A Finite-Particle Convergence Rate for Stein Variational Gradient Descent

Jiaxin Shi[*] JIAXINS@STANFORD.EDU
Stanford University

Lester Mackey LMACKEY@MICROSOFT.COM
Microsoft Research New England

Abstract

We provide a first finite-particle convergence rate for Stein variational gradient descent (SVGD). Specifically, whenever the target distribution satisfies Talagrand's inequality, SVGD with n particles and an appropriate step size sequence drives the kernel Stein discrepancy to zero at an order $1/\sqrt{\log \log n}$ rate. We suspect that the dependence on n can be improved, and we hope that our explicit, non-asymptotic proof strategy will serve as a template for future refinements.

1. Introduction

Stein variational gradient descent [SVGD, 11] is an algorithm for approximating a target distribution P with a collection of n particles. The algorithm iteratively evolves the particle locations to approach the target distribution through optimization in the space of probability measures. It has demonstrated encouraging results for a wide variety of inferential tasks, including approximate inference [11, 18, 19], generative modeling [17], and reinforcement learning [8, 13].

Despite the popularity of SVGD, relatively little is known about its convergence. A first analysis by Liu [10, Thm. 3.3] showed that an infinite-particle analogue of SVGD converges to P in kernel Stein discrepancy [KSD, 2, 6, 12]. Follow-up work by Korba et al. [9], Salim et al. [14], Sun et al. [15] sharpened this result with path-independent constants, weaker smoothness conditions, and explicit rates of convergence. In addition, Duncan et al. [4] analyzed the continuous-time limit of the infinite-particle analogue to provide conditions for exponential convergence. However, each of these analyses applies only to the infinite-particle analogue of SVGD and not to the finite-particle algorithm used in practice.

To bridge this gap, Liu [10, Thm. 3.2] showed that n-particle SVGD converges to its infinite-particle analogue in bounded-Lipschitz distance but only under boundedness assumptions violated by most common uses of SVGD. To provide a more broadly applicable proof of convergence, Gorham et al. [7, Thm. 7] showed that n-particle SVGD converges to its infinite-particle analogue in 1-Wasserstein distance under assumptions commonly satisfied in SVGD applications. However, both convergence results are asymptotic, providing neither explicit error bounds nor rates of convergence.

In this work, we derive the first explicit error bounds and rates of convergence for finite-particle SVGD. To achieve this, we first bound the 1-Wasserstein error between each round of finite- and

[*] Part of this work was done at Microsoft Research New England.

© J. Shi & L. Mackey.

infinite-particle SVGD in Theorem 1. We next bound the KSD in terms of the 1-Wasserstein distance in Theorem 2. Finally, Theorem 3 combines our results with the established infinite-particle KSD analysis of SVGD to arrive at an explicit KSD error bound for n-particle SVGD.

2. Notation and Assumptions

Throughout, we fix a reproducing kernel $k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$, let $\mathcal{H}$ denote its induced reproducing kernel Hilbert space (RKHS), and let $\mathcal{H}^d \triangleq \bigotimes_{i=1}^d \mathcal{H}$ denote the product RKHS [1]. For probability measures μ and ν, we let $W_1(\mu, \nu) \triangleq \inf_{X\sim\mu, Z\sim\nu} \mathbb{E}[\|Z - X\|_2]$ denote the 1-Wasserstein distance between them and introduce the shorthand $m_\mu \triangleq \mathbb{E}_\mu[\|\cdot\|]_2$, $m_{\mu,P} \triangleq \mathbb{E}_{X\sim\mu \perp\!\!\!\perp Z\sim P}[\|X - Z\|_2]$, and $M_{\mu,P} \triangleq \mathbb{E}_{X\sim\mu \perp\!\!\!\perp Z\sim P}[\|X - Z\|_2^2]$. We allow each of these quantities to take on the value ∞ when the random variables are not suitably integrable. We further define the Kullback-Leibler divergence as $\mathrm{KL}(\mu\|\nu) \triangleq \mathbb{E}_\mu[\log(\frac{d\mu}{d\nu})]$ when μ is absolutely continuous with respect to ν and as ∞ otherwise.

Our analysis will make use of the following standard assumptions on the SVGD kernel and target distribution.

Assumption 1 (Bounded kernel derivatives) $\sup_{x\in\mathbb{R}^d}\left(D_x^I D_y^I k(x, y)|_{y=x}\right) \leq \kappa^2$ *for any multi-index* $I = (I_1, I_2, \ldots, I_d)$ *with* $|I| \triangleq \sum_{i=1}^d I_i \leq 2$. *Here,* D^I *is the differential operator defined as* $D_x^I = \frac{d^{|I|}}{dx_1^{I_1} dx_2^{I_2} \ldots dx_d^{I_d}}$.

Under Assumption 1, we could show that for any $f \in \mathcal{H}$,

$$|f(x)| \leq \|f\|_{\mathcal{H}} \sqrt{k(x, x)} \leq \kappa \|f\|_{\mathcal{H}};$$
$$|D^I f(x)| \leq \|f\|_{\mathcal{H}} \sqrt{D_x^I D_y^I k(x, y)|_{y=x}} \leq \kappa \|f\|_{\mathcal{H}}.$$

Assumption 2 (Decaying kernel derivatives) *There exists* $\gamma > 0$ *such that*

$$\sup_{x,y\in\mathbb{R}^d, \|x-y\|_2\geq r} \|\nabla_x k(x, y)\|_2 \leq \gamma/r.$$

Assumption 3 (Lipschitz score function) *The target distribution* P *has a differentiable density* p *on* $\mathbb{R}^d$ *and an* L*-Lipschitz* score function $s_p \triangleq \nabla \log p$, *i.e.,* $\|s_p(x) - s_p(y)\|_2 \leq L\|x - y\|_2$ *for any* $x \neq y$. *We let* x^* *be any point that satisfies* $s_p(x^*) = 0$.

In line with Salim et al. [14], we also assume the distribution P satisfies Talagrand's inequality T1 [16, Def. 22.1]. We note that this assumption is only necessary for leveraging the infinite-particle convergence result of Salim et al. [14]. In case it does not hold, one can alternatively resort to the path-dependent assumptions in Korba et al. [9], Liu [10] .

Assumption 4 (Talagrand's inequality T1 [16, Def. 22.1]) *There exists* $\lambda > 0$ *such that for all* μ *with* $\mathbb{E}_\mu[\|\cdot\|_2] < \infty$

$$W_1(\mu, P) \leq \sqrt{2\mathrm{KL}(\mu\|P)/\lambda}.$$

Finally we make use of the following notation specific to the SVGD algorithm.

Definition 1 *The* Langevin Stein operator [5] *for a target measure P supported on $\mathbb{R}^d$ is defined by*

$$(\mathcal{T}_P g)(x) \triangleq \langle s_p(x), g(x)\rangle + \nabla \cdot g(x)$$

for any vector-valued function $g : \mathbb{R}^d \to \mathbb{R}^d$.

Definition 2 *The* vector-valued Langevin Stein operator [12] *for a target measure P on $\mathbb{R}^d$ is defined by*

$$(\mathcal{A}_P h)(x) \triangleq s_p(x)h(x) + \nabla h(x)$$

with components

$$(\mathcal{A}_P^j h)(x) \triangleq (s_p(x))_j\, h(x) + \nabla_j h(x)$$

for any function $h : \mathbb{R}^d \to \mathbb{R}$.

Definition 3 *The* SVGD transport map [11] *for a kernel k, target measure P, approximating measure μ, and step size ϵ is given by*

$$T_{\mu,\epsilon}(x) \triangleq x + \epsilon \mathbb{E}_{X\sim\mu}[(\mathcal{A}_P k(\cdot, x))(X)].$$

Definition 4 *The* SVGD pushforward $\Phi_\epsilon(\mu)$ *represents the distribution of $T_{\mu,\epsilon}(X)$ when $X \sim \mu$.*

Definition 5 *The* Langevin kernel Stein discrepancy [KSD, 2, 6, 12] *with base kernel k, target measure P, and approximating measure μ is given by*

$$\mathrm{KSD}(\mu, P) \triangleq \sup_{\|g\|_{\mathcal{H}^d}\leq 1} \mathbb{E}_\mu[\mathcal{T}_P g].$$

3. Discretization Error of SVGD

Our first main result concerns the discretization error of SVGD and shows that n-particle SVGD does not stray too far from its infinite-particle limit when its step sizes are chosen appropriately.

Theorem 1 (Discretization error of SVGD) *Suppose Assumptions 1, 2, and 3 hold. Let μ_r^n, μ_r^∞ denote the approximation given by n-particle and infinite-number-of-particle SVGD with step size ϵ_r at step r. And let $b_r \triangleq \sum_{s=0}^r \epsilon_s$. Then*

$$W_1(\mu_{r+1}^n, \mu_{r+1}^\infty) \leq W_1(\mu_0^n, \mu_0^\infty)\exp(b_r(A + B\exp(Cb_r))),$$

for $A = (c_1 + c_2)(1 + m_P)$, $B = c_1 m_{\mu_0^n,P} + c_2 m_{\mu_0^\infty,P}$, and $C = \kappa^2(3L + d)$. Here $c_1 = \max(\sqrt{d}\kappa^2 L, \sqrt{d}\kappa^2 L\|x^*\|_2 + d\kappa^2)$, $c_2 = \kappa^2 L + d\kappa^2 + (\gamma + \sqrt{d}\kappa^2)(1 + \|x^*\|_2)$.

The proof of Theorem 1 in Appendix A relies on two lemmas. The first, due to Gorham et al. [7], shows that the one-step SVGD mapping Φ_ϵ is pseudo-Lipschitz with respect to the 1-Wasserstein distance whenever the score function $\nabla \log p$ and kernel k fulfill a commonly-satisfied pseudo-Lipschitz condition.

Lemma 1 (Wasserstein pseudo-Lipschitzness of SVGD [7, Lem. 12]) *Suppose that, for some constants $c_1, c_2 > 0$, the following pseudo-Lipschitz bounds hold:*

$$\sup_{z\in\mathbb{R}^d} \|\nabla_z(s_p(x)k(x,z) + \nabla_x k(x,z))\|_{\mathrm{op}} \le c_1(1+\|x\|_2),$$
$$\sup_{x\in\mathbb{R}^d} \|\nabla_x(s_p(x)k(x,z) + \nabla_x k(x,z))\|_{\mathrm{op}} \le c_2(1+\|z\|_2).$$

Then,

$$W_1(\Phi_\epsilon(\mu), \Phi_\epsilon(\nu)) \le W(\mu,\nu)(1+\epsilon c_{\mu,\nu}),$$

where $c_{\mu,\nu} = c_1(1+m_\mu) + c_2(1+m_\nu)$.

The second lemma, proved in Appendix B, controls first and second absolute moment growth under SVGD using P as a reference.

Lemma 2 (SVGD moment growth) *Suppose Assumptions 1 and 3 hold. Let μ_r denote the approximation given by SVGD at step r. Then,*

$$\begin{aligned} m_{\mu_r} &\le m_{\mu_0,P} \textstyle\prod_{s=0}^{r-1}(1+\epsilon_s C) + m_P \le m_{\mu_0,P}\exp(Cb_{r-1}) + m_P, \\ M_{\mu_r,P} &\le M_{\mu_0,P} \textstyle\prod_{s=0}^{r-1}(1+2\epsilon_s C + \epsilon_s^2 C^2) \le M_{\mu_0,P}\exp((2C+\epsilon_0 C^2)b_{r-1}) \end{aligned} \tag{1}$$

for $C = \kappa^2(3L+d)$.

4. From Wasserstein to KSD

The above infinite-particle SVGD convergence rate is computed with respect to KSD. To relate it to the Wasserstein discretization error bound in Theorem 1, we establish the following KSD-Wasserstein bound.

Theorem 2 (KSD-Wasserstein bound) *Suppose Assumptions 1 and 3 hold. Let μ_r^n, μ_r^∞ denote the approximation by n particle and infinitely many particle SVGD at iteration r. Then,*

$$\begin{aligned} \mathrm{KSD}(\mu_r^n, P) \le{}& \kappa(d+L)W_1(\mu_r^n,\mu_r^\infty) + d^{1/4}\kappa L\exp((C+\epsilon_0 C^2/2)b_{r-1})\sqrt{2M_{\mu_0^\infty,P}W_1(\mu_r^n,\mu_r^\infty)} \\ &+ \mathrm{KSD}(\mu_r^\infty, P). \end{aligned}$$

Proof Using the result of Lemma 3, Cauchy-Schwarz, Eq. (1) of Lemma 2, and $\min(a,b)^2 \le ab$, we have

$$\begin{aligned} \mathrm{KSD}(\mu_r^n, P) &= \sup_{\|g\|_{\mathcal{H}^d}\le 1} \mathbb{E}_{\mu_r^n}[\mathcal{T}_P g] - \mathbb{E}_{\mu_r^\infty}[\mathcal{T}_P g] + \mathbb{E}_{\mu_r^\infty}[\mathcal{T}_P g] \\ &\le \sup_{\|g\|_{\mathcal{H}^d}\le 1} \mathbb{E}_{\mu_r^n}[\mathcal{T}_P g] - \mathbb{E}_{\mu_r^\infty}[\mathcal{T}_P g] + \sup_{\|g\|_{\mathcal{H}^d}\le 1} \mathbb{E}_{\mu_r^\infty}[\mathcal{T}_P g] \\ &\le \kappa(d+L)W_1(\mu_r^n,\mu_r^\infty) + L\mathbb{E}_{X\sim\mu_r^n, Y\sim\mu_r^\infty, Z\sim P}[\|Y-Z\|_2 \min(2\kappa, \sqrt{d}\kappa\|X-Y\|_2)] \\ &\quad + \mathrm{KSD}(\mu_r^\infty, P) \\ &\le \kappa(d+L)W_1(\mu_r^n,\mu_r^\infty) + LM_{\mu_r^\infty,P}^{1/2}\mathbb{E}_{X\sim\mu_r^n, Y\sim\mu_r^\infty}[\min(2\kappa, \sqrt{d}\kappa\|X-Y\|_2)^2]^{1/2} \\ &\quad + \mathrm{KSD}(\mu_r^\infty, P) \\ &\le \kappa(d+L)W_1(\mu_r^n,\mu_r^\infty) + \sqrt{2M_{\mu_r^\infty,P}}d^{1/4}\kappa L\mathbb{E}_{X\sim\mu_r^n, Y\sim\mu_r^\infty}[\|X-Y\|_2]^{1/2} \\ &\quad + \mathrm{KSD}(\mu_r^\infty, P). \end{aligned}$$

Taking the infinimum over the joint distribution of (X, Y) leads to

$$\mathrm{KSD}(\mu_r^n, P) \leq \kappa(d+L)W_1(\mu_r^n, \mu_r^\infty) + d^{1/4}\kappa L \exp((C + \epsilon_0 C^2/2)b_{r-1})\sqrt{2M_{\mu_0^\infty,P} W_1(\mu_r^n, \mu_r^\infty)} + \mathrm{KSD}(\mu_r^\infty, P).$$

■

The proof of Theorem 2 uses the following lemma, a generalization of Gorham and Mackey [6, Lem. 18] that we prove in Appendix C, which shows that the mean discrepancy between two $\mathcal{T}_P$ transformed functions is controlled by the 1-Wasserstein distance.

Lemma 3 (Single function Stein discrepancy bound) *Suppose Assumptions 1 and 3 hold. Let μ, ν be two probability measures on $\mathbb{R}^d$ and $g \in \mathcal{H}^d$ satisfying $\|g\|_{\mathcal{H}^d}^2 \triangleq \sum_{i=1}^d \|g_i\|_{\mathcal{H}}^2 \leq 1$. Then,*

$$\mathbb{E}_\mu[\mathcal{T}_P g] - \mathbb{E}_\nu[\mathcal{T}_P g] \leq \kappa(d+L)W_1(\mu,\nu) + L\mathbb{E}_{(X\sim\mu, Y\sim\nu)\perp\!\!\!\perp Z\sim P}[\|Y-Z\|_2 \min(2\kappa, \sqrt{d}\kappa\|X-Y\|_2)].$$

5. A Finite-particle Convergence Rate for SVGD

To establish our main SVGD convergence result, we combine Theorems 1 and 2 with the following infinite-particle SVGD convergence rate due to Salim et al. [14] (see also Korba et al. [9], Liu [10]).

Lemma 4 (Infinite-particle SVGD descent lemma [14, Theorem 3.2]) *Suppose Assumptions 1, 3, and 4 hold. For any constant $\alpha > 1$ and $\epsilon_r < \min\left(\frac{2}{\kappa^2(L+\alpha^2)}, R\right)$, where $R \triangleq (\alpha-1)(1 + L\mathbb{E}_{\mu_0}[\|\cdot - x^*\|_2] + 2L\sqrt{2\mathrm{KL}(\mu_0^\infty\|P)/\lambda})$, SVGD with infinite number of particles decreases KL and drives KSD to zero:*

$$\mathrm{KL}(\mu_{r+1}^\infty\|P) - \mathrm{KL}(\mu_r^\infty\|P) \leq -\epsilon_r\left(1 - \frac{\kappa^2(L+\alpha^2)}{2}\epsilon_r\right)\mathrm{KSD}(\mu_r^\infty, P)^2. \tag{2}$$

By summing (2) over $r = 0, \ldots, t$, we have the following corollary:

Corollary 1 *Let $c(\epsilon) \triangleq \epsilon\left(1 - \frac{\kappa^2(L+\alpha^2)}{2}\epsilon\right)$. If $\epsilon_r \leq \min\left(\frac{1}{\kappa^2(L+\alpha^2)}, R\right)$, then we have $\frac{\epsilon_r}{2} \leq c(\epsilon_r) < \epsilon_r$ and thereby*

$$\frac{1}{\sum_{r=0}^t c(\epsilon_r)}\sum_{r=0}^t c(\epsilon_r)\mathrm{KSD}(\mu_r^\infty, P)^2 \leq \frac{1}{\sum_{r=0}^t c(\epsilon_r)}\mathrm{KL}(\mu_0^\infty\|P) \leq \frac{2}{b_t}\mathrm{KL}(\mu_0^\infty\|P).$$

Finally, we arrive at our main result that shows finite-particle SVGD with appropriately chosen step size sequences drives KSD to zero as $W_1(\mu_0^n, \mu_0^\infty) \to 0$.

Theorem 3 (KSD error of finite-particle SVGD) *Suppose Assumptions 1, 2, 3, and 4 hold. Define $\pi_r \triangleq \frac{c(\epsilon_r)}{\sum_{r=0}^{t-1} c(\epsilon_r)}$ and $w_0 \triangleq W_1(\mu_0^n, \mu_0^\infty)$. Let $b_t = \sum_{r=0}^t \epsilon_t$. Then,*

$$\min_{0\leq r<t}\mathrm{KSD}(\mu_r^n, P) \leq \sum_{r=0}^{t-1}\pi_r\mathrm{KSD}(\mu_r^n, P) \leq a_t + \left(\frac{2}{b_{t-1}}\mathrm{KL}(\mu_0^\infty\|P)\right)^{1/2}, \tag{3}$$

where $a_t = \kappa(d+L)w_0\exp(b_{t-1}(A + B\exp(Cb_{t-1}))) + d^{1/4}\kappa L\sqrt{2M_{\mu_0^\infty,P}w_0}\exp(((2C + \epsilon_0 C^2 + A + B\exp(Cb_{t-1}))/2)b_{t-1})$, and A, B, C are defined as in Theorem 1.

Proof Let $w_r \triangleq W_1(\mu_r^n, \mu_r^\infty)$. From Theorem 2, we know

$$\mathrm{KSD}(\mu_r^n, P) \le \kappa(d+L)w_r + d^{1/4}\kappa L \exp((C+\epsilon_0 C^2/2)b_{r-1})\sqrt{2M_{\mu_0^\infty,P} w_r} + \mathrm{KSD}(\mu_r^\infty, P).$$

Plugging in Theorem 1's result

$$w_r \le w_0 \exp(b_{r-1}(A + B\exp(Cb_{r-1}))),$$

we have $\mathrm{KSD}(\mu_r^n, P) - a_r \le \mathrm{KSD}(\mu_r^\infty, P)$, where

$$\begin{aligned} a_r = {} & \kappa(d+L)w_0 \exp(b_{r-1}(A + B\exp(Cb_{r-1}))) \\ & + d^{1/4}\kappa L\sqrt{2M_{\mu_0^\infty,P} w_0}\exp((2C + \epsilon_0 C^2 + A + B\exp(Cb_{r-1}))/2)b_{r-1}). \end{aligned}$$

Taking square on both sides and the weighted sum over $r = 0, \dots, t-1$ with weights $\pi_r \triangleq \frac{c(\epsilon_r)}{\sum_{r=0}^{t-1} c(\epsilon_r)}$, we obtain

$$\textstyle\sum_{r=0}^{t-1} \pi_r (\mathrm{KSD}(\mu_r^n, P) - a_r)^2 \le \sum_{r=0}^{t-1} \pi_r \mathrm{KSD}(\mu_r^\infty, P)^2 \le \frac{2}{b_{t-1}} \mathrm{KL}(Q_0^\infty \| P), \tag{4}$$

where the last inequality follows from Corollary 1. Moreover, by Cauchy-Schwarz,

$$\textstyle\sum_{r=0}^{t-1} \pi_r (\mathrm{KSD}(\mu_r^n, P) - a_r)^2 \ge \left(\sum_{r=0}^{t-1} \pi_r \mathrm{KSD}(\mu_r^n, P) - \sum_{r=0}^{t-1} \pi_r a_r\right)^2 \tag{5}$$

Combining (4) and (5), we have

$$\textstyle\sum_{r=0}^{t-1} \pi_r \mathrm{KSD}(\mu_r^n, P) \le \sum_{r=0}^{t-1} \pi_r a_r + \left(\frac{2}{b_{t-1}} \mathrm{KL}(\mu_0^\infty \| P)\right)^{1/2}.$$

We finish the proof by noticing that $\sum_{r=0}^{t-1} \pi_r a_r \le \max_{0 \le r < t} a_r = a_{t-1} \le a_t$. ■

The following corollary, proved in Appendix D, provides an explicit rate of SVGD by choosing the step size sequence and t such that the resulting b_{t-1} balance the three terms on the right hand side of (3).

Corollary 2 (A finite-particle convergence rate for SVGD) *Define the shorthand* $\psi_{B,C}(x, y, \beta) \triangleq \frac{1}{C}\log\left(\frac{1}{B}(\frac{1}{\beta}\log\frac{1}{x} - y)\right)$. *If* $\max_{0 \le r < t} \epsilon_r \le \min\left(\frac{1}{\kappa^2(L+\alpha^2)}, R\right)$ *and*

$$\begin{aligned} b_{t-1} = \textstyle\sum_{r=0}^{t-1} \epsilon_r = {} & \min\Big(\psi_{B,C}\big(w_0\sqrt{\log\log\tfrac{1}{w_0}}, A, \beta_1\big), \psi_{B,C}\big(w_0 \log\log\tfrac{1}{w_0}, A + 2C + \epsilon_0 C^2, \beta_2\big)\Big), \\ & \textit{for } \beta_1 \triangleq \max\Big(1, \psi_{B,C}\big(w_0\sqrt{\log\log\tfrac{1}{w_0}}, A, 1\big)\Big) \textit{ and} \\ & \beta_2 \triangleq \max\Big(1, \psi_{B,C}\big(w_0 \log\log\tfrac{1}{w_0}, A + 2C + \epsilon_0 C^2, 1\big)\Big), \end{aligned}$$

then,

$$\min_{0 \le r < t} \mathrm{KSD}(\mu_r^n, P) = O\Big(1/\sqrt{\log\log\tfrac{1}{w_0}}\Big).$$

If, in addition, $\mu_0^n = \frac{1}{n}\sum_{i=1}^n \delta_{x_i}$ *for* $x_i \overset{i.i.d.}{\sim} \mu_0^\infty$, *then*

$$\min_{0 \le r < t} \mathrm{KSD}(\mu_r^n, P) = O\Big(\tfrac{1}{\sqrt{\log\log n}}\Big).$$

References

[1] Alain Berlinet and Christine Thomas-Agnan. *Reproducing kernel Hilbert spaces in probability and statistics*. Springer Science & Business Media, 2011.

[2] Kacper Chwialkowski, Heiko Strathmann, and Arthur Gretton. A kernel test of goodness of fit. In *International Conference on Machine Learning*, pages 2606–2615, 2016.

[3] Richard Mansfield Dudley. The speed of mean Glivenko-Cantelli convergence. *The Annals of Mathematical Statistics*, 40(1):40–50, 1969.

[4] Andrew Duncan, Nikolas Nüsken, and Lukasz Szpruch. On the geometry of Stein variational gradient descent. *arXiv preprint arXiv:1912.00894*, 2019.

[5] Jackson Gorham and Lester Mackey. Measuring sample quality with Stein's method. In *Advances in Neural Information Processing Systems*, pages 226–234, 2015.

[6] Jackson Gorham and Lester Mackey. Measuring sample quality with kernels. In *International Conference on Machine Learning*, pages 1292–1301, 2017.

[7] Jackson Gorham, Anant Raj, and Lester Mackey. Stochastic Stein discrepancies. *Advances in Neural Information Processing Systems*, 33:17931–17942, 2020.

[8] Tuomas Haarnoja, Haoran Tang, Pieter Abbeel, and Sergey Levine. Reinforcement learning with deep energy-based policies. In *International Conference on Machine Learning*, pages 1352–1361, 2017.

[9] Anna Korba, Adil Salim, Michael Arbel, Giulia Luise, and Arthur Gretton. A non-asymptotic analysis for Stein variational gradient descent. *Advances in Neural Information Processing Systems*, 33, 2020.

[10] Qiang Liu. Stein variational gradient descent as gradient flow. In *Advances in Neural Information Processing Systems*, pages 3115–3123, 2017.

[11] Qiang Liu and Dilin Wang. Stein variational gradient descent: A general purpose Bayesian inference algorithm. *Advances in Neural Information Processing Systems*, 29:2378–2386, 2016.

[12] Qiang Liu, Jason Lee, and Michael Jordan. A kernelized Stein discrepancy for goodness-of-fit tests. In *International Conference on Machine Learning*, pages 276–284, 2016.

[13] Yang Liu, Prajit Ramachandran, Qiang Liu, and Jian Peng. Stein variational policy gradient. In *33rd Conference on Uncertainty in Artificial Intelligence*, 2017.

[14] Adil Salim, Lukang Sun, and Peter Richtarik. A convergence theory for SVGD in the population limit under Talagrand's inequality T1. In *International Conference on Machine Learning*, pages 19139–19152. PMLR, 2022.

[15] Lukang Sun, Avetik Karagulyan, and Peter Richtarik. Convergence of Stein variational gradient descent under a weaker smoothness condition. *arXiv preprint arXiv:2206.00508*, 2022.

[16] Cédric Villani. *Optimal transport: old and new*, volume 338. Springer, 2009.

[17] Dilin Wang and Qiang Liu. Learning to draw samples: With application to amortized MLE for generative adversarial learning. *arXiv preprint arXiv:1611.01722*, 2016.

[18] Dilin Wang, Zhe Zeng, and Qiang Liu. Stein variational message passing for continuous graphical models. In *International Conference on Machine Learning*, pages 5219–5227, 2018.

[19] Jingwei Zhuo, Chang Liu, Jiaxin Shi, Jun Zhu, Ning Chen, and Bo Zhang. Message passing Stein variational gradient descent. In *International Conference on Machine Learning*, pages 6018–6027, 2018.

Appendix A. Proof of Theorem 1: Discretization error of SVGD

We first show that the pseudo-Lipshitz conditions in Lemma 1 holds given our assumptions. According to Assumption 1, we have

$$\nabla_{z_i} k(x,z) = \langle \nabla_{z_i} k(z,\cdot), k(x,\cdot)\rangle_{\mathcal{H}} \le (\nabla_{z_i}\nabla_{z_i'} k(z,z')|_{z'=z} k(x,x))^{1/2} \le \kappa^2,$$
$$\|\nabla_z k(x,z)\|_2 = \sqrt{\textstyle\sum_{i=1}^d (\nabla_{z_i} k(x,z))^2} \le \sqrt{d}\kappa^2.$$
$$\nabla_{z_j}\nabla_{x_i} k(x,z) = \langle \nabla_{z_j} k(z,\cdot), \nabla_{x_i} k(x,\cdot)\rangle_{\mathcal{H}} \le (\nabla_{z_j}\nabla_{z_j'} k(z,z')|_{z'=z}\nabla_{x_i}\nabla_{x_i'} k(x,x')|_{x'=x})^{1/2} \le \kappa^2,$$
$$\|\nabla_z\nabla_x k(x,z)\|_{\mathrm{op}} \le \|\nabla_z\nabla_x k(x,z)\|_F = \sqrt{\textstyle\sum_{i=1}^d\sum_{j=1}^d (\nabla_{z_j}\nabla_{x_i} k(x,z))^2} \le d\kappa^2,$$

Recall that x^* satisfies $s_p(x^*) = 0$ by Assumption 3. Then, by triangle inequality, the definition of $\|\cdot\|_{\mathrm{op}}$, and Cauchy-Schwartz,

$$\begin{aligned}
&\|\nabla_z(s_p(x)k(x,z) + \nabla_x k(x,z))\|_{\mathrm{op}} \\
&= \left\|(s_p(x) - s_p(x^*))\nabla_z k(x,z)^\top\right\|_{\mathrm{op}} + \|\nabla_z\nabla_x k(x,z)\|_{\mathrm{op}} \\
&\le \sup_{\|u\|_2\le 1}(\|s_p(x) - s_p(x^*)\|_2 |\nabla_z k(x,z)^\top u|) + d\kappa^2 \\
&\le L\|x - x^*\|_2 \|\nabla_z k(x,z)\|_2 + d\kappa^2 \\
&\le \sqrt{d}\kappa^2 L(\|x\|_2 + \|x^*\|_2) + d\kappa^2 \\
&\le \max(\sqrt{d}\kappa^2 L, \sqrt{d}\kappa^2 L\|x^*\|_2 + d\kappa^2)(1 + \|x\|_2).
\end{aligned}$$

Letting $c_1 = \max(\sqrt{d}\kappa^2 L, \sqrt{d}\kappa^2 L\|x^*\|_2 + d\kappa^2)$ and taking supremum over z proves the first pseudo-Lipschitz condition. Similarly, we have

$$\begin{aligned}
&\|\nabla_x(s_p(x)k(x,z) + \nabla_x k(x,z))\|_{\mathrm{op}} \\
&= \|\nabla s_p(x)\|_{\mathrm{op}} k(x,z) + \left\|(s_p(x) - s_p(x^*))\nabla_x k(x,z)^\top\right\|_{\mathrm{op}} + \left\|\nabla_x^2 k(x,z)\right\|_{\mathrm{op}} \\
&\le \kappa^2 L + L\|x - x^*\|_2 \|\nabla_x k(x,z)\|_2 + d\kappa^2,
\end{aligned} \tag{6}$$

where we used

$$k(x,z) = \langle k(x,\cdot), k(z,\cdot)\rangle_{\mathcal{H}} \le \sqrt{k(x,x)k(z,z)} \le \kappa^2,$$
$$\left\|\nabla_x^2 k(x,z)\right\|_{\mathrm{op}} \le \left\|\nabla_x^2 k(x,z)\right\|_F = \sqrt{\textstyle\sum_{|I|=2}(D_x^I k(x,z))^2} \le d\kappa^2.$$

The last inequality is due to

$$|D_x^I k(x,z)| = |\langle D_x^I k(x,\cdot), k(z,\cdot)\rangle_{\mathcal{H}}| \le \sqrt{k(z,z) D_x^I D_{x'}^I k(x,x')|_{x'=x}} \le \kappa^2.$$

According to Assumption 2, there exists $\gamma > 0$ such that $\|\nabla_x k(x,z)\|_2 \le \gamma\|x - z\|_2^{-1}$. Therefore, for $\|x - z\|_2 \ge 1$,

$$\begin{aligned}
\|x - x^*\|_2 \|\nabla_x k(x,z)\|_2 &\le \gamma\|x - x^*\|_2 / \|x - z\|_2 \\
&\le \gamma(1 + \|z - x^*\|_2 / \|x - z\|_2) \\
&\le \gamma(1 + \|z - x^*\|_2).
\end{aligned} \tag{7}$$

And for $\|x - z\|_2 < 1$,

$$\begin{aligned}\|x - x^*\|_2 \|\nabla_x k(x, z)\|_2 &\leq \sqrt{d}\kappa^2(\|x - z\|_2 + \|z - x^*\|_2) \\ &\leq \sqrt{d}\kappa^2(1 + \|z - x^*\|_2). \end{aligned} \tag{8}$$

Combining (7) and (8),

$$\begin{aligned}\|x - x^*\|_2 \|\nabla_x k(x, z)\|_2 &\leq (\gamma + \sqrt{d}\kappa^2)(1 + \|z - x^*\|_2) \\ &\leq (\gamma + \sqrt{d}\kappa^2)(1 + \|x^*\|_2 + \|z\|_2). \end{aligned} \tag{9}$$

Plugging (9) back into (6), we can show the second pseudo Lipschitzness condition holds for $c_2 = \kappa^2 L + d\kappa^2 + (\gamma + \sqrt{d}\kappa^2)(1 + \|x^*\|_2)$.

Now that the pseudo Lipschitz conditions hold, by repeated application of Lemma 1 and the inequality $(1 + x) \leq e^x$, we have

$$\begin{aligned}W_1(\mu_{r+1}^n, \mu_{r+1}^\infty) &= W_1(\Phi_{\epsilon_r}(\mu_r^n), \Phi_{\epsilon_r}(\mu_r^\infty)) \leq (1 + \epsilon_r C_r) W(\mu_r^n, \mu_r^\infty) \\ &\leq W_1(\mu_0^n, \mu_0^\infty) \prod\nolimits_{s=0}^r (1 + \epsilon_s C_s) \leq W_1(\mu_0^n, \mu_0^\infty) \exp(\sum\nolimits_{s=0}^r \epsilon_s C_s) \end{aligned} \tag{10}$$

for $C_s = c_1(1 + m_{\mu_s^n}) + c_2(1 + m_{\mu_s^\infty})$.

Using the result from Lemma 2, we have

$$C_{s+1} \leq A + B \exp(\kappa^2(3L + d)b_s)$$

for $A = (c_1 + c_2)(1 + m_P)$ and $B = c_1 m_{\mu_0^n, P} + c_2 m_{\mu_0^\infty, P}$. Therefore

$$\begin{aligned}\textstyle\sum_{s=0}^r \epsilon_s C_s &\leq \max_{0 \leq s \leq r} C_s \textstyle\sum_{s=0}^r \epsilon_s \\ &\leq b_r(A + B \exp(\kappa^2(3L + d)b_{r-1})) \\ &\leq b_r(A + B \exp(\kappa^2(3L + d)b_r)). \end{aligned}$$

Plugging this back into (10) proves the result.

Appendix B. Proof of Lemma 2: SVGD moment growth

From Assumption 1 we know

$$\begin{aligned}&|k(y, x)| \leq |\langle k(y, \cdot), k(x, \cdot)\rangle_{\mathcal{H}}| \leq \|k(y, \cdot)\|_{\mathcal{H}} \|k(x, \cdot)\|_{\mathcal{H}} = \sqrt{k(y, y)k(x, x)} \leq \kappa^2, \\ &|D_y^I k(y, x)| = |\langle D_y^I k(y, \cdot), k(x, \cdot)\rangle_{\mathcal{H}}| \leq \sqrt{k(x, x) D_y^I D_{y'}^I k(y, y')|_{y'=y}} \leq \kappa^2, \\ &\left\|\nabla_y^2 k(y, x)\right\|_{op} \leq \left\|\nabla_y^2 k(y, x)\right\|_F = (\textstyle\sum_{|I|=2} (D_y^I k(y, x))^2)^{1/2} \leq d\kappa^2. \end{aligned}$$

Let μ be any probability measure. Using Jensen's inequality and the facts that $\mathbb{E}_P[s_p(\cdot)] = 0$ and $\mathbb{E}_{Z\sim P}[(\mathcal{A}_P k(\cdot, x))(Z)] = 0$, we have

$$\begin{aligned}
\|T_{\mu,\epsilon}(x) - x\|_2 &\leq \epsilon \|\mathbb{E}_{X\sim\mu}[(\mathcal{A}_P k(\cdot, x))(X)]\|_2 \\
&= \epsilon \|\mathbb{E}_{X\sim\mu}[(\mathcal{A}_P k(\cdot, x))(X)] - \mathbb{E}_{Z\sim P}[(\mathcal{A}_P k(\cdot, x))(Z)]\|_2 \\
&= \epsilon \|\mathbb{E}_{X\sim\mu \perp\!\!\!\perp Z\sim P}[k(Z, x)(s_p(X) - s_p(Z)) \\
&\quad + (k(X, x) - k(Z, x))(s_p(X) - \mathbb{E}_P[s_p(\cdot)]) + (\nabla k(X, x) - \nabla k(Z, x))]\|_2 \\
&\leq \epsilon \mathbb{E}_{X\sim\mu \perp\!\!\!\perp Z\sim P}[|k(Z, x)| \|s_p(X) - s_p(Z)\|_2 \\
&\quad + (|k(X, x)| + |k(Z, x)|)\|s_p(X) - \mathbb{E}_P[s_p(\cdot)]\|_2 + \|\nabla k(X, x) - \nabla k(Z, x)\|_2] \\
&\leq \epsilon \mathbb{E}_{X\sim\mu \perp\!\!\!\perp Z\sim P}[\kappa^2 L \|X - Z\|_2 + 2\kappa^2 \|s_p(X) - \mathbb{E}_P[s_p(Y)]\|_2 + d\kappa^2 \|X - Z\|_2] \\
&\leq \epsilon \mathbb{E}_{X\sim\mu \perp\!\!\!\perp Z\sim P}[\kappa^2 (L + d)\|X - Z\|_2] + \epsilon 2\kappa^2 L \mathbb{E}_{X\sim\mu \perp\!\!\!\perp Y\sim P}[\|X - Y\|_2] \\
&= \epsilon \kappa^2 (3L + d) \mathbb{E}_{X\sim\mu \perp\!\!\!\perp Z\sim P}[\|X - Z\|_2].
\end{aligned}$$

Let $m_{\mu_r,P} \triangleq \mathbb{E}_{X\sim\mu_r \perp\!\!\!\perp Z\sim P}[\|X - Z\|_2]$, $M_{\mu_r,P} \triangleq \mathbb{E}_{X\sim\mu_r \perp\!\!\!\perp Z\sim P}[\|X - Z\|_2^2]$, and $C = \kappa^2(3L+d)$. Then,

$$\begin{aligned}
m_{\mu_{r+1},P} &= \mathbb{E}_{X\sim\mu_r \perp\!\!\!\perp Z\sim P}[\|T_{\mu_r,\epsilon_r}(X) - Z\|_2] \\
&\leq \mathbb{E}_{X\sim\mu_r \perp\!\!\!\perp Z\sim P}[\|T_{\mu_r,\epsilon_r}(X) - X\|_2 + \|X - Z\|_2] \\
&\leq \epsilon_r C \mathbb{E}_{X\sim\mu_r \perp\!\!\!\perp Z\sim P}[\|X - Z\|_2] + \mathbb{E}_{X\sim\mu_r \perp\!\!\!\perp Z\sim P}[\|X - Z\|_2] \\
&= (1 + \epsilon_r C) m_{\mu_r,P}. \\
M_{\mu_{r+1},P} &= \mathbb{E}_{X\sim\mu_r \perp\!\!\!\perp Z\sim P}[\|T_{\mu_r,\epsilon_r}(X) - Z\|_2^2] \\
&\leq \mathbb{E}_{X\sim\mu_r \perp\!\!\!\perp Z\sim P}[\|T_{\mu_r,\epsilon_r}(X) - X\|_2^2 + \|X - Z\|_2^2 + 2\|T_{\mu_r,\epsilon_r}(X) - X\|_2 \|X - Z\|_2] \\
&\leq (\epsilon_r^2 C^2 + 2\epsilon_r C) m_{\mu_r,P}^2 + M_{\mu_r,P} \\
&\leq (1 + 2\epsilon_r C + \epsilon_r^2 C^2) M_{\mu_r,P},
\end{aligned}$$

where the last step used Jensen's inequality $m_{\mu_r,P}^2 \leq M_{\mu_r,P}$. Then

$$\begin{aligned}
M_{\mu_r,P} &\leq M_{\mu_0,P} \textstyle\prod_{s=0}^{r-1}(1 + 2\epsilon_s C + \epsilon_s^2 C^2) \leq M_{\mu_0,P} e^{\sum_{s=0}^{r-1}(2\epsilon_s C + \epsilon_s^2 C^2)} \leq M_{\mu_0,P} e^{(2C + \epsilon_0 C^2)\sum_{s=0}^{r-1}\epsilon_s}. \\
m_{\mu_r} &= \mathbb{E}_{\mu_r}[\|X\|_2] \leq m_{\mu_r,P} + \mathbb{E}_P[\|Z\|_2] \leq m_{\mu_0,P} \textstyle\prod_{s=0}^{r-1}(1 + \epsilon_s C) + m_P \\
&\leq m_{\mu_0,P} \exp(C b_{r-1}) + m_P.
\end{aligned}$$

The final inequality uses the relation $1 + x \leq e^x$.

Appendix C. Proof of Lemma 3

From Assumption 1 we know

$$\begin{aligned}
&\|g(x)\|_2^2 \leq \textstyle\sum_{i=1}^d \kappa^2 \|g_i\|_{\mathcal{H}}^2 \leq \kappa^2, \\
&\|\nabla g(x)\|_{op}^2 \leq \|\nabla g(x)\|_F^2 = \textstyle\sum_{i=1}^d \sum_{j=1}^d |\nabla_{x_i} g_j(x)|^2 \leq \sum_{i=1}^d \sum_{j=1}^d \kappa^2 \|g_j\|_{\mathcal{H}}^2 \leq d\kappa^2, \\
&\|\nabla(\nabla \cdot g(x))\|_2^2 = \textstyle\sum_{i=1}^d \left(\sum_{j=1}^d \nabla_{x_i} \nabla_{x_j} g_j(x)\right)^2 \leq d \sum_{i=1}^d \sum_{j=1}^d |\nabla_{x_i} \nabla_{x_j} g_j(x)|^2 \leq d^2\kappa^2.
\end{aligned}$$

Suppose X, Y, Z are distributed so that (X, Y) is a 1-Wasserstein optimal coupling of (μ, ν) and Z is independent of (X, Y). Since $\mathbb{E}_P[s_p(\cdot)] = 0$, repeated use of Cauchy-Schwarz gives

$$\begin{aligned}
&\mathbb{E}_\mu[\mathcal{T}_P g] - \mathbb{E}_\nu[\mathcal{T}_P g] \\
&= \mathbb{E}[\nabla \cdot g(X) - \nabla \cdot g(Y)] + \mathbb{E}[\langle s_p(X) - s_p(Y), g(X)\rangle] + \mathbb{E}[\langle s_p(Y) - s_p(Z), g(X) - g(Y)\rangle] \\
&\leq \kappa(d + L)W_1(\mu, \nu) + L\mathbb{E}[\|Y - Z\|_2 \min(2\kappa, \sqrt{d}\kappa\|X - Y\|_2)].
\end{aligned}$$

Appendix D. Proof of Corollary 2: A finite-particle convergence rate for SVGD

We first state and prove a useful lemma.

Lemma 5 *Suppose f is a monotonic decreasing function. Let $x = f(\beta)$ for $\beta = \max(1, f(1))$. Then $x \leq f(x)$.*

Proof If $\beta = 1 \geq f(1)$, then $x = f(\beta) = f(1) \leq 1$. Because f is monotonic decreasing, $f(x) \geq f(1) = x$. Otherwise, $\beta = f(1) > 1$ and hence $x = f(\beta) < f(1) = \beta$. Again, due to monotonicity, $f(x) > f(\beta) = x$. Combining the two cases finishes the proof. ■

Now we are ready to prove Corollary 2. Let $b_{t-1}^{(1)} = \psi_{B,C}(w_0\sqrt{\log\log\frac{1}{w_0}}, A, \beta_1)$ and $b_{t-1}^{(2)} = \psi_{B,C}(w_0 \log\log\frac{1}{w_0}, A + 2C + \epsilon_0 C^2, \beta_2)$. According to Lemma 5,

$$b_{t-1}^{(1)} \leq \psi_{B,C}(w_0\sqrt{\log\log\frac{1}{w_0}}, A, b_{t-1}^{(1)}).$$

Rearranging the terms, we have

$$w_0 \exp(b_{t-1}^{(1)}(A + B\exp(Cb_{t-1}^{(1)}))) \leq \frac{1}{\sqrt{\log\log\frac{1}{w_0}}}. \tag{11}$$

Similarly, we have $b_{t-1}^{(2)} \leq \psi_{B,C}(w_0 \log\log\frac{1}{w_0}, A + 2C + \epsilon_0 C^2, b_{t-1}^{(2)})$ and

$$\sqrt{w_0}\exp(b_{t-1}^{(2)}(2C + \epsilon_0 C^2 + (A + B\exp(Cb_{t-1}^{(2)}))/2)) \leq \frac{1}{\sqrt{\log\log\frac{1}{w_0}}}. \tag{12}$$

Since $b_{t-1} = \min(b_{t-1}^{(1)}, b_{t-1}^{(2)})$, we can substitute b_{t-1} for $b_{t-1}^{(1)}$ and $b_{t-1}^{(2)}$ in (11) and (12), respectively. Also, from the definition of b_{t-1} we know $\frac{1}{b_{t-1}} = O\left(\frac{1}{\log\log\frac{1}{w_0}}\right)$. Plugging them into (3) proves the first claim. The second claim follows from the $\Theta(n^{-1/d})$ convergence rate of an empirical measure to its population measure in 1-Wasserstein distance [3].