) - F^*]}{\tau_3}. \]

The remaining part of the present paper is about finding bounds for these errors. Section 2 summarizes technical conditions and the main results. Comparison of our contributions to previous studies is discussed in Section 3. Proofs are given in Section 4.

Notation and conventions. For \(l \geq 1\), scalar product in \(\mathbb{R}^l\) is denoted by \(\langle \cdot, \cdot \rangle\). We use \(\| \cdot \|\) to denote the Euclidean norm (where the dimension of the space may vary). \(B(\mathbb{R}^l)\) denotes the Borel \(\sigma\)-field of \(\mathbb{R}^l\). For any \(\mathbb{R}^l\)-valued random variable \(X\) and for any \(1 \leq p < \infty\), let us set \(\|X\|_p := E^{1/p} |X|^p\). We denote by \(L^p\) the set of \(X\) with \(\|X\|_p < \infty\). The Wasserstein distance of order \(p \in [1, \infty)\) between two probability measures \(\mu\) and \(\nu\) on \(B(\mathbb{R}^l)\) is defined by
\[ W_p(\mu, \nu) = \left( \inf_{\pi \in \Pi(\mu, \nu)} \int_{\mathbb{R}^l} \|x - y\|^p d\pi(x, y) \right)^{1/p}, \]
where \(\Pi(\mu, \nu)\) is the set of couplings of \((\mu, \nu)\), see e.g. [Vil98]. For two \(\mathbb{R}^l\)-valued random variables \(X, Y\), we denote \(\mathbb{M}_2(X, Y) := W_2(\mathcal{L}(X), \mathcal{L}(Y))\), where \(\mathcal{L}(X)\) is the law of \(X\). We do not indicate \(l\) in the notation and it may vary.
2 Assumptions and main results

The following conditions are required throughout the paper.

**Assumption 2.1.** The function \( f \) is continuously differentiable, takes non-negative values, and there are constants \( A_0, B \geq 0 \) such that for any \( z \in \mathbb{Z} \),

\[
\|f(0, z)\| \leq A_0, \quad \|\nabla f(0, z)\| \leq B.
\]

**Assumption 2.2.** There is \( M > 0 \) such that, for each \( z \in \mathbb{Z} \),

\[
\|\nabla f(x_1, z) - \nabla f(x_2, z)\| \leq M\|x_1 - x_2\|, \quad \forall x_1, x_2 \in \mathbb{R}^d.
\]

**Assumption 2.3** (Dissipative). There exists a constant \( M > 0 \) such that

\[
(x, f(x, z)) \geq M\|x\|^2 - b, \quad \forall x \in \mathbb{R}^d, z \in \mathbb{Z}.
\]

**Assumption 2.4.** For each \( u \in U \), it holds that \( \|g(0, u)\| \leq B \) and

\[
\|g(x_1, u) - g(x_2, u)\| \leq M\|x_1 - x_2\|, \quad \forall x_1, x_2 \in \mathbb{R}^d.
\]

**Assumption 2.5.** There exists a constant \( \delta > 0 \) such that for every \( z \in \mathbb{Z}^n \),

\[
E\|g(x, U_k) - \nabla F_k(x)\|^2 \leq 2\delta(M^2\|x\|^2 + B^2).
\]

**Assumption 2.6.** The law \( \mu_0 \) of the initial state \((x_0, v_0)\) satisfies

\[
\int_{\mathbb{R}^d} e^{\mathcal{V}(x,v)} d\mu_0(x,v) < \infty,
\]

where \( \mathcal{V} \) is the Lyapunov function defined in \([17]\) below.

**Remark 2.7.** If the set of global minimizers is bounded, we can always redefine the function \( f \) to be quadratic outside a compact set containing the origin while maintaining its minimizers. Hence, Assumption 2.3 can be satisfied in practice. Assumption 2.4 means that the estimated gradient is also Lipschitz when using the same minibatch of size \( \ell \). Notice that for each \( \ell \), \( g(x, U_k) \) is the scaled Brownian motion. Let

\[
\hat{V}(t, s, (v, x)) = \frac{1}{\ell} \sum_{j=1}^{\ell} \nabla f(x, z_{I_j}),
\]

which is clearly unbiased and Assumption 2.4 will be satisfied whenever Assumptions 2.5 and 2.6 are in force.

An auxiliary continuous time process is needed in the subsequent analysis. For a step size \( \lambda > 0 \), denote by \( B_t^\lambda := \sqrt{\lambda}B_t \) the scaled Brownian motion. Let \( \hat{V}(t, s, (v, x)), \hat{X}(t, s, (v, x)) \) be the solutions of

\[
\begin{align*}
d\hat{V}(t, s, (v, x)) &= -\lambda \left( \gamma \hat{V}(t, s, (v, x)) + \nabla F_k(\hat{X}(t, s, (v, x))) \right) dt + \sqrt{2\gamma\lambda \beta^{-1} dB_t^\lambda}, \\
d\hat{X}(t, s, (v, x)) &= \lambda \hat{V}(t, s, (v, x)) dt,
\end{align*}
\]

with initial condition \( \hat{V}_s = v, \hat{X}_s = x \) where \( v, x \) may be random but independent of \( (B_t^\lambda)_{t \geq 0} \).

Our first result tracks the discrepancy between the SGHMC algorithm \([9, 10]\) and the auxiliary processes \([13, 14]\).

**Theorem 2.8.** Let \( 1 \leq p \leq 2 \). There exists a constant \( \tilde{C} > 0 \) such that for all \( k \in \mathbb{N} \),

\[
\mathbb{M}_p((V_k^\lambda, X_k^\lambda), (\hat{V}(k, 0, (v_0, x_0)), \hat{X}(k, 0, (v_0, x_0)))) \leq \tilde{C}(\lambda^{1/2p} + \delta^{1/2p}).
\]

**Proof.** The proof of this theorem is given in Section 4.2

The following is the main result of the paper.
Theorem 2.9. Let $1 < p \leq 2$. Suppose that the SGHMC iterates $(V_k^\lambda, X_k^\lambda)$ are defined by [4], [17]. The expected population risk can be bounded as

$$E[F(X_k^\lambda)] - F^* \leq B_1 + B_2 + B_3,$$

where

$$B_1 := (M \sigma + B) \left( \tilde{C}(\lambda^{1/(2p)} + \delta^{1/(2p)}) + C_*(W_p(\mu_0, \pi_\lambda))^{1/p} \exp(-c, k\lambda) \right),$$

$$B_2 := \frac{4\beta c_{LS}}{n} \left( \frac{M^2}{m} (b + d/\beta) + B^2 \right),$$

$$B_3 := \frac{d}{2\beta} \log \left( \frac{eM}{m} \left( \frac{b\beta}{d} + 1 \right) \right),$$

where $\tilde{C}, C_*, c_*, c_{LS}$ are appropriate constants and $W_p$ is the metric defined in [27] below.

Proof. The proof of this theorem is given in Section 4.3.

Corollary 2.10. Let $1 \leq p \leq 2, \varepsilon > 0$ We have

$$W_p(\mathcal{L}(X_k^\lambda), \pi_\lambda) \leq \varepsilon$$

whenever

$$(\lambda^{1/(2p)} + \delta^{1/(2p)}) \leq \frac{1}{2\tilde{C}} \varepsilon, \quad k \geq \left( \frac{2\tilde{C}}{C_*} \frac{1}{\varepsilon^{2p}} \log \left( \frac{C_*(W_p(\mu_0, \pi_\lambda))^{1/p}}{\varepsilon} \right) \right).$$

Proof. From the proof of Theorem 2.9 or more precisely from [40], we need to choose $\lambda$ and $k$ such that

$$\tilde{C}(\lambda^{1/(2p)} + \delta^{1/(2p)}) + C_*(W_p(\mu_0, \pi_\lambda))^{1/p} \leq \varepsilon.$$ 

First, we choose $\lambda$ and $\delta$ so that $\tilde{C}(\lambda^{1/(2p)} + \delta^{1/(2p)}) < \varepsilon/2$ and then

$$C_*(W_p(\mu_0, \pi_\lambda))^{1/p} \exp(-c, k\lambda) \leq \varepsilon/2$$

will hold for $k$ large enough.

3 Related work and our contributions

Non-asymptotic convergence rate Langevin dynamics based algorithms for approximate sampling log-concave distributions are intensively studied in recent years. For example, overdamped Langevin dynamics are discussed in [WT11], [Dal17b], [DM16], [DK17], [DM17] and others. Recently, [BCM18] treats the case of non-i.i.d. data streams with a certain mixing property. Underdamped Langevin dynamics are examined in [CFG14], [Nec11], [CCBJ17], etc. Further analysis on HMC are discussed on [BBLG17], [Bet17]. Subsampling methods are applied to speed up HMC for large datasets, see [DQK17], [QKV18].

The use of momentum to accelerate optimization methods are discussed intensively in literature, for example [AP16]. In particular, performance of SGHMC is experimentally proved better than SGLD in many applications, see [CDC15], [CFG14]. An important advantage of the underdamped SDE is that convergence to its stationary distribution is faster than that of the overdamped SDE in the 2-Wasserstein distance, as shown in [ECZ17].

Finding an approximate minimizer is similar to sampling distributions concentrate around the true minimizer. This well known connection gives rise to the study of simulated annealing algorithms, see [Hwa80], [Gla85], [Haj85], [CHS87], [HKS89], [GM91], [GM93]. Recently, there are many studies further investigate this connection by means of non asymptotic convergences of Langevin based algorithms and in stochastic non-convex optimization and large-scale data analysis, [CCG16], [Dal17a].

Relaxing convexity is a more challenging issue. In [CCAY18], the problem of sampling from a target distribution $\exp(-F(x))$ where $F$ is L-smooth everywhere and $m$-strongly convex outside a ball of finite radius is considered. They provide upper bounds for the number of steps to be within a given precision level $\varepsilon$ of the 1-Wasserstein distance between the HMC algorithm and the equilibrium distribution. In a similar setting, [MMS18] obtains bounds in both the $W_1$ and $W_2$ distances for overdamped Langevin dynamics with stochastic gradients. [XCZ18] studies the convergence of the SGLD algorithm and the variance reduced SGLD to global minima of nonconvex functions satisfying the dissipativity condition.

Our work continues these lines of research, the most similar setting to ours is the recent paper [CGZ18]. We summarize our contributions below:
• Diffusion approximation. In Lemma 10 of [GGZ18], the upper bound for the 2-Wasserstein distance between the SGHMC algorithm at step $k$ and underdamped SDE at time $t = k\lambda$ is (up to constants) given by
\[ (\delta^{1/4} + \lambda^{1/4})\sqrt{k\lambda} \log(k\lambda), \]
which depends on the number of iteration $k$. Therefore obtaining a precision $\varepsilon$ requires a careful choice of $k, \lambda$ and even $k\lambda$. By introducing the auxiliary SDEs [13], [14], we are able to achieve the rate
\[ (\delta^{1/4} + \lambda^{1/4}), \]
see Theorem 2.8 for the case $p = 2$. This upper bound is better in the number of iterations and hence, improves Lemma 10 of [GGZ18]. Our analysis for variance of the algorithm is also different. The iteration does not accumulate mean squared errors, as the number of step goes to infinity.

• Our proof for Theorem 2.8 is relatively simple and we do not need to adopt the techniques of [RRT17] which involve heavy functional analysis, e.g. the weighted Csiszár - Kullback - Pinsker inequalities in [BV05] is not needed.

• If we consider the $p$-Wasserstein distance for $1 < p \leq 2$, in particular, when $p \to 1$, Theorem 2.8 gives tighter bounds, compared to Theorem 2 of [GGZ18].

• Dependence structure of the dataset in the sampling mechanism, can be arbitrary, see the proof of Theorem 2.8. The i.i.d assumption on dataset is used only for the generalization error. We could also incorporate non-i.i.d data in our analysis, see Remark 1.20 but this is left for further research.

4 Proofs

4.1 A contraction result

In this section, we recall a contraction result of [EGZ17]. First, it should be noticed that the constant $c$ stands for “contraction”. Using the upper bound of Lemma 5.1 for $f$ below, there exist constants $\lambda_c \in (0, \min\{1/4, m/(M + 2B + \gamma^2/2)\})$ small enough and $A_c \geq \beta/2(b + 2B + A_0)$ such that
\[ \langle x, \nabla F_\ast(x) \rangle \geq m \|x\|^2 - b \geq 2\lambda_c(F_\ast(x) + \gamma^2 \|x\|^2/4) - 2A_c/\beta. \] (16)

Therefore, Assumption 2.1 of [EGZ17] is satisfied, noting that $L_c := \beta M$ and
\[ \|\nabla F_\ast(x) - \nabla F_\ast(y)\| \leq \beta^{-1}L_c\|x - y\|. \]

We define the Lyapunov function
\[ V(x, v) = \beta F_\ast(x) + \frac{\beta}{4} \gamma^2 \left( \|x + \gamma^{-1}v\|^2 + \|\gamma^{-1}v\|^2 - \lambda_c\|x\|^2 \right), \] (17)
For any $(x_1, v_1), (x_2, v_2) \in \mathbb{R}^{2d}$, we set
\[ r((x_1, v_1), (x_2, v_2)) = \alpha_c\|x_1 - x_2\| + \|x_1 - x_2 + \gamma^{-1}(v_1 - v_2)\|, \] (18)
\[ \rho((x_1, v_1), (x_2, v_2)) = h(r((x_1, v_1), (x_2, v_2))) (1 + \varepsilon_cV(x_1, v_1) + \varepsilon_cV(x_2, v_2)), \] (19)
where $\alpha_c, \varepsilon_c > 0$ are suitable positive constants to be fixed later and $h : [0, \infty) \to [0, \infty)$ is continuous, non-decreasing concave function such that $h(0) = 0$, $h$ is $C^2$ on $(0, R_1)$ for some constant $R_1 > 0$ with right-sided derivative $h'_+(0) = 1$ and left-sided derivative $h'_-(R_1) > 0$ and $h$ is constant on $[R_1, \infty)$. For any two probability measures $\mu, \nu$ on $\mathbb{R}^{2d}$, we define
\[ W_p(\mu, \nu) := \inf_{(X_1, V_1) \sim \mu, (X_2, V_2) \sim \nu} \mathbb{E}[\rho((X_1, V_1), (X_2, V_2))]. \] (20)

Note that $\rho$ and $W_p$ are semimetrics but not necessarily metrics. A result from [EGZ17] is recalled below.

For a probability measure $\mu$ on $\mathcal{B}(\mathbb{R}^{2d})$, we denote by $\mu\{X_t\}$ the law of $(V_t, X_t)$ when $L(V_0, X_0) = \mu$.

Theorem 4.1. There exists a continuous non-decreasing concave function $h$ with $h(0) = 0$ such that for all probability measures $\mu, \nu$ on $\mathbb{R}^{2d}$, and $1 \leq p \leq 2$, we have
\[ W_p(\mu\{X_t\}, \nu\{X_t\}) \leq C \left( W_p(\mu, \nu) \right)^{1/p} \exp(-c_s t), \quad \forall t \geq 0, \] (21)
where the following relations hold:

\[ c_* = \frac{7}{384p} \min \{ \lambda_c M \gamma^{-2}, \Lambda_c^1 e^{-\Lambda_c} M \gamma^{-2}, \Lambda_c^1 e^{-\Lambda_c} \}, \]

\[ C_* = 2^{1/p} e^{2/p + \Lambda_c/\gamma} \frac{1 + \gamma}{\min \{1, \Lambda_c\}} \left( \max \left\{ 1, \frac{1, R_p^{p-2}}{\min \{1, R_1\}} \right\} (1 + 2 \alpha_c + 2 \alpha_c^2)(d + A_c) \beta^{-1} \gamma^{-1} c_*^{-1} \right)^{1/p} , \]

\[ \Lambda_c = \frac{12}{5} (1 + 2 \alpha_c + 2 \alpha_c^2)(d + A_c) \gamma^{-2} \Lambda_c^{-1} (1 - 2 \lambda_c)^{-1}, \]

\[ \alpha_c = (1 + \Lambda_c^{-1}) \gamma^{-2} > 0, \]

\[ \varepsilon_c = 4 \gamma^{-1} \Lambda_c^{-1} / (d + A_c) > 0, \]

\[ R_1 = 4 \cdot (6/5)^{1/2} (1 + 2 \alpha_c + 2 \alpha_c^2)^{1/2} (d + A_c)^{1/2} \beta^{-1/2} \Lambda_c^{-1} (\lambda_c - 2 \lambda_c^2)^{-1/2}. \]

The function \( h \) is constant on \([R_1, \infty), C^2 \) on \((0, R_1)\) with

\[ f(r) = \int_0^{\gamma R_1} \varphi(s) g(s) \, ds, \]

\[ \varphi(s) = \exp \left\{ -(1 + \eta_c) L_c s^2 / 8 - \gamma^2 \beta \varepsilon_c \max \{1, (2 \alpha_c^{-1}) \} s^2 / 2 \right\}, \]

\[ g(s) = 1 - \frac{9}{4} c_s \gamma \beta \int_0^s \varphi(s) \, ds, \quad \varphi(s) = \int_0^s \varphi(x) \, dx \]

and \( \eta_c \) satisfies \( \alpha_c = (1 + \eta_c) L_c \beta^{-1} \gamma^{-2} \).

**Proof.** From (5.15) of [EGZ17], we get

\[ \|(x_1, v_1) - (x_2, v_2)\|^p \leq \left( \frac{1 + \gamma}{\min \{1, \Lambda_c\}} \right)^p \cdot r((x_1, v_1), (x_2, v_2))^p. \]

Furthermore, from the proof of Corollary 2.6 of [EGZ17], if \( r := r((x_1, v_1), (x_2, v_2)) \leq \min \{1, R_1\}, \)

\[ r^2 \leq r \leq 2 \varepsilon_c \rho((x_1, v_1), (x_2, v_2)) \]

and if \( r \geq \min \{1, R_1\} \) then

\[ r^p \leq \max \{1, R_1^{p-2}\} r^{p-2} \left( \frac{\max \{1, R_1^{p-2}\}}{\min \{1, R_1\}} \right) 2 \varepsilon_c \rho((x_1, v_1), (x_2, v_2)). \]

These bounds and Theorem 2.3 of [EGZ17] imply that

\[ W_p(\mu \nu, \nu \nu) \leq C_* \left( W_p(\mu, \nu) \right)^{1/p} \exp(-c_* \lambda t). \]

The proof is complete.

4.2 **Proof of Theorem 2.8**

Here, we summarize our approach. For a given step size \( \lambda > 0 \), we divide the time axis into intervals of length \( T = [1/\lambda] \). For each time step \( k \in [nT, (n + 1)T], n \in \mathbb{N} \), we compare the SGHMC to the version with exact gradients relying on the Doob inequality, and then compare the later to the auxiliary continuous-time diffusion \( \tilde{V}(k, 0, (v_0, x_0)), \tilde{X}(k, 0, (v_0, x_0)) \) with the scaled Brownian motion. At this stage we reply on the contraction result from [EGZ17] and uniform boundedness of the Langevin diffusion and its discrete time versions. Since the auxiliary dynamics evolves slower than the original Langevin dynamics, or more precisely at the same speed as that of the SGHCM, our upper bounds do not accumulate errors and are independent from the number of iterations.

**Proof.** For each \( k \in \mathbb{N} \), we define

\[ \mathcal{H}_k := \sigma(U_{k, i}, 1 \leq i \leq k) \lor \sigma(\xi_j, j \in \mathbb{N}). \]
Let \( \tilde{v}, \tilde{x} \) be \( \mathbb{R}^d \)-valued random variables satisfying Assumption 2.4. For any \( 0 \leq i \leq j \), we recursively define 
\[
\tilde{V}^\lambda(i, i, (\tilde{v}, \tilde{x})) := \tilde{v}, \quad \tilde{X}^\lambda(i, i, (\tilde{v}, \tilde{x})) := \tilde{x}
\]
and
\[
\tilde{V}^\lambda(j + 1, i, (\tilde{v}, \tilde{x})) = \tilde{V}^\lambda(j, i, (\tilde{v}, \tilde{x})) - \lambda [\gamma \tilde{V}^\lambda(j, i, (\tilde{v}, \tilde{x})) + \nabla F_{\hat{x}}(\tilde{X}^\lambda(j, i, (\tilde{v}, \tilde{x})))] + \sqrt{2\gamma/\beta} \lambda \xi_{j+1}, \quad (22)
\]
\[
\tilde{X}^\lambda(j + 1, i, (\tilde{v}, \tilde{x})) = \tilde{X}^\lambda(j, i, (\tilde{v}, \tilde{x})) + \lambda \tilde{V}^\lambda(j, i, (\tilde{v}, \tilde{x})).
\]

Let \( T := [1/\lambda] \). For each \( n \in \mathbb{N} \), and for each \( nT \leq k < (n + 1)T \), we set
\[
\tilde{V}_k := \tilde{V}^\lambda(k, nT; (V_{nT}^\lambda, X_{nT}^\lambda)), \quad \tilde{X}_k := \tilde{X}^\lambda(k, nT; (V_{nT}^\lambda, X_{nT}^\lambda)). \quad (24)
\]
For each \( n \in \mathbb{N} \), it holds by definition that \( V_{nT}^\lambda = \tilde{V}_{nT}^\lambda \) and the triangle inequality implies for \( nT \leq k < (n + 1)T \),
\[
\|V_k^\lambda - \tilde{V}_k\| \leq \lambda \sum_{i=nT}^{k-1} \left| g(X_i^\lambda, U_{z,i}) - \nabla F_{z}(\tilde{X}_i^\lambda) \right|
\]
and
\[
\|X_k^\lambda - \tilde{X}_k\| \leq \lambda \sum_{i=nT}^{k-1} \|V_i^\lambda - \tilde{V}_i\|. \quad (25)
\]
Denote \( g_{k,nT}(x) := E[g(x, U_{a,k})|\mathcal{H}_{nT}], x \in \mathbb{R}^d \). By Assumption 2.4, the estimation continues as follows
\[
\|V_k^\lambda - \tilde{V}_k\| \leq \lambda \sum_{i=nT}^{k-1} \left| g(X_i^\lambda, U_{z,i}) - \nabla F_{z}(\tilde{X}_i^\lambda) \right| \leq \lambda \sum_{i=nT}^{k-1} \|g(X_i^\lambda, U_{z,i}) - g(\tilde{X}_i^\lambda, U_{z,i})\|
\]
\[
+ \lambda \sum_{i=nT}^{k-1} \|g_i,nT(\tilde{X}_i^\lambda) - \nabla F_{z}(\tilde{X}_i^\lambda)\| \leq \lambda M \sum_{i=nT}^{k-1} \|X_i^\lambda - \tilde{X}_i\| + \lambda \max_{nT \leq m < (n+1)T} \sum_{i=nT}^{m} \|g_i(\tilde{X}_i^\lambda, U_{z,i}) - g_i,nT(\tilde{X}_i^\lambda)\|
\]
\[
+ \lambda \sum_{i=nT}^{(n+1)T-1} \|g_i,nT(\tilde{X}_i^\lambda) - \nabla F_{z}(\tilde{X}_i^\lambda)\|. \quad (26)
\]
Using (25), one obtains
\[
\sum_{i=nT}^{k-1} \|X_i^\lambda - \tilde{X}_i\| \leq \lambda T \|V_{nT}^\lambda - \tilde{V}_{nT}^\lambda\| + ... + \lambda T \|V_{k-1}^\lambda - \tilde{V}_{k-1}\|
\]
\[
\leq \sum_{i=nT}^{k-1} \|V_i^\lambda - \tilde{V}_i\|, \quad (27)
\]
noting that \( T \lambda \leq 1 \). Therefore, the estimation in (20) continues as
\[
\|V_k^\lambda - \tilde{V}_k\| \leq \lambda M \sum_{i=nT}^{k-1} \|V_i^\lambda - \tilde{V}_i\| + \lambda \max_{nT \leq m < (n+1)T} \sum_{i=nT}^{m} \|g(\tilde{X}_i^\lambda, U_{z,i}) - g_i,nT(\tilde{X}_i^\lambda)\|
\]
\[
+ \lambda \sum_{i=nT}^{(n+1)T-1} \|g_i,nT(\tilde{X}_i^\lambda) - \nabla F_{z}(\tilde{X}_i^\lambda)\|. \quad (28)
\]
Applying the discrete-time version of Grönwall’s lemma and taking squares, noting also that \( (x + y)^2 \leq 2(x^2 + y^2) \), \( x, y \in \mathbb{R} \) yield
\[
\|V_k^\lambda - \tilde{V}_k\|^2 \leq 2\lambda^2 e^{2MT\lambda} \max_{nT \leq m < (n+1)T} \left[ \sum_{i=nT}^{m} \|g(\tilde{X}_i^\lambda, U_{z,i}) - g_i,nT(\tilde{X}_i^\lambda)\|^2 + \xi_n^2 \right],
\]
where
\[
\xi_n := \sum_{i=nT}^{(n+1)T-1} \|g_i,nT(\tilde{X}_i^\lambda) - \nabla F_{z}(\tilde{X}_i^\lambda)\|.
\]
Taking conditional expectation with respect to $\mathcal{H}_{nT}$, the estimation becomes

\[
E \left[ \|V_k^\lambda - \tilde{V}_k^\lambda\|^2 \bigg| \mathcal{H}_{nT} \right] \leq 2\lambda^2 e^{2M} E \left[ \max_{nT \leq m < (n+1)T} \left\| \sum_{i=nT}^{m} g(\tilde{X}_i^\lambda, U_{x,i}) - g_{i,nT}(\tilde{X}_i^\lambda) \right\|^2 \bigg| \mathcal{H}_{nT} \right] + 2\lambda^2 e^{2M} E [\Xi^\lambda_{nT} | \mathcal{H}_{nT}].
\]

Since the random variables $U_{x,i}$ are independent, the sequence of random variables $g(\tilde{X}_i^\lambda, U_{x,i}) - g_{i,nT}(\tilde{X}_i^\lambda)$, $nT \leq i < (n+1)T$ are independent conditionally on $\mathcal{H}_{nT}$, noting that $\tilde{X}_i^\lambda$ is measureable with respect to $\mathcal{H}_{nT}$. In addition, they have zero mean by the tower property of conditional expectation. By Assumption 2.3

\[
\|g(x,u)\| \leq M \|x\| + B
\]

and thus

\[
E \left[ \|g(\tilde{X}_i^\lambda, U_{x,i})\|^2 \big| \mathcal{H}_{nT} \right] \leq 2M^2 E \left[ \|\tilde{X}_i^\lambda\|^2 \right] + 2B^2.
\]

(29)

by the independence of $U_{x,i}, i > nT$ from $\mathcal{H}_{nT}$. Doob’s inequality and (29) imply

\[
E \left[ \max_{nT \leq m < (n+1)T} \sum_{i=nT}^{m} g(\tilde{X}_i^\lambda, U_{x,i}) - g_{i,nT}(\tilde{X}_i^\lambda) \bigg| \mathcal{H}_{nT} \right] \leq 8M^2 \sum_{i=nT}^{(n+1)T-1} E \left[ \|\tilde{X}_i^\lambda\|^2 \right] + 8B^2 T.
\]

Taking one more expectation and using Lemma 5.3 give

\[
E \left[ \max_{nT \leq m < (n+1)T} \sum_{i=nT}^{m} g(\tilde{X}_i^\lambda, U_{x,i}) - g_{i,nT}(\tilde{X}_i^\lambda) \bigg| \mathcal{H}_{nT} \right] \leq 8M^2 \sum_{i=nT}^{(n+1)T-1} E \left[ \|\tilde{X}_i^\lambda\|^2 \right] + 8B^2 T
\]

\[
\leq (8M^2 C_x^n + 8B^2) T.
\]

By Lemma 13 we have $E[\Xi^\lambda_{nT}] < 2T^2\delta(M^2 C_x^n + B^2)$, and therefore,

\[
E^{1/2} \left[ \|V_k^\lambda - \tilde{V}_k^\lambda\|^2 \right] \leq c_2 \sqrt{\lambda} + c_3 \sqrt{\delta}
\]

(30)

where we define

\[
c_2 = 4e^{M\sqrt{(M^2 C_x^n + B^2)}}, \quad c_3 = 2e^{M\sqrt{M^2 C_x^n + B^2}}.
\]

Consequently, we have from (29)

\[
E^{1/2} \left[ \|X_k^\lambda - \tilde{X}_k^\lambda\|^2 \right] \leq \lambda \sum_{i=nT}^{(k-1)T} E^{1/2} \left[ \|V_i^\lambda - \tilde{V}_i^\lambda\|^2 \right] \leq \lambda T(c_2 \sqrt{\lambda} + c_3 \sqrt{\delta})
\]

\[
\leq c_2 \sqrt{\lambda} + c_3 \sqrt{\delta}.
\]

(31)

Let $\tilde{V}_{\text{int}}^\lambda$ and $\tilde{X}_{\text{int}}^\lambda$ be the continuous-time interpolation of $\tilde{V}_k^\lambda$, and of $\tilde{X}_k^\lambda$ on $[nT, (n+1)T)$, respectively,

\[
d\tilde{V}_{\text{int}}^\lambda = -\lambda \gamma \tilde{V}_{\text{int}}^\lambda dt - \lambda \nabla F_{\lambda} (\tilde{X}_{\text{int}}^\lambda) dt + \sqrt{2\gamma \lambda \beta - 1} dB_t^\lambda;
\]

\[
d\tilde{X}_{\text{int}}^\lambda = \lambda \nabla F_{\lambda} (\tilde{X}_{\text{int}}^\lambda) dt,
\]

with the initial conditions $\tilde{V}_{\text{int}}^\lambda(0) = \tilde{V}_{\text{int}}^\lambda(nT) = V_{\text{int}}^\lambda(nT)$ and $\tilde{X}_{\text{int}}^\lambda = \tilde{X}_{\text{int}}^\lambda(nT) = X_{\text{int}}^\lambda(nT)$. For each $n \in \mathbb{N}$ and for $nT \leq t < (n+1)T$, define also

\[
\tilde{V}_t = \tilde{V}(t, nT, (V_{\text{int}}^\lambda(nT), X_{\text{int}}^\lambda(nT)));
\]

\[
\tilde{X}_t = \tilde{X}(t, nT, (V_{\text{int}}^\lambda(nT), X_{\text{int}}^\lambda(nT)));
\]

where the dynamics of $\tilde{V}, \tilde{X}$ are given in (13), (14). In this way, the processes $(\tilde{V}_t)_{t \geq 0}, (\tilde{X}_t)_{t \geq 0}$ are right continuous with left limits. From Lemma 4.4 we obtain for $nT \leq t < (n+1)T$

\[
E^{1/2} \left[ \|\tilde{V}_{\text{int}}^\lambda - \tilde{V}_t\|^2 \right] \leq c_7 \sqrt{\lambda}, \quad E^{1/2} \left[ \|\tilde{X}_{\text{int}}^\lambda - \tilde{X}_t\|^2 \right] \leq c_7 \sqrt{\lambda}.
\]

(35)

Combining (30), (31) and (33) gives

\[
E^{1/2} \left[ \|V_k^\lambda - \tilde{V}_k\|^2 \right] \leq (c_2 + c_7) \sqrt{\lambda} + c_3 \sqrt{\delta}, \quad E^{1/2} \left[ \|X_k^\lambda - \tilde{X}_k\|^2 \right] \leq (c_2 + c_7) \sqrt{\lambda} + c_3 \sqrt{\delta}.
\]

(36)
Define $\tilde{A}_t = (\tilde{V}_t, \tilde{X}_t)$ and $\tilde{B}(t, s, (v_s, x_s)) = (\tilde{V}(t, s, (v_s, x_s)), \tilde{X}(t, s, (v_s, x_s)))$ for $s \leq t$ and $v_s, x_s$ are $\mathbb{R}^d$-valued random variables. The triangle inequality and Theorem 4.4 imply that for $nT \leq t < (n + 1)T$, and for $1 \leq p \leq 2$,

$$\mathcal{W}_p(\tilde{A}_t, \tilde{B}(t, 0, (v_0, x_0))) \leq \sum_{i=1}^{n} \mathcal{W}_p(\tilde{B}(t, iT, (V^\lambda_{iT}(\cdot), X^\lambda_{iT}(\cdot))), \tilde{B}(t, (i - 1)T, (V^\lambda_{(i-1)T}(\cdot), X^\lambda_{(i-1)T}(\cdot))))$$

$$= \sum_{i=1}^{n} \mathcal{W}_p(\tilde{B}(t, iT, (V^\lambda_{iT}(\cdot), X^\lambda_{iT}(\cdot))), \tilde{B}(t, iT, \tilde{B}(t, (i - 1)T, (V^\lambda_{(i-1)T}(\cdot), X^\lambda_{(i-1)T}(\cdot))))$$

$$\leq C_n \sum_{i=1}^{n} e^{-c\lambda(t-iT)}\mathcal{W}_{1/p}((\mathcal{L}(V^\lambda_{iT}(\cdot), X^\lambda_{iT}(\cdot)), \mathcal{L}(\tilde{B}(t, (i - 1)T, (V^\lambda_{(i-1)T}(\cdot), X^\lambda_{(i-1)T}(\cdot))))))\right),$$

noting the rate of contraction of $(\tilde{V}_t, \tilde{X}_t)$ is $e^{-c\lambda t}$. Using Lemma 5.3, we obtain

$$\mathcal{W}_p((\mathcal{L}(V^\lambda_{iT}(\cdot), X^\lambda_{iT}(\cdot)), \mathcal{L}(\tilde{V}(i, (i - 1)T, (V^\lambda_{(i-1)T}(\cdot), X^\lambda_{(i-1)T}(\cdot))), \tilde{X}(i, (i - 1)T, (V^\lambda_{(i-1)T}(\cdot), X^\lambda_{(i-1)T}(\cdot))))))$$

$$\leq c_{17} \left(1 + e_c \sup_{k \in \mathbb{N}} \sqrt{EV^2(V^\lambda_{iT}(\cdot), X^\lambda_{iT}(\cdot))} + e_c \sup_{k \in \mathbb{N}} \sqrt{EV^2(\tilde{V}(i, (i - 1)T, (V^\lambda_{(i-1)T}(\cdot), X^\lambda_{(i-1)T}(\cdot))), \tilde{X}(i, (i - 1)T, (V^\lambda_{(i-1)T}(\cdot), X^\lambda_{(i-1)T}(\cdot))))} \right),$$

where

$$c_{17} = c_{17} \left(1 + e_c \sup_{k \in \mathbb{N}} \sqrt{EV^2(V^\lambda_{iT}(\cdot), X^\lambda_{iT}(\cdot))} \right).$$

Now, we compute

$$||V^\lambda_{iT} - \tilde{V}(i, (i - 1)T, (V^\lambda_{(i-1)T}(\cdot), X^\lambda_{(i-1)T}(\cdot)))||$$

$$\leq ||V^\lambda_{iT} - \tilde{V}(iT - 1, (i - 1)T, (V^\lambda_{(i-1)T}(\cdot), X^\lambda_{(i-1)T}(\cdot)))||$$

$$+ \lambda \gamma \left|\int_{iT-1}^{iT} \left(\tilde{V}(i, (i - 1)T, (V^\lambda_{(i-1)T}(\cdot), X^\lambda_{(i-1)T}(\cdot))) - \tilde{V}(i, (i - 1)T, (V^\lambda_{(i-1)T}(\cdot), X^\lambda_{(i-1)T}(\cdot)))\right) dt\right|$$

$$+ \lambda \left|\int_{iT-1}^{iT} \left(\tilde{V}(i, (i - 1)T, (V^\lambda_{(i-1)T}(\cdot), X^\lambda_{(i-1)T}(\cdot))) - \tilde{V}(i, (i - 1)T, (V^\lambda_{(i-1)T}(\cdot), X^\lambda_{(i-1)T}(\cdot)))\right) dt\right|$$

$$+ \sqrt{\lambda} ||\xi_{iT} - (B^\lambda_{iT} - B^\lambda_{iT-1})||.$$

In $L^2$ norm, the first and second terms of $||V^\lambda_{iT} - \tilde{V}(i, (i - 1)T, (V^\lambda_{(i-1)T}(\cdot), X^\lambda_{(i-1)T}(\cdot)))||$ are bounded by $(c_2 + c_7)\sqrt{\lambda} + c_3\sqrt{\sigma}$, see [30] and the fifth term is estimated by $\sqrt{\lambda}$. We consider the third term in [35]. From the dynamics of $\tilde{V}$, we find that for $i T - 1 \leq t \leq iT$,

$$\tilde{V}(iT - 1, (i - 1)T, (V^\lambda_{(i-1)T}(\cdot), X^\lambda_{(i-1)T}(\cdot))) - \tilde{V}(t, (i - 1)T, (V^\lambda_{(i-1)T}(\cdot), X^\lambda_{(i-1)T}(\cdot)))$$

$$= \lambda \int_{iT-1}^{t} \left(\gamma \tilde{V}(s, (i - 1)T, (V^\lambda_{(i-1)T}(\cdot), X^\lambda_{(i-1)T}(\cdot))) + \nabla F(x) \tilde{X}(s, (i - 1)T, (V^\lambda_{(i-1)T}(\cdot), X^\lambda_{(i-1)T}(\cdot)))\right) ds$$

$$- \sqrt{2\lambda\beta^{-1}} (B^\lambda_{iT} - B^\lambda_{iT-1}).$$

Hölder's inequality yields

$$E \left[||\tilde{V}(iT - 1, (i - 1)T, (V^\lambda_{(i-1)T}(\cdot), X^\lambda_{(i-1)T}(\cdot))) - \tilde{V}(t, (i - 1)T, (V^\lambda_{(i-1)T}(\cdot), X^\lambda_{(i-1)T}(\cdot)))||^2\right]$$

$$\leq 3\lambda^2 \lambda^2 \int_{iT-1}^{t} E \left[||\tilde{V}(s, (i - 1)T, (V^\lambda_{(i-1)T}(\cdot), X^\lambda_{(i-1)T}(\cdot)))||^2\right] ds$$

$$+ 3\lambda^2 \int_{iT-1}^{t} E \left[||\nabla F(x) \tilde{X}(s, (i - 1)T, (V^\lambda_{(i-1)T}(\cdot), X^\lambda_{(i-1)T}(\cdot)))||^2\right] ds + 6\gamma \beta^{-1} \lambda$$

$$\leq c_{14} \lambda,$$
where the last inequality uses Lemma 5.3 and Assumption 2.2 and $c_{14} := 3\gamma^2 C_n^x + 6M^2 C_x^\gamma + 6B^2 + 6\gamma^2 \beta^{-1}$. For the fourth term of (38), we have

$$E \left[ \|g(X_{i(T-1)}^\lambda, U_{\mathbf{x}(T-1)}) - \int_{(T-1)}^{iT} \nabla F_\mathbf{z}(X^\lambda_i(t, (i-1)T, (V^\lambda_{(i-1)T}, X^\lambda_{(i-1)T}))) dt \|^{2} \right]$$

$$\leq 2E \left[ \|g(X_{i(T-1)}^\lambda, U_{\mathbf{x}(T-1)}) - \nabla F_\mathbf{z}(X^\lambda_{(i-1)T}) \|^{2} \right]$$

$$+ 2E \left[ \left\| \int_{(T-1)}^{iT} \nabla F_\mathbf{z}(X^\lambda_i(t, (i-1)T, (V^\lambda_{(i-1)T}, X^\lambda_{(i-1)T}))) dt \right\|^{2} \right]$$

$$\leq 2E \left[ \|g(X_{i(T-1)}^\lambda, U_{\mathbf{x}(T-1)}) - \nabla F_\mathbf{z}(X^\lambda_{(i-1)T}) \|^{2} \right]$$

$$+ 2M^2 E \left[ \left\| X^\lambda_{i(T-1)} - \hat{X}(t, (i-1)T, (V^\lambda_{(i-1)T}, X^\lambda_{(i-1)T})) \right\|^{2} dt \right]$$

$$\leq 2\delta (M^2 C_n^x + B^2) + 2M^2 (2(c_2 + c_7)^2 \lambda + 2c_1 \rho)$$

$$\leq c_15(\lambda + \delta),$$

where the last inequality uses Assumption 2.4, Lemma 5.3 and (39) and $c_{15} := \max\{2(M^2 C_n^x + B^2) + 4M^2 c_3^2, 4M^2 (c_2 + c_7)^2\}$. A similar estimate holds for

$$E^{1/2} \left[ \left\| X^\lambda_{iT} - \hat{X}(iT, (i-1)T, (V^\lambda_{(i-1)T}, X^\lambda_{(i-1)T})) \right\|^2 \right].$$

Letting $c_{16} := \max\{c_2 + c_7, c_3, \sqrt{c_{14}}, \sqrt{c_{15}}\}$, the estimate (39) continues as

$$\mathbb{M}_{p}(\hat{A}_i, \hat{B}(t, 0, (v_0, x_0))) \leq \sum_{i=1}^{n} C_{\ast} e^{-c_1 (n-i)} \left( c_{18} C_{16}(\sqrt{\lambda} + \sqrt{\delta}) \right)^{1/p} \leq C_{\ast} (c_{18} C_{16})^{1/p} \frac{e^{-c_1 (n-i)}}{1 - e^{-c_1 (n-i)}} (\lambda^{1/(2p)} + \delta^{1/(2p)}).$$

(39)

Therefore, from (39), (45), (49), the triangle inequality implies for $nT \leq k < (n+1)T$,

$$\mathbb{M}_{p}(V_k, X_k^\lambda), (\hat{V}_k(0, (v_0, x_0)), \hat{X}(k, 0, (v_0, x_0)))$$

$$\leq \mathbb{M}_{p}(V_k, X_k^\lambda), (\hat{V}_k, \hat{X}_k^\lambda)) + \mathbb{M}_{p}(V_k, \hat{X}_k^\lambda) \leq \mathbb{M}_{p}(V_k, X_k^\lambda), (\hat{V}_k, \hat{X}_k^\lambda) \leq \tilde{C}(\lambda^{1/(2p)} + \delta^{1/(2p)}),$$

where $\tilde{C} = 2 \max\{c_2, c_3, c_7, c_\ast (c_{18} C_{16})^{1/p} \frac{e^{-c_1 (n-i)}}{1 - e^{-c_1 (n-i)}} \}$.

The proof is complete. \hfill \Box

Remark 4.2. It is important to remark from the proof above that the data structure of Z can be arbitrary, and only the independence of random elements $U_{\mathbf{z}, k}, k \in \mathbb{N}$ is used.

**Lemma 4.3.** The quantity $\Xi_n$ defined in (28) has second moments and

$$\sup_{n \in \mathbb{N}} E[\Xi_n^2] < \infty.$$

**Proof.** Noting that for each $nT \leq i < (n+1)T - 1$, the random variable $\hat{X}_i^\lambda$ is $H_{n+T}$-measurable. Using Assumption 2.4, the Cauchy-Schwarz inequality implies

$$E[\Xi_n^2] \leq T \sum_{i=nT}^{(n+1)T-1} E \left[ \|g_{i,nT}(\hat{X}_i^\lambda) - \nabla F_\mathbf{z}(\hat{X}_i^\lambda) \|^2 \right]$$

$$= T \sum_{i=nT}^{(n+1)T-1} E \left[ \left\| E \left[ g(\hat{X}_i^\lambda, U_{\mathbf{z}, k}) | H_{nT} \right] - \nabla F_\mathbf{z}(\hat{X}_i^\lambda) \right\|^2 \right]$$

$$\leq T \sum_{i=nT}^{(n+1)T-1} E \left[ \left\| g(\hat{X}_i^\lambda, U_{\mathbf{z}, k}) - \nabla F_\mathbf{z}(\hat{X}_i^\lambda) \right\|^2 \right]$$

$$\leq 2T \delta \sum_{i=nT}^{(n+1)T-1} (M^2 E \left[ \|\hat{X}_i^\lambda\|^2 \right] + B^2)$$

$$\leq 2T^2 \delta (M^2 C_n^x + B^2),$$

where the last inequality uses Lemma 5.3. \hfill \Box
This lemma provides variance control for the algorithm. Each term in $\Xi_n$ has an error of order $\delta$, the total variance in $\Xi_n$ is of order $T^3$. However, unlike RRT17, GCZ18, our technique does not accumulate variance errors over time, as shown in [10]. Recently in [BCM+18], the authors imposed no condition for variance of the estimated gradient, but employ the conditional L-mixing property of data stream, and hence variance is controlled by the decay of mixing property, see their Lemma 8.6.

**Lemma 4.4.** For every $nT \leq t < (n+1)T$, it holds that

$$E^{1/2} \left[ \left\| \hat{V}^{\text{int}}_t - \hat{V}_t \right\|^2 \right] \leq c_7 \sqrt{\lambda}, \quad E^{1/2} \left[ \left\| \hat{X}^{\text{int}}_t - \hat{X}_t \right\|^2 \right] \leq c_7 \sqrt{\lambda}.$$

**Proof.** Noting that $\hat{V}^{\text{int}}_{nt} = \hat{V}_{nt} = V^{nt}_{nt}$, we use the triangle inequality and Assumption 2.2 to estimate

$$\left\| \hat{V}^{\text{int}}_t - \hat{V}_t \right\| \leq \lambda \int_{nt}^t \left\| \hat{V}^{\text{int}}_s - \hat{V}_s \right\| ds \leq \lambda \int_{nt}^t \left\| \hat{V}^{\text{int}}_s - \hat{V}_s \right\| ds + \lambda \int_{nt}^t \left\| \nabla F_x(\hat{X}^{\text{int}}_s) - \nabla F_x(\hat{X}_s) \right\| ds \leq \lambda \int_{nt}^t \left\| \hat{V}^{\text{int}}_s - \hat{V}_s \right\| ds + \lambda \int_{nt}^t \left\| \hat{X}^{\text{int}}_s - \hat{X}_s \right\| ds.$$

For notational convenience, we define for every $nT \leq t < (n+1)T$

$$I_t := \left\| \hat{V}^{\text{int}}_t - \hat{V}_t \right\|, \quad J_t := \left\| \hat{X}^{\text{int}}_t - \hat{X}_t \right\|.$$

Then (40) becomes

$$I_t \leq \lambda \int_{nt}^t I_s ds + \lambda M \int_{nt}^t J_s ds + \lambda \int_{nt}^t \left\| \hat{V}^{\text{int}}_s - \hat{V}^{\text{int}}_s \right\| ds + \lambda M \int_{nt}^t \left\| \hat{X}^{\text{int}}_s - \hat{X}^{\text{int}}_s \right\| ds. \quad (41)$$

Furthermore,

$$J_t \leq \lambda \int_{nt}^t \left\| \hat{V}^{\text{int}}_s - \hat{V}_s \right\| ds + \lambda \int_{nt}^t \left\| \hat{V}^{\text{int}}_s - \hat{V}^{\text{int}}_s \right\| ds \leq \lambda \int_{nt}^t I_s ds + \lambda \int_{nt}^t \left\| \hat{V}^{\text{int}}_s - \hat{V}^{\text{int}}_s \right\| ds. \quad (42)$$

We estimate

$$\left\| \hat{V}^{\text{int}}_{[t]} - \hat{V}^{\text{int}}_t \right\|^2 \leq \lambda \int_{[t]}^t \left\| \hat{V}^{\text{int}}_s \right\|^2 ds + \lambda \int_{[t]}^t \left\| \nabla F_x(\hat{X}^{\text{int}}_s) \right\| ds + \sqrt{2\gamma \lambda \beta^{-1}} \left\| B^{\lambda}_t - B^{\lambda}_{[t]} \right\|^2.$$

Noting that $0 \leq t - [t] \leq 1$, the Cauchy-Schwarz inequality and Lemma 5.1 imply

$$\left\| \hat{V}^{\text{int}}_{[t]} - \hat{V}^{\text{int}}_t \right\|^2 \leq 3\lambda^2 \gamma^2 \int_{[t]}^t \left\| \hat{V}^{\text{int}}_s \right\|^2 ds + 6\lambda^2 M^2 \int_{[t]}^t \left\| \hat{X}^{\text{int}}_s \right\|^2 ds
+ 6\lambda^2 B^2 + 6\gamma \lambda \beta^{-1} \left\| B^{\lambda}_t - B^{\lambda}_{[t]} \right\|^2.$$

Taking expectation both sides and noting that $(\hat{V}^{\text{int}}_{k}, \hat{X}^{\text{int}}_{k})$ has the same distribution as $(\hat{V}^{\Lambda}_k, \hat{X}^{\Lambda}_k), k \in \mathbb{N}$, Lemma 5.3 leads to

$$E \left[ \left\| \hat{V}^{\text{int}}_{[t]} - \hat{V}^{\text{int}}_t \right\|^2 \right] \leq 3\lambda^2 \gamma^2 C_v^a + 6\lambda^2 M^2 C_x^a + 6\lambda^2 B^2 + 6\gamma \beta^{-1} \lambda \leq c_8 \lambda, \quad (43)$$

for $c_8 := 3\gamma^2 C_v^a + 6M^2 C_x^a + 6B^2 + 6\gamma \beta^{-1}$. Similarly,

$$E \left[ \left\| \hat{X}^{\text{int}}_{[t]} - \hat{X}^{\text{int}}_t \right\|^2 \right] = \lambda^2 \int_{[t]}^t E \left[ \left\| \hat{V}^{\text{int}}_s \right\|^2 \right] ds \leq \lambda^2 C_v^a. \quad (44)$$

Taking squares and expectation of (41), (42), applying (43), (44) we obtain for $nT \leq t < (n+1)T$

$$E \left[ I_t^2 \right] \leq 4\lambda^2 \int_{nt}^t E \left[ I_s^2 \right] ds + 4\lambda M^2 \int_{nt}^t E \left[ J_s^2 \right] ds + c_9 \lambda,$nT \leq t < (n+1)T$

$$E \left[ J_t^2 \right] \leq 2\lambda \int_{nt}^t E \left[ J_s^2 \right] ds + c_9 \lambda,$$
Therefore, an upper bound for $E[I_t^2 + J_t^2]$ is

$$E[I_t^2 + J_t^2] \leq c_{10} \lambda \int_{nT}^{t} E[I_s^2 + J_s^2] ds + 2c_9 \lambda,$$

where $c_{10} := \max\{4\gamma^2 + 2, 4M^2\}$ and then Gronwall’s lemma shows

$$E[I_t^2 + J_t^2] \leq 2c_9 \lambda e^{c_{10} t},$$

noting that $t \mapsto E[I_t^2 + J_t^2]$ is continuous. The proof is complete by setting $c_7 = \sqrt{2c_9 \lambda e^{c_{10} t}}$, which is of order $\sqrt{d}$.

### 4.3 Proof of Theorem 2.9

Denote $\mu_{x,k} := \mathcal{L}((V_0^x, X_0^x) \mid Z = z)$. Let $(\tilde{X}, \tilde{V})$ and $(\tilde{X}^*, \tilde{V}^*)$ be such that $\mathcal{L}((\tilde{X}, \tilde{V}) \mid Z = z) = \mu_{x,k}$ and $\mathcal{L}((\tilde{X}^*, \tilde{V}^*) = \pi_x$. We decompose the population risk by

$$E \left[ F(\tilde{X}) - F^* \right] = \left( E \left[ F(\tilde{X}) - E \left[ F(\tilde{X}^*) \right] \right] + \left( E \left[ F(\tilde{X}^*) - E \left[ F_x(\tilde{X}_x^*) \right] \right] \right) \right. + \left( E \left[ F_x(\tilde{X}_x^*) - F^* \right] \right).$$

#### 4.3.1 The first term $\mathcal{T}_1$

The first term in the right-hand side of (45) is rewritten as

$$E \left[ F(\tilde{X}) - F^* \right] = \int_{\mathbb{R}^d} \mu^{\otimes n}(dz) \left( \int_{\mathbb{R}^d} F_x(x) \mu_{x,k}(dx, dv) - \int_{\mathbb{R}^d} F_x(x) \pi_x(dx, dv) \right),$$

where $\mu^{\otimes n}$ is the product of laws of independent random variables $Z_1, ..., Z_n$. By Assumptions 2.1 and 2.2, the function $F_x$ satisfies $\|\nabla F_x(x)\| \leq M \|x\| + B$. Using Lemma 5.2 we have

$$\int_{\mathbb{R}^d} F_x(x) \mu_{x,k}(dx, dv) - \int_{\mathbb{R}^d} F_x(x) \pi_x(dx, dv) \leq (M \sigma + B) W_p(\mu_{x,k}, \pi_x),$$

where $p > 1, q \in \mathbb{N}, 1/p + 1/(2q) = 1$,

$$\sigma = \max \left\{ \left( \int_{\mathbb{R}^d} \|x\|^{2q} \mu_{x,k}(dx, dv) \right)^{1/(2q)}, \left( \int_{\mathbb{R}^d} \|x\|^{2q} \pi_x(dx, dv) \right)^{1/(2q)} \right\} < \infty$$

by Lemma 5.3. On the other hand, Theorems 2.8 and 4.1 imply

$$W_p(\mu_{x,k}, \pi_x) \leq W_p(\mathcal{L}((V_0^x, X_0^x) \mid Z = z), \mathcal{L}((\tilde{V}(k, 0, v_0), \tilde{X}(k, 0, x_0)) \mid Z = z)) + W_p(\mathcal{L}((\tilde{V}(k, 0, v_0), \tilde{X}(k, 0, x_0)) \mid Z = z), \pi_x) \leq \tilde{C}(\lambda^{1/(2p)} + \delta^{1/(2p)}) + C_* \left( W_p(\mu_0, \pi_x) \right)^{1/p} \exp(-c_* k \lambda).$$

Therefore, an upper bound for $\mathcal{T}_1$ is given by

$$\mathcal{T}_1 \leq (M \sigma + B) \left( \tilde{C}(\lambda^{1/(2p)} + \delta^{1/(2p)}) + C_* \left( W_p(\mu_0, \pi_x) \right)^{1/p} \exp(-c_* k \lambda) \right).$$

#### 4.3.2 The second term $\mathcal{T}_2$

Since the $x$-marginal of $\pi_x(dx, dv)$ is $\pi_x(dx)$, the Gibbs measure of $\pi_x$, we compute

$$\int_{\mathbb{R}^d} F_x(x) \pi_x(dx, dv) = \int_{\mathbb{R}^d} F_x(x) \pi_x(dx).$$

Therefore the argument in [RRTT12] is adopted,

$$E \left[ F(\tilde{X}^*) \right] - E \left[ F_x(\tilde{X}_x^*) \right] \leq \frac{4\beta_{C_{LS}}}{n} \left( \frac{M^2}{m} (b + d/\beta) + B^2 \right).$$
The constant $c_{LS}$ comes from the logarithmic Sobolev inequality for $\pi_z$ and

$$c_{LS} \leq \frac{2m^2 + 8M^2}{m^2M\beta} + \frac{1}{\lambda_*} \left( \frac{6M(d + \beta)}{m} + 2 \right),$$

where $\lambda_*$ is the uniform spectral gap for the overdamped Langevin dynamics

$$\lambda_* = \inf_{x \in \mathbb{R}^n} \inf \left\{ \int_{\mathbb{R}^d} \|\nabla g\|^2 d\pi_x : g \in C^1(\mathbb{R}^d) \cap L^2(\pi_x), g \neq 0, \int_{\mathbb{R}^d} g d\pi_x = 0 \right\}.$$

**Remark 4.5.** One can also find an upper bound for $\mathcal{T}_2$ when the data $z$ is a realization of some non-Markovian processes. For example, if we assume that $f$ is Lipschitz on the second variable $z$ and $Z$ satisfies a certain mixing property discussed in [CKRST16] then the term $\mathcal{T}_2$ is bounded by $1/\sqrt{\lambda}$ times a constant, see Theorem 2.5 therein.

### 4.3.3 The third term $\mathcal{T}_3$

For the third term, we follow [RRT17]. Let $x^*$ be any minimizer of $F(x)$. We compute

$$E \left[ F_Z(\hat{X}^*) - F^* \right] = E \left[ F_Z(\hat{X}^*) - \min_{x \in \mathbb{R}^d} F_Z(x) \right] + E \left[ \min_{x \in \mathbb{R}^d} F_Z(x) - F_Z(x^*) \right]$$

$$\leq E \left[ F_Z(\hat{X}^*) - \min_{x \in \mathbb{R}^d} F_Z(x) \right]$$

$$\leq \frac{d}{2\beta} \log \left( \frac{eM}{m} \left( \frac{b\beta}{d} + 1 \right) \right),$$

where the last inequality comes from Proposition 3.4 of [RRT17]. The condition $\beta \geq 2m$ is not used here, see the explanation in Lemma 16 of [GGZ18].

## 5 Technical lemmas

**Lemma 5.1.** Under Assumptions 2.1, 2.2 for any $x \in \mathbb{R}^d$ and $z \in U$,

$$\|\nabla f(x, z)\| \leq M\|x\| + B,$$

and

$$\frac{m}{3} \|x\|^2 - \frac{b}{2} \log 3 \leq f(x, z) \leq \frac{M}{2} \|x\|^2 + B\|x\| + A_0.$$

**Proof.** See Lemma 2 of [RRT17].

The next lemma generalizes continuity for functions of quadratic growth in Wasserstein distances given in [PW16].

**Lemma 5.2.** Let $\mu, \nu$ be two probability measures on $\mathbb{R}^{2d}$ with finite second moments and let $G : \mathbb{R}^{2d} \to \mathbb{R}$ be a $C^1$ function with

$$\|\nabla G(u)\| \leq c_1\|u\| + c_2$$

for some $c_1 > 0, c_2 \geq 0$. Then for $p > 1, q > 1$ such that $1/p + 1/q = 1$, we have

$$\left| \int_{\mathbb{R}^{2d}} Gd\mu - \int_{\mathbb{R}^{2d}} Gd\nu \right| \leq (c_1\sigma + c_2)\mathcal{W}_p(\mu, \nu),$$

where

$$\sigma = \frac{1}{2} \max \left\{ \left( \int_{\mathbb{R}^{2d}} \|v\|^q \nu(dv) \right)^{1/q}, \left( \int_{\mathbb{R}^{2d}} \|u\|^q \mu(du) \right)^{1/q} \right\}.$$

**Proof.** Using the Cauchy-Schwarz inequality, we compute

$$|G(u) - G(v)| = \left| \int_0^1 (\nabla G(tu + (1 - t)v), u - v) \, dt \right|$$

$$\leq \left| \int_0^1 (c_1\|v\| + c_1(1 - t)\|u\| + c_2)\|u - v\| \, dt \right|$$

$$= (c_1\|v\|/2 + c_1\|u\|/2 + c_2)\|u - v\|.$$
Then for any $\xi \in \Pi(\mu, \nu)$ we have

$$
\left| \int_{\mathbb{R}^d} G(u)\mu(du) - \int_{\mathbb{R}^d} G(v)\nu(dv) \right| \leq \int_{\mathbb{R}^d} (c_1 \|v\|^2 + c_1 \|u\|^2 + c_2) \|u - v\|\xi(du, dv)
$$

$$
\leq \frac{c_1}{2} \left( \int_{\mathbb{R}^d} \|v\|^q \nu(dv) \right)^{1/q} \left( \int_{\mathbb{R}^d} \|u\|^p \xi(du, dv) \right)^{1/p} + \frac{c_1}{2} \left( \int_{\mathbb{R}^d} \|u\|^q \mu(du) \right)^{1/q} \left( \int_{\mathbb{R}^d} \|v\|^p \xi(du, dv) \right)^{1/p} + c_2 \left( \int_{\mathbb{R}^d} \|u - v\|^p \xi(du, dv) \right)^{1/p}.
$$


Since this inequality holds true for any $\xi \in \Pi(\mu, \nu)$, the proof is complete. \hfill \square

**Lemma 5.3.** The continuous time processes $[4], [5]$ are uniformly bounded in $L^2$, more precisely,

$$
\sup_{t \geq 0} E_{\nu} \left[ \|X_t\|^2 \right] \leq C_{\nu} := \frac{8}{(1 - 2\lambda_c)^{\beta} \gamma^2} \left( \int_{\mathbb{R}^d} \nu(x, v)d\mu_0(x, v) + \frac{5(d + A_c)}{\lambda_c} \right) < \infty,
$$

$$
\sup_{t \geq 0} E_{\nu} \left[ \|V_t\|^2 \right] \leq C_{\nu} := \frac{4}{(1 - 2\lambda_c)^{\beta}} \left( \int_{\mathbb{R}^d} \nu(x, v)d\mu_0(x, v) + \frac{5(d + A_c)}{\lambda_c} \right) < \infty.
$$

For $0 < \lambda \leq \min \left\{ \frac{\gamma}{\sqrt{\gamma} A}, \frac{\gamma^2}{2\sqrt{\gamma}} \right\}$, where

$$
K_1 := \max \left\{ \frac{32M^2(1 + \gamma + \delta)}{(1 - 2\lambda_c)^{\beta} \gamma^2}, \frac{8(d + A_c) + \frac{\gamma^2}{\lambda (1 - 2\lambda_c)} + \gamma} \right\}
$$

and

$$
k_2 := 2B^2 \left( \frac{1}{2} + \gamma + \delta \right),
$$

the SGHMC [2], [7] satisfy

$$
\sup_{k \in \mathbb{N}} E_{\nu} \left[ \|X_k\|^2 \right] \leq C_{\nu} := \frac{8}{(1 - 2\lambda_c)^{\beta} \gamma^2} \left( \int_{\mathbb{R}^d} \nu(x, v)d\mu_0(x, v) + \frac{8(d + A_c)}{\lambda_c} \right) < \infty,
$$

$$
\sup_{k \in \mathbb{N}} E_{\nu} \left[ \|V_k\|^2 \right] \leq C_{\nu} := \frac{4}{(1 - 2\lambda_c)^{\beta}} \left( \int_{\mathbb{R}^d} \nu(x, v)d\mu_0(x, v) + \frac{8(d + A_c)}{\lambda_c} \right) < \infty.
$$

Furthermore, the processes defined in [24], [25] are also uniformly bounded in $L^2$ with the upper bounds $C_{\nu}^c, C_{\nu}^z, C_{\nu}^v, C_{\nu}^z$, respectively.

**Proof.** The uniform boundedness in $L^2$ of the processes in [4], [5], [9], [10] are given in Lemma 8 of [GGZT18]. From (A.4) of [GGZT18], it holds that

$$
\nu(v, x) \geq \max \left\{ \frac{1}{8}(1 - 2\lambda_c)\beta \gamma^2 \|x\|^2, \frac{\beta}{4}(1 - 2\lambda_c)\|v\|^2 \right\}.
$$

(48)

Using the notations in their Lemma 8, we denote

$$
L_t = E_{\nu} \left[ \nu(V_t, X_t) \right], \quad L_2(k) = E_{\nu} \left[ \nu(V_k, X_k) / \beta \right],
$$

then the following relations hold

$$
L_t \leq L_4 e^{-\gamma \lambda_c (t - s)} + \frac{d + A_c}{\lambda_c}(1 - e^{-\gamma \lambda_c (t - s)}), \quad \text{for } s \leq t, \tag{49}
$$

$$
L_2(k) \leq L_2(j) + \frac{4(d / \beta + A_c / \beta)}{\lambda_c} \quad \text{for } j \leq k. \tag{50}
$$

Taking $j = 0$ in (50) gives

$$
E_{\nu} \left[ \nu(V_0, X_0) \right] \leq E_{\nu} \left[ \nu(V_0, X_0) \right] + \frac{4(d + A_c)}{\lambda_c}.
$$

(51)

Therefore, by (19) we obtain for $nT \leq t < (n + 1)T, n \in \mathbb{N}$

$$
E_{\nu} \left[ \nu(\tilde{V}(t, nT, V_{nT}), \tilde{X}(t, nT, V_{nT})) \right] \leq E_{\nu} \left[ \nu(V_{nT}, X_{nT}) \right] + \frac{d + A_c}{\lambda_c}.
$$

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Then the processes in (54) is uniformly bounded in $L^2$ by (18) and (51),
\[
\sup_{c_0 \geq 0} E \left[ \| \tilde{V}_t \|^2 \right] \leq \frac{4}{(1 - 2 \lambda_c) \beta} \left( \int_{\mathbb{R}^d} \mathcal{V}(x, v) d\mu_0(x, v) + \frac{5(d + A_c)}{\lambda_c} \right) = C_c^v,
\]
and
\[
\sup_{c \geq 0} E \left[ \| \tilde{X}_t \|^2 \right] \leq \frac{8}{(1 - 2 \lambda_c) \beta^2 \gamma} \left( \int_{\mathbb{R}^d} \mathcal{V}(x, v) d\mu_0(x, v) + \frac{5(d + A_c)}{\lambda_c} \right) = C_c^x.
\]

Similarly, from (50) and (51), we obtain for $nT \leq k < (n + 1)T, n \in \mathbb{N}$,
\[
E_x \left[ \mathcal{V}(\tilde{V}_k^x, \tilde{X}_k^x) \right] \leq E_x \left[ \mathcal{V}(\tilde{V}_0^x, X_0^x) \right] + \frac{8(d + A_c)}{\lambda_c},
\]
and the upper bounds for $\sup_{k \in \mathbb{N}} E[\| \tilde{V}_k^x \|^2], \sup_{k \in \mathbb{N}} E[\| \tilde{X}_k^x \|^2]$ are $C_v^a, C_x^a$, respectively.

\begin{lemma}
Let $\mu, \nu$ be any two probability measures on $\mathbb{R}^{2d}$. It holds that
\[
W_\rho(\mu, \nu) \leq c_{17} \left( 1 + e_c \left( \int \mathcal{V}^2 d\mu \right)^{1/2} + e_c \left( \int \mathcal{V}^2 d\nu \right)^{1/2} \right) W_2(\mu, \nu),
\]
where $c_{17} := 3 \max\{1 + \alpha, \gamma^{-1}\}$.
\end{lemma}

\begin{proof}
From (2.11) of [CGZT17], we have that $h(x) \leq x$, for $x \geq 0$, and from (18), $r((x_1, v_1), (x_2, v_2)) \leq c_{17}/3\|(x_1, v_1) - (x_2, v_2)\|$. By definition (20), we estimate
\[
W_\rho(\mu, \nu) = \inf_{\xi \in \Pi(\mu, \nu)} \int_{\mathbb{R}^{2d}} \rho((x_1, v_1), (x_2, v_2)) \xi(d(x_1, v_1)d(x_2, v_2))
\leq \inf_{\xi \in \Pi(\mu, \nu)} \int_{\mathbb{R}^{2d}} r((x_1, v_1), (x_2, v_2)) (1 + e_c \mathcal{V}(x_1, v_1) + e_c \mathcal{V}(x_2, v_2)) \xi(d(x_1, v_1)d(x_2, v_2))
\leq c_{17}/3 \inf_{\xi \in \Pi(\mu, \nu)} \int_{\mathbb{R}^{2d}} \|(x_1, v_1) - (x_2, v_2)\| (1 + e_c \mathcal{V}(x_1, v_1) + e_c \mathcal{V}(x_2, v_2)) \xi(d(x_1, v_1)d(x_2, v_2))
\leq c_{17} \left( 1 + e_c \left( \int \mathcal{V}^2 d\mu \right)^{1/2} + e_c \left( \int \mathcal{V}^2 d\nu \right)^{1/2} \right) W_2(\mu, \nu).
\]
\end{proof}

\begin{lemma}
Let $1 \leq q \in \mathbb{N}$. It holds that

$C_v^{2q} := \sup_{k \in \mathbb{N}} E[\| \tilde{V}_k^x \|^{2q}] < \infty$, \quad $C_x^{2q} := \sup_{k \in \mathbb{N}} E[\| \tilde{X}_k^x \|^{2q}] < \infty$.
\end{lemma}

\begin{proof}
We will use the arguments in the proof of Lemma 12 of [CGZT18] to obtain the contraction for $\mathcal{V}(X_k^x, V_k^x)$ and in Lemma 3.9 of [CMR+18] to obtain high moment estimates. First, we have
\[
F_\rho(X_{k+1}^x, V_{k+1}^x) - F_\rho(X_k^x, V_k^x) = \int_0^1 \langle \nabla F_\rho(X_k^x, \gamma V_k^x), \lambda \mathcal{V}_k^x \rangle d\tau
\leq \int_0^1 \| \nabla F_\rho(X_k^x, \gamma V_k^x) - \nabla F_\rho(X_k^x) \| \| \mathcal{V}_k^x \| d\tau
\leq \frac{1}{2} M \lambda^2 \| \mathcal{V}_k^x \|^2.
\]
Denoting $\Delta_k^x = V_k^x - \lambda [\gamma V_k^x + g(X_k^x, U_{x,k})]$, we compute
\[
\| \Delta_{k+1}^x \|^2 = \| \Delta_k^x \|^2 + 2 \gamma \beta^{-1} \lambda \| \xi_{k+1} \|^2 + 2 \sqrt{2} \gamma \beta^{-1} \lambda \langle \Delta_k^x, \xi_{k+1} \rangle
\leq \| V_k^x - \lambda [\gamma V_k^x + g(X_k^x, U_{x,k})] - \nabla F_\rho(X_k^x, \lambda \mathcal{V}_k^x) \| \| \mathcal{V}_k^x \| d\tau
\leq (1 - \lambda)^2 \| V_k^x \|^2 - 2 \lambda (1 - \lambda) \langle \nabla F_\rho(X_k^x), V_k^x \rangle + 2 \lambda^2 \| F_\rho(X_k^x) \|^2 + 2 \lambda^2 \| g(X_k^x, U_{x,k}) - \nabla F_\rho(X_k^x) \|^2
\leq (1 - \lambda)^2 \| V_k^x \|^2 - 2 \lambda (1 - \lambda) \langle \nabla F_\rho(X_k^x), V_k^x \rangle + 3 \lambda^2 (M \| X_k^x \| + B)^2 + 2 \gamma \beta^{-1} \lambda \| \xi_{k+1} \|^2 + 2 \sqrt{2} \gamma \beta^{-1} \lambda \langle \Delta_k^x, \xi_{k+1} \rangle.
\]
Similarly, we have
\[
\|X_{k+1}^l\|^2 = \|X_k^l\|^2 + 2\lambda \langle X_k^l, V_k^l \rangle + \lambda^2 \|V_k^l\|^2.
\] (54)

Denoting \(\Delta_k^l = X_k^l + \gamma^{-1}V_k^l - \lambda\gamma^{-1}g(X_k^l, U_{x,k})\), we compute that
\[
\begin{align*}
\|X_{k+1}^l + \gamma^{-1}V_{k+1}^l\|^2 &= \|X_k^l + \gamma^{-1}V_k^l - \lambda\gamma^{-1}g(X_k^l, U_{x,k}) + \sqrt{2\gamma^{-1}\beta^{-1}\lambda}\xi_{k+1}\|^2 \\
&= \|X_k^l + \gamma^{-1}V_k^l - \lambda\gamma^{-1}g(X_k^l, U_{x,k})\|^2 + 2\gamma^{-1}\beta^{-1}\lambda\xi_{k+1}\|^2 + 2\sqrt{2\gamma^{-1}\beta^{-1}\lambda}\langle \Delta_k^l, \xi_{k+1}\rangle \\
&\leq \|X_k^l + \gamma^{-1}V_k^l - \lambda\gamma^{-1}\nabla F_k(X_k^l)\|^2 + \lambda^2\gamma^{-2}\|g(X_k^l, U_{x,k}) - F_k(X_k^l)\|^2 \\
&\quad + 2\gamma^{-1}\beta^{-1}\lambda\xi_{k+1}\|^2 + 2\sqrt{2\gamma^{-1}\beta^{-1}\lambda}\langle \Delta_k^l, \xi_{k+1}\rangle \\
&\leq \|X_k^l + \gamma^{-1}V_k^l\|^2 + 2\gamma^{-1}\nabla F_k(X_k^l)\|^2 + \lambda^2\gamma^{-1}\lambda\xi_{k+1}\|^2 + 3\lambda^2\gamma^{-2}(M\|X_k^l\| + B)^2 \\
&\quad + 2\gamma^{-1}\beta^{-1}\lambda\xi_{k+1}\|^2 + 2\sqrt{2\gamma^{-1}\beta^{-1}\lambda}\langle \Delta_k^l, \xi_{k+1}\rangle .
\end{align*}
\] (55)

Let us denote \(V_k = \nabla(X_k^l, V_k^l)\). From (54), (55), and (56) we compute that
\[
\begin{align*}
\frac{V_{k+1} - V_k}{\beta} &\leq \lambda \langle \nabla F_k(X_k^l), V_k^l \rangle + \frac{1}{4} M\lambda^2\|V_k^l\|^2 \\
&\quad - \frac{1}{2} \lambda \gamma \langle \nabla F_k(X_k^l), X_k^l + \gamma^{-1}V_k^l \rangle + \frac{3}{4} \lambda^2 \|X_k^l\| + B)^2 + \\
&\quad + \frac{1}{2} \gamma^{-1}\lambda\xi_{k+1}\|^2 + \frac{1}{4} \sqrt{2\gamma^{-1}\beta^{-1}\lambda}\langle \Delta_k^l, \xi_{k+1}\rangle \\
&\quad + \frac{1}{2} (-2 \lambda \gamma + \lambda^2\gamma^{-2})\|V_k^l\|^2 - \frac{1}{2} \lambda \gamma \langle \nabla F_k(X_k^l), V_k^l \rangle + \frac{3}{4} \lambda^2 \|X_k^l\| + B)^2 + \\
&\quad + \frac{1}{2} \gamma^{-1}\lambda\xi_{k+1}\|^2 + \frac{1}{4} \sqrt{2\gamma^{-1}\beta^{-1}\lambda}\langle \Delta_k^l, \xi_{k+1}\rangle \\
&\quad - \frac{1}{2} \lambda \gamma \langle \nabla F_k(X_k^l), X_k^l \rangle \right) \|V_k^l\|^2 \\
&\quad - \frac{1}{2} \lambda \gamma \|V_k^l\|^2 - \frac{1}{2} \lambda \gamma \langle X_k^l, V_k^l \rangle + \lambda^2\xi_k \\
&\quad + \gamma^{-1}\lambda\xi_{k+1}\|^2 + \Sigma_k,
\end{align*}
\]

where
\[
\begin{align*}
\xi_k &:= \left(\frac{1}{2} M + \frac{1}{4} \gamma - \frac{1}{4} \gamma^2\lambda_c\right) \|V_k^l\|^2 + \frac{3}{2} \|X_k^l\|^2 + B)^2 + \frac{1}{2} \gamma \langle \nabla F_k(X_k^l), V_k^l \rangle, \\
\Sigma_k &:= \frac{1}{2} \gamma^2 \sqrt{2\gamma^{-1}\beta^{-1}\lambda}\langle \Delta_k^l, \xi_{k+1}\rangle + \frac{1}{2} \sqrt{2\gamma^{-1}\beta^{-1}\lambda}\langle \Delta_k^l, \xi_{k+1}\rangle .
\end{align*}
\]

Using the inequality (50), we obtain
\[
\frac{V_{k+1} - V_k}{\beta} \leq -\lambda \gamma \langle X_k^l, V_k^l \rangle - \frac{1}{4} \gamma^3\lambda_c\|X_k^l\|^2 + \lambda \gamma \langle X_k^l, V_k^l \rangle + \lambda^2\xi_k \\
+ \gamma^{-1}\lambda\xi_{k+1}\|^2 + \Sigma_k.
\] (57)

The quantity \(\xi_k\) is bounded as follows
\[
\xi_k \leq \left(\frac{1}{2} M + \frac{1}{4} \gamma - \frac{1}{4} \gamma^2\lambda_c + \gamma \right) \|V_k^l\|^2 + M^2(3 + 2\gamma)\|X_k^l\|^2 + B^2(3 + 2\gamma).
\]

As in [GGZ18], we deduce that
\[
\frac{V_k}{\beta} \geq \max \left\{ \frac{1}{8} (1 - 2\lambda_c) \gamma^2 \|X_k^l\|^2, \frac{1}{4} (1 - 2\lambda_c) \|V_k^l\|^2 \right\} \\
\geq \frac{1}{16} (1 - 2\lambda_c) \gamma^2 \|X_k^l\|^2 + \frac{1}{8} (1 - 2\lambda_c) \|V_k^l\|^2.
\] (58)

And then we get that
\[
\xi_k \leq K_1 V_k + K_2
\] (59)
where
\[ K_1 = \max \left\{ \frac{M^2(3 + 2\gamma)}{16(1 - 2\lambda)c_4\gamma^2}, \frac{(M/2 + \gamma^2/4 - \gamma^2c_4/4 + \gamma)}{\delta(1 - 2\lambda)} \right\}, \quad K_2 = B^2(3 + 2\gamma). \]

Similarly, we bound \( \Sigma_k \), using \( \lambda \leq 2 \) and the definitions of \( \Delta_k, \Sigma_k \),

\[
\|\Sigma_k\|^2 \leq 2\gamma^3 - \lambda \|\Delta_k\|^2 \|\xi_{k+1}\|^2 + 2\gamma^2 \lambda \|\Delta_k\|^2 \|\xi_{k+1}\|^2 + 2\gamma \lambda \|\xi_{k+1}\|^2 \|\xi_{k+1}\|^2 + 2||V_k^\lambda - \lambda \gamma V_k^\lambda + g(X_k^\lambda, U_{x,k})||^2 + 2\lambda \|\xi_{k+1}\|^2 (3\gamma^2 + 3(\|X_k^\lambda\|^2 + 3(M\|X_k^\lambda\| + B)^2 + 2(1 - \gamma^2)^2 ||V_k^\lambda||^2 + 2(M\|X_k^\lambda\| + B)^2)
\]

and thus
\[
\|\Sigma_k\|^2 \leq (P_1 V_k / \beta + P_2) \lambda \|\xi_{k+1}\|^2
\]

where
\[
P_1 = 2 \max \left\{ \frac{2\gamma - (3\gamma^2 + 10M^2)}{16(1 - 2\lambda)c_4\gamma^2}, \frac{2 \gamma^2 (3 + 2(1 - \lambda\gamma^2))^2}{\delta(1 - 2\lambda)} \right\}, \quad P_2 = 20\gamma\beta - B^2.
\]

Noting that \( \lambda_c \leq 1/4 \), we have
\[
V_k / \beta = F_k(X_k^\lambda) + \frac{1}{4} \gamma^2 (1 - \lambda_c) \|X_k^\lambda\|^2 + \frac{1}{2} \gamma \|X_k^\lambda, V_k^\lambda\| + \frac{1}{2} \|V_k^\lambda\|^2
\]

From \([57], [58]\) we obtain
\[
\frac{V_{k+1} - V_k}{\beta} \leq -\lambda \gamma \lambda_c \left( F_k(X_k^\lambda) + \frac{1}{4} \gamma^2 \|X_k^\lambda\|^2 - A_c / (\beta \lambda_c) + \frac{1}{2\lambda_c} \|V_k^\lambda\|^2 + \frac{1}{2} \gamma \|X_k^\lambda, V_k^\lambda\| \right) + \lambda^2 \epsilon_k + \gamma \beta^{-1} \lambda \|\xi_{k+1}\|^2 + \Sigma_k
\]

\[
\leq \lambda \gamma (A_c / \beta - \lambda_c V_k / \beta) + (K_1 V_k / \beta + K_2) \lambda^2 + \gamma \beta^{-1} \lambda \|\xi_{k+1}\|^2 + \Sigma_k.
\]

Therefore, for \( 0 < \lambda < \frac{\lambda}{4\lambda_1} \),
\[
V_{k+1} \leq \phi V_k + K_{k+1}
\]

where
\[
\phi := 1 - \lambda \gamma \lambda_c / 2, \quad K_{k+1} := \lambda \gamma A_c + \lambda^2 \beta K_2 + \gamma \lambda \|\xi_{k+1}\|^2 + \beta \Sigma_k.
\]

Define \( E_k[\cdot] := E[\cdot(X_k^\lambda, V_k^\lambda), Z = z] \). We then compute as follows,
\[
E_k[V_{k+1}^q] \leq E_k \left[ (|\phi V_k|^q + 2|\phi V_k|^{q-1}) E_k \left[ \phi V_k K_{k+1} \right] + \sum_{k=2}^{2q} C_{2q}^k C_k E_k \left[ |\phi V_k|^{2q-k} K_{k+1} \right] \right]^q
\]

where the last inequality is due to Lemma A.3 of \([\text{CMR+18}]\). Denoting \( c_{19} := \gamma A_c + \beta K_2 + \gamma d \), we continue
\[
E_k[V_{k+1}^q] \leq |\phi V_k|^q + 2\lambda c_{19} q |\phi V_k|^{2q-1} + \sum_{t=0}^{2q-2} \left( \frac{2q}{\ell + 2} \right) E_k \left[ |\phi V_k|^{2q-2-\ell} K_{k+1} |K_{k+1}|^\ell \right]
\]

\[
\leq |\phi V_k|^q + 2\lambda c_{19} |\phi V_k|^{2q-1} + \left( \frac{2q}{2} \right) \sum_{t=0}^{q-2} \left( \frac{2q - 2}{\ell} \right) C_{2q-2}^{q-2} E_k \left[ |\phi V_k|^{2q-2-\ell} K_{k+1} |K_{k+1}|^\ell \right]
\]

\[
\leq |\phi V_k|^q + 2\lambda c_{19} |\phi V_k|^{2q-1} + q(2q - 1) E_k \left[ (|\phi V_k|^q + |K_{k+1}|) |K_{k+1}|^q \right]
\]

\[
\leq |\phi V_k|^q + 2\lambda c_{19} |\phi V_k|^{2q-1} + q(2q - 1) 2^{q-3} E_k \|K_{k+1}\|^{2q}. \tag{63}
\]

Clearly we have
\[
E_k[K_{k+1}]^q \leq 3\lambda(\gamma A_c + \beta K_2)^2 + 3\lambda \gamma^2 E[|\xi_{k+1}|^4 + 3\lambda \beta d P_1 |V_k| + 3\lambda^2 d P_2,
\]

\[
E_k[K_{k+1}]^{2q} \leq 2^{q-1} \lambda E \left( \gamma A_c + \beta K_2 + \gamma 2 |\xi_{k+1}|^2 + \beta \sqrt{P_2} ||\xi_{k+1}||^2 + 2^{q-1} \lambda^2 P_1 |V_k|^q E[|\xi_{k+1}|]^{2q}. \tag{64}
\]
Define
\[
\tilde{M}_1 := \max \left\{ \frac{(\gamma A_c + \beta K_2)^2 + \gamma^2 E\|\xi_{k+1}\|^4 + \beta^2 dP_2}{\beta dP_1}, \left( \frac{E (\gamma A_c + \beta K_2 + \gamma\|\xi_{k+1}\|^2 + \beta \sqrt{P_2}\|\xi_{k+1}\|)^{2q}}{\beta P_1 E^{1/q}\|\xi_{k+1}\|^{2q}} \right)^{1/q} \right\}.
\]

On \( \{\mathcal{V}_k \geq \tilde{M}_1\} \) we have
\[
E_k\|\tilde{K}_{k+1}\|^2 \leq 6\lambda\beta dP_1|\mathcal{V}_k|,
\]
and thus
\[
E_k|\mathcal{V}_{k+1}|^{2q} \leq 2^{2q}\lambda^q P_1^q|\mathcal{V}_k|E\|\xi_{k+1}\|^{2q}.
\]

If we choose
\[
\tilde{M} := \max \left\{ \tilde{M}_1, \frac{2\gamma c_1 q}{\gamma c}, \frac{72q(2q-1)2^{q-3}\beta dP_1}{\gamma c}, \left( \frac{12q(2q-1)2^{q-3}\beta^q P_1^q E\|\xi_{k+1}\|^{2q}}{\gamma c} \right)^{1/q} \right\}
\]
then on \( \{\mathcal{V}_k \geq \tilde{M}\} \), the second, the third and the fourth term in the RHS of (64) are bounded by 0 and then
\[
E_k|\mathcal{V}_{k+1}|^2 \leq (1 - \lambda\gamma c/4)|\mathcal{V}_k|^2.
\]

On \( \{\mathcal{V}_k < \tilde{M}\} \), we have
\[
E_k|\mathcal{V}_{k+1}|^2 \leq (1 - \lambda\gamma c/4)|\mathcal{V}_k|^2 + \lambda\tilde{N},
\]
where \( \tilde{N} = 2c_1 q\tilde{M}^{q-1} + 6q(2q-1)2^{q-3}\beta dP_1\tilde{M}^{2q-1} + q(2q-1)2^{q-3}\beta^q P_1^q E\|\xi_{k+1}\|^{2q}\tilde{M}^q \). For sufficiently small \( \lambda \), we get from these bounds
\[
E|\mathcal{V}_k^2| \leq (1 - \lambda\gamma c/4)k|\mathcal{V}_0^2 + \frac{4\tilde{N}}{\gamma c}.
\]

The proof is complete by using (55). \( \square \)

5.1 Explicit dependence of constants on important parameters

Similar to [GGZ18], we choose \( \mu_0 \) in such a way that
\[
\int_{\mathbb{R}^{2d}} \mathcal{V}(x,v) d\mu_0(dx,dv) = \mathcal{O}(\beta), \quad \int_{\mathbb{R}^{2d}} e^{\mathcal{V}(x,v)} d\mu_0(dx,dv) = \mathcal{O}(e^\beta).
\]
Then we get \( C_x = C_v = C_c = C_v = \mathcal{O}((\beta + d)/\beta) \). It follows that
\[
c_2 = c_3 = c_7 = c_{16} = \mathcal{O}(\sqrt{1 + d/\beta}).
\]

It is checked that
\[
A_c = \mathcal{O}(\beta), \quad \alpha_c = \mathcal{O}(1), \quad \Lambda_c = \mathcal{O}(\beta + d), \quad R_1 = \mathcal{O}(\sqrt{1 + d/\beta}),
\]
and
\[
c_* = \mathcal{O}(\sqrt{1 + d} e^{-\mathcal{O}(\beta^2+d)}),
\]
\[
C_* = \mathcal{O}(e^{\Lambda_c/p} \left( \frac{R_1^p - \beta^d}{\beta c_*} \right)^{1/p}) = \mathcal{O} \left( \frac{(d + \beta)^{1/2 - 1/(2p)}}{\beta^{1/2 - 1/(2p)} \Lambda_c^{1/2}} \right) = \mathcal{O} \left( \frac{(d + \beta)^{1/2}}{\beta^{1/2 - 1/(2p)} c_*^{2/p}} \right).
\]
The constant $c_*, C_*$ are $\mu_*$ and $C$ respectively in [GGZ18]. In addition, we check
\[
c_{19} = O(d + \beta), \quad \tilde{M} = \tilde{M}_1 = O((d + \beta)^2/d),
\]
\[
\tilde{N} = O\left(\frac{(d + \beta)^{4q - 1}}{d^{2q - 1}}\right), \quad c_{18} = O((d + \beta)^{3/2}/d^{1/2})
\]
and hence
\[
\tilde{C} = O\left(\frac{(d + \beta)^{1/2 + 2/p}}{\beta^{1/2}d^{1/2p}}\frac{e^{-c_*}}{c_*^{2/p}(1 - e^{-c_*})}\right).
\]
From Lemma 16 of [GGZ18], we get
\[
W_p(\mu_0, \pi_x) = O\left(\sqrt{\frac{\beta + d}{\beta}}\right).
\]
Furthermore, it is observed that
\[
\sigma = O\left(\frac{(d + \beta)^{1-1/(4q)}}{d^{1/2 - 1/(4q)}}\right).
\]
Therefore, for a fixed $k$, the term $B_1$ is bounded by
\[
B_1 = O\left(\frac{(d + \beta)^{3/2 + 2/p - 1/(4q)}}{\beta^{1/2}d^{1/2 + 1/(4q)}c_*^{2/p}(1 - e^{-c_*})}\right)(\lambda^{1/(2p)} + \tilde{\delta}^{1/(2p)})
\]
\[
+ O\left(\frac{(d + \beta)^{3/2 + 1/(2p) - 1/(4q)}}{d^{1/2 - 1/(4q)}(\beta + \beta)}\right)e^{-c_*k\lambda}.
\]
Since $c_*$ is exponentially small in $(\beta + d)$, our bound for $B_1$ is worse than that of $J_1(\varepsilon) + J_0(\varepsilon)$ given in [GGZ18].

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