Ergodicity and Long-Time Behavior of Random Batch Method for Interacting Particle Systems

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1 Problem Setting

- Simulation of large-size interacting particle systems is an important task in computational physics.
- A simple model of common interest is the following first-order Langevin dynamics of the N particles $\{X_t^i\}_{i=1}^N$ in $\mathbb{R}^d$:

$$\dot{X}_t^i = b(X_t^i) + \frac{1}{N-1}\sum_{j\neq i} K(X_t^i - X_t^j) + \sigma \dot{W}_t^i, \qquad \text{(IPS)}$$

  where $b : \mathbb{R}^d \to \mathbb{R}^d$ is the drift force in $\mathbb{R}^d$, $K : \mathbb{R}^d \to \mathbb{R}^d$ is the interaction force in $\mathbb{R}^d$, $\sigma > 0$ is the fixed diffusion constant, and $\{W_t^i\}_{i=1}^N$ are independent Wiener processes in $\mathbb{R}^d$.
- Our goal is to design efficient numerical methods to sample the invariant distribution $\pi \in \mathcal{P}(\mathbb{R}^{dN})$ of the (IPS).
- When $b = -\nabla V$ and $K = -\nabla W$ are gradients for some potential functions V and W, then $\pi \propto e^{-U}$ with the potential function

$$U(x) = \sum_{i=1}^N V(x^i) + \frac{1}{N-1}\sum_{1\leqslant i<j\leqslant N} W(x^i - x^j)$$

1 Classical Results

The analytical results of the (IPS) are fruitful.

- As the number of the particles $N \to \infty$, the (IPS) converges to the following McKean–Vlasov process of the single particle $\bar{X}_t$ in $\mathbb{R}^d$:

$$\dot{\bar{X}}_t = b(\bar{X}_t) + \int_{\mathbb{R}^d} K(\bar{X}_t - z)\nu_t(\mathrm{d}z) + \sigma \dot{W}_t, \qquad \text{(MVP)}$$

  where $\nu_t = \mathrm{Law}(\bar{X}_t)$ is the distribution law of the random variable $\bar{X}_t$, and W_t is the Wiener process. This is classical in the theory of the propagation of chaos [Chaintron22].

- When the interaction force K is moderately small, the (IPS) has uniform-in-N ergodicity[1], which can be proved by either reflection coupling [Eberle16] or functional inequalities [Guillin22]. In this case the (MVP) has a unique invariant distribution $\bar{\pi} \in \mathcal{P}(\mathbb{R}^d)$.

Given the results above, our goal comprises sampling $\pi \in \mathcal{P}(\mathbb{R}^{dN})$ using the (IPS) and sampling $\bar{\pi}$ using the (MVP).

[1] The convergence rate towards the equilibrium is uniform in the number of particles N

1 Random Batch Method

- The Random Batch Method [Jin20] is a novel simulation tool for the interacting particle systems. In the (IPS), it requires $\mathcal{O}(N^2)$ cost to compute the interaction forces, which is a burden when N is large.
- To resolve this, pick a small integer $p \geqslant 2$, randomly divide the N particles into $q = N/p$ batches, denoted by $\mathcal{D} = \{\mathcal{C}_1, \cdots, \mathcal{C}_q\}$. Then approximate the interaction forces within the batches, i.e., construct the random batch interacting particle system $\{Y_t^i\}_{i=1}^N$ by

$$\dot{Y}_t^i = b(Y_t^i) + \frac{1}{N-1} \sum_{j \neq i, j \in \mathcal{C}} K(Y_t^i - Y_t^j) + \sigma \dot{W}_t^i, \qquad \text{(RB-IPS)}$$

  where for each $i \in \{1, \cdots, N\}$, $\mathcal{C} \in \mathcal{D}$ is the unique batch that contains the index i.
- The most important feature of the IPS is that the random division $\mathcal{D}$ is renewed for each time step. Fix the time step $\tau > 0$, then for each $n \in \mathbb{N}$, the (RB-IPS) in the time interval $[n\tau, (n+1)\tau)$ is evolved with an independent choice of $\mathcal{D}$.

- Using the Euler–Maruyama discretization, we obtain the numerical scheme of $\{\tilde{Y}_n^i\}$ in $\mathbb{R}^{dN}$, which is given by

$$\tilde{Y}_n^i = b(\tilde{Y}_n^i)\tau + \frac{1}{N-1}\sum_{j\neq i, j\in\mathcal{C}} K(\tilde{Y}_n^i - \tilde{Y}_n^j)\tau + \sigma\sqrt{\tau}\xi_n^i, \quad \text{(discrete RB-IPS)}$$

  where $\{\xi_n^i\}_{i=1}^N$ are independent normal random variables, and $\tilde{Y}_n^i$ is expected to be an approximation of $Y_{n\tau}^i$.

- The (discrete RB-IPS) reduces the computational cost from $\mathcal{O}(N^2)$ to $\mathcal{O}(pN)$, which largely accelerates the simulation. In this way, the (discrete RB-IPS) is an efficient numerical method for the (IPS).

- Given the parameters τ (time step) and p (batch size), how accurately does the (discrete RB-IPS) sample the distribution $\pi \in \mathcal{P}(\mathbb{R}^{dN})$?

2 Main Results

We state our main results on the long-time behavior of the (RB-IPS) and the (discrete RB-IPS), which requires the following assumptions:

Assumption 1 (global Lipschitz condition)

For the drift force b, there exists a constant L_0 such that

$$|b(x)| \leqslant L_0(|x| + 1), \quad \forall x \in \mathbb{R}^d.$$

For the interaction force K, there exists a constant L_1 such that

$$\max\{|K(x)|, |\nabla K(x)|, |\nabla^2 K(x)|\} \leqslant L_1, \quad \forall x \in \mathbb{R}^{dN}.$$

Assumption 2 (drift condition)

There exists the function $\kappa(r)$ in $r \in (0, +\infty)$ satisfying

$$\kappa(r) \leqslant \left\{ -\frac{2}{\sigma^2} \frac{(x-y)\cdot(b(x)-b(y))}{|x-y|^2} : x, y \in \mathbb{R}^d, |x-y| = r \right\}.$$

and the following conditions:

1. $\kappa(r)$ is continuous for $r \in (0, +\infty)$;
2. $\kappa(r)$ has a lower bound for $r \in (0, +\infty)$;
3. $\varliminf_{r\to\infty} \kappa(r) > 0$.

[JinLiYeZhou23] Ergodicity and long-time behavior of the Random Batch Method for interacting particle systems.

Theorem 1 (ergodicity of the RB-IPS)

Under Assumptions 1 and 2, there exist constants $L_{\max}, C, \beta$ independent of N, τ, p such that if the constant $L_1 < L_{\max}$, then

$$\mathcal{W}_1(\mu q_{n\tau}, \nu q_{n\tau}) \leqslant C e^{-\beta n\tau} \mathcal{W}_1(\mu, \nu), \quad \forall t \geqslant 0,$$

where μ, ν are probability distributions in $\mathbb{R}^{dN}$, and $q_{n\tau}$ is the transition semigroup of the (RB-IPS).

Here, $\mathcal{W}_1(\mu, \nu)$ is the normalized Wasserstein distance

$$\mathcal{W}_1(\mu, \nu) = \inf_{\gamma \in \Pi(\mu,\nu)} \int_{\mathbb{R}^{dN} \times \mathbb{R}^{dN}} \left(\frac{1}{N} \sum_{i=1}^{N} |x^i - y^i| \right) \gamma(\mathrm{d}x\mathrm{d}y).$$

As a consequence, the RB-IPS has a unique invariant distribution in $\mathbb{R}^{dN}$.

[JinLiYeZhou23] Ergodicity and long-time behavior of the Random Batch Method for interacting particle systems.

Corollary 1 (long-time behavior of the RB-IPS)

Under Assumptions 1 and 2, there exist constants $L_{\max}, C, \beta$ independent of N, τ, p such that if the constant $L_1 < L_{\max}$, then

$$\mathcal{W}_1(\mathrm{Law}(Y_{n\tau}), \pi) \leqslant C\sqrt{\tau^2 + \frac{\tau}{p-1}} + Ce^{-\beta n\tau}, \quad \forall n \geqslant 0.$$

Here, the first part corresponds to the strong error of the (RB-IPS) in a finite time period, and the second part corresponds to the uniform ergodicity of the (RB-IPS).

[YeZhou23] Error analysis of time-discrete Random Batch Method for interacting particle systems and associated mean-field limits.

Theorem 2 (long-time behavior of the discrete RB-IPS)

Under Assumptions 1 and 2, there exist constants $L_{\max}, \tau_{\max}, C, \lambda$ independent of N, τ, p such that if the constants $L_1 < L_{\max}$, $\tau < \tau_{\max}$, then

$$\mathcal{W}_1(\mathrm{Law}(\tilde{Y}_n), \pi) \leqslant C\sqrt{\tau} + Ce^{-\lambda n\tau}, \quad \forall n \geqslant 0.$$

Here, $\tilde{Y}_n \in \mathbb{R}^{dN}$ is the state of The convergence rate λ here can be smaller than β in Theorem 1, but it can be guaranteed that λ is also independent of N, τ, p. Theorem 2 characterizes the long-time sampling error of the (discrete RB-IPS), which comprises the discretization error in terms of the time step τ and the exponential convergence term.

[YeZhou23] Error analysis of time-discrete Random Batch Method for interacting particle systems and associated mean-field limits.

Corollary 2 (long-time behavior of the discrete RB-IPS)

Under Assumptions 1 and 2, there exist constants $L_{\max}, \tau_{\max}, C, \lambda$ independent of N, τ, p such that if the constants $L_1 < L_{\max}$, $\tau < \tau_{\max}$, then

$$\mathcal{W}_1(\mu_{n\tau}^{\mathrm{RB}}, \bar{\pi}) \leqslant C\sqrt{\tau} + Ce^{-\lambda n\tau} + \frac{C}{\sqrt{N}}, \quad \forall n \geqslant 0,$$

where $\mu_{n\tau}^{\mathrm{RB}}$ is the empirical distribution of the particles $\{\tilde{Y}_n^i\}_{i=1}^N$,

$$\mu_{n\tau}^{\mathrm{RB}} = \frac{1}{N}\sum_{i=1}^N \delta(x - \tilde{Y}_n^i) \in \mathcal{P}(\mathbb{R}^d).$$

This characterizes the sampling accuracy of the invariant distribution $\bar{\pi}$ for the (MVP).

3 Outline

3 Reflection Coupling

The main mathematical tool to prove the uniform-in-N ergodicity of the (RB-IPS) is the reflection coupling technique introduced in [Eberle16].

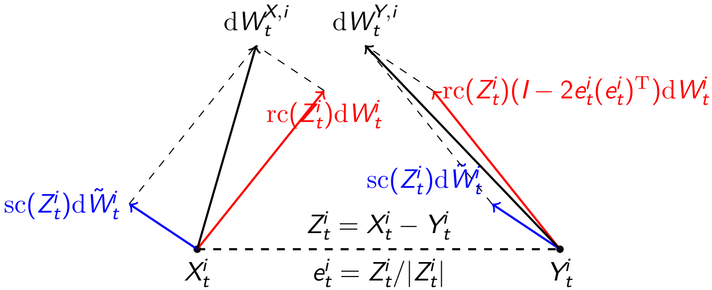

Figure 1: A schematic show of the reflection coupling method.

With the reflection coupling of the Wiener processes of two duplicates of RB-IPS, one can prove the uniform ergodicity in the $\mathcal{W}_1$-distance.

For completeness, we explicitly write the coupling scheme for the IPS (1.1). The coupled dynamics $\{(X_t, Y_t)\}_{t\geqslant 0}$ in $\mathbb{R}^{Nd}\times\mathbb{R}^{Nd}$ is given by

$$\begin{cases} \mathrm{d}X_t^i = b(X_t^i)\mathrm{d}t + \dfrac{1}{N-1}\displaystyle\sum_{j\neq i} K(X_t^i - X_t^j)\mathrm{d}t \\ \qquad\qquad + \sigma\Big(\mathrm{rc}(Z_t^i)\mathrm{d}W_t^i + \mathrm{sc}(Z_t^i)\mathrm{d}\tilde{W}_t^i\Big), \\ \mathrm{d}Y_t^i = b^i(Y_t)\mathrm{d}t + \dfrac{1}{N-1}\displaystyle\sum_{j\neq i} K(Y_t^i - Y_t^j)\mathrm{d}t \\ \qquad\qquad + \sigma\Big(\mathrm{rc}(Z_t^i)(I - 2e_t^i(e_t^i)^{\mathrm{T}})\mathrm{d}W_t^i + \mathrm{sc}(Z_t^i)\mathrm{d}\tilde{W}_t^i\Big), \end{cases} \tag{2.43}$$

for $i = 1, \cdots, N$. Theorem 2.1 then immediately implies

[JinLiYeZhou23] The coupled dynamics for the (RB-IPS).

3 Triangle Inequality Framework

The study of the long-time behavior of the (discrete RB-IPS) employs the triangle inequality framework described below.

Lemma (triangle inequality)

Let $\{X_t\}_{t\geqslant 0}, \{\tilde{X}_t\}_{t\geqslant 0}$ be stochastic processes in $\mathbb{R}^d$ with transition probabilities $(p_t)_{t\geqslant 0}$, $(\tilde{p}_t)_{t\geqslant 0}$. Given the metric $d(\cdot,\cdot)$ on $\mathcal{P}(\mathbb{R}^d)$, assume $(p_t)_{t\geqslant 0}$ has an invariant distribution $\pi \in \mathcal{P}(\mathbb{R}^d)$ and there exist constants $C, \beta > 0$ such that

$$d(\nu p_t, \pi) \leqslant Ce^{-\beta t} d(\nu, \pi), \quad \forall \nu \in \mathcal{P}(\mathbb{R}^d);$$

and for any $T > 0$, there exists a constant $\varepsilon(T)$ such that

$$\sup_{0\leqslant t\leqslant T} d(\nu \tilde{p}_t, \nu p_t) \leqslant \varepsilon(T), \quad \forall \nu \in \mathcal{P}(\mathbb{R}^d).$$

Then there exist constants $T_0, \lambda > 0$ such that

$$d(\nu \tilde{p}_t, \pi) \leqslant 2\varepsilon(T_0) + 2M_0 e^{-\lambda t}, \quad \forall t \geqslant 0,$$

where $M_0 := \sup_{s\in[0,T_0]} d(\nu \tilde{p}_s, \pi)$.

[YeZhou21] Preconditioned Langevin dynamics: sampling thermal equilibrium of high dimensional quantum systems.

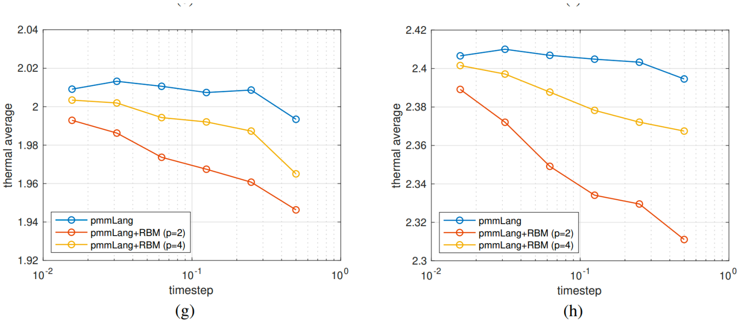

Figure 3: Error of the (RB-IPS) converges to 0 as the time step decreases.

5 Outline

5 References

[Chaintron22] Chaintron, L. P., & Diez, A. (2022). Propagation of chaos: a review of models, methods and applications. I. Models and methods. arXiv preprint arXiv:2203.00446.

[Guillin22] Guillin, A., Liu, W., Wu, L., & Zhang, C. (2022). Uniform Poincaré and logarithmic Sobolev inequalities for mean field particle systems. The Annals of Applied Probability, 32(3), 1590-1614.

[Eberle16] Eberle, Andreas. "Reflection couplings and contraction rates for diffusions." Probability theory and related fields 166 (2016): 851-886.

[Jin20] Jin, S., Li, L., & Liu, J. G. (2020). Random batch methods (RBM) for interacting particle systems. Journal of Computational Physics, 400, 108877.

[JinLiYeZhou23] Jin, S., Li, L., Ye, X., & Zhou, Z. (2023). Ergodicity and long-time behavior of the random batch method for interacting particle systems. Mathematical Models and Methods in Applied Sciences, 33(01), 67-102.

[YeZhou23] Error analysis of time-discrete random batch method for interacting particle systems and associated mean-field limits.

[YeZhou21] Ye, X., & Zhou, Z. (2021). Efficient sampling of thermal averages of interacting quantum particle systems with random batches. The Journal of Chemical Physics, 154(20).