A Non-Asymptotic Analysis for Stein Variational Gradient Descent

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Abstract

We study the Stein Variational Gradient Descent (SVGD) algorithm, which optimizes a set of particles to approximate a target probability distribution $\pi \propto e^{-V}$ on $\mathbb{R}^d$. In the population limit, SVGD performs gradient descent in the space of probability distributions on the KL divergence with respect to $\pi$, where the gradient is smoothed through a kernel integral operator. In this paper, we provide a novel finite time analysis for the SVGD algorithm. We obtain a descent lemma establishing that the algorithm decreases the objective at each iteration, and provably converges, with less restrictive assumptions on the step size than required in earlier analyses. We further provide a guarantee on the convergence rate in Kullback-Leibler divergence, assuming $\pi$ satisfies a Stein log-Sobolev inequality as in [Duncan et al., 2019], which takes into account the geometry induced by the smoothed KL gradient.

1 Introduction

The task of sampling from a target distribution is common in Bayesian inference, where the distribution of interest is the posterior distribution of the parameters. Unfortunately, the posterior distribution is generally difficult to compute due to the presence of an intractable integral. This sampling problem can be formulated from an optimization point of view [Wibisono, 2018]. We assume that the target distribution $\pi$ admits a density proportional to $\exp(-V)$ with respect to Lebesgue measure over $\mathcal{X} = \mathbb{R}^d$, where $V : \mathcal{X} \to \mathbb{R}$ is referred to as the potential function. In this setting, the target distribution $\pi$ is the solution to the optimization problem defined on the set $\mathcal{P}_2(\mathcal{X})$ of probability measures $\mu$ such that $\int \|x\|^2 d\mu(x) < \infty$ by:

$$\min_{\mu \in \mathcal{P}_2(\mathcal{X})} \text{KL}(\mu | \pi),$$

where KL denotes the Kullback-Leibler divergence, and assuming $\pi \in \mathcal{P}_2(\mathcal{X})$. Many existing methods for the sampling task can be related to this optimization problem. Variants of the Langevin
Monte Carlo algorithm (Durmus and Moulines, 2016), Dalalyan and Karagulyan, 2019) can be seen as time-discretized schemes of the gradient flow of the relative entropy. These methods generate a Markov chain whose law converges to \( \pi \) under mild assumptions, but the rates of convergence deteriorate quickly in high dimensions (Durmus et al. 2018). Variational inference methods instead restrict the search space of problem (1) to a family of parametric distributions (Zhang et al. 2018; Ranganath et al. 2014). These methods are much more tractable in the large scale setting, since they benefit from efficient optimization methods (parallelization, stochastic optimization), however they can only return an approximation of the target distribution.

Recently, the Stein Variational Gradient Descent (SVGD) algorithm (Liu and Wang, 2016) was introduced as a non-parametric alternative to variational inference methods. It uses a set of interacting particles to approximate the target distribution, and applies iteratively to these particles a form of gradient descent of the relative entropy, where the descent direction is restricted to belong to a unit ball in a Reproducing Kernel Hilbert space (RKHS) Steinwart and Christmann (2008). In particular, this algorithm can be seen as a discretization of the gradient flow of the relative entropy on the space of probability distributions, equipped with a distance depending on the kernel (Liu, 2017; Feng et al., 2017; Liu and Zhu, 2018; Feng et al., 2017; Liu and Zhu, 2018; Detommaso et al., 2018), learning deep probabilistic models (Wang and Liu, 2016; Pu et al., 2017), or reinforcement learning (Liu et al., 2017). In the limit of infinite particles, the algorithm is known to converge to the target distribution under appropriate growth assumptions on the potential (Lu et al., 2019). Its non-asymptotic analysis remains incomplete, however: in particular, to the best of our knowledge, quantitative rates of convergence have yet to be obtained. The present paper aims at answering this question. Our first contribution is to provide in the infinite-particle regime a descent lemma showing that SVGD decreases at each iteration for a sufficiently small but constant step-size, with an analysis different from Liu (2017). We view this problem as an optimization problem over \( P_2(\mathcal{X}) \) equipped with the Wasserstein distance, and use this framework and optimization techniques to obtain our results. Then, by leveraging a kernel version of the log-Sobolev inequality, called the Stein log-Sobolev inequality as proposed by Duncan et al., (2019), we derive rates of convergence in terms of the KL objective.

This paper is organized as follows. Section 2 introduces the background needed on optimal transport, while Section 3 presents the point of view adopted to study SVGD in the infinite number of particles regime and reviews related work. Section 4 studies the continuous time dynamics of SVGD, and presents the Stein log Sobolev inequality that will be used in this paper. Our main result is presented in Section 5, where we provide a descent lemma and rates of convergence for the SVGD algorithm. The complete proofs, toy experiments and an auxiliary convergence result of the finite particle system to its population version are deferred to the appendix.

2 Preliminaries on optimal transport

Let \( \mathcal{X} = \mathbb{R}^d \). We denote by \( C^l(\mathcal{X}) \) the space of \( l \) continuously differentiable functions on \( \mathcal{X} \). If \( \psi : \mathcal{X} \to \mathbb{R}^p \), \( p \geq 0 \), is differentiable, we denote by \( J\psi : \mathcal{X} \to \mathbb{R}^{p \times d} \) the Jacobian matrix of \( \psi \). If \( p = 1 \), the gradient of \( \psi \) denoted \( \nabla \psi \) is seen as a column vector. Moreover, if \( \nabla \psi \) is differentiable, the Jacobian of \( \nabla \psi \) is the Hessian of \( \psi \) denoted \( H_{\psi} \). If \( p = d \), \( div(\psi) \) denotes the divergence of \( \psi \), i.e. the trace of the Jacobian. The Hilbert-Schmidt norm of a matrix is denoted \( \|\cdot\|_{HS} \) and the operator norm denoted \( \|\cdot\|_{op} \).

2.1 The Wasserstein space and the continuity equation

In this section, we recall some background from optimal transport. The reader may refer to Ambrosio et al. (2008) for more details.

Consider the set \( P_2(\mathcal{X}) \) of probability measures \( \mu \) on \( \mathcal{X} \) with finite second order moment. For any \( \mu \in P_2(\mathcal{X}) \), \( L^2(\mu) \) is the space of functions \( f : \mathcal{X} \to \mathbb{R} \) such that \( \int \|f\|^2 d\mu < \infty \). If \( \mu \in P_2(\mathcal{X}) \), we denote by \( \|\cdot\|_{L^2(\mu)} \) and \( \langle\cdot,\cdot\rangle_{L^2(\mu)} \) respectively the norm and the inner product of the Hilbert space \( L^2(\mu) \). Given a measurable map \( T : \mathcal{X} \to \mathcal{X} \) and \( \mu \in P_2(\mathcal{X}) \), we denote by \( T\#\mu \) the pushforward measure of \( \mu \) by \( T \), characterized by the transfer lemma \( \int \phi(T(x)) d\mu(x) = \int \phi(y) dT\#\mu(y) \), for any measurable and bounded function \( \phi \). Consider \( \mu, \nu \in P_2(\mathcal{X}) \), the 2-nd order Wasserstein distance is defined by \( W_2^2(\mu, \nu) = \inf_{s \in S(\mu, \nu)} \int \|x - y\|^2 ds(x, y) \), where \( S(\mu, \nu) \) is the set of couplings between \( \mu \) and \( \nu \), i.e. the set of nonnegative measures \( s \) over \( \mathcal{X} \times \mathcal{X} \) such that \( P_{\#} s = \mu \) (resp.
When the kernel is integrally strictly positive definite, then $v$ with 
\begin{equation}
Q_{#s} = v)
\end{equation}
where $P : (x, y) \mapsto x$ (resp. $Q : (x, y) \mapsto y$) denote the projection onto the first (resp. the second) component. The Wasserstein distance is a distance over $P_2(\mathcal{X})$. The metric space $(P_2(\mathcal{X}), W_2)$ is called the Wasserstein space.

Let $T > 0$. Consider a weakly continuous map $\mu : (0, T) \to P_2(\mathcal{X})$. The family $(\mu_t)_{t \in (0, T)}$ satisfies a continuity equation if there exists $(v_t)_{t \in (0, T)}$ such that $v_t \in L^2(\mu_t)$ and 
\begin{equation}
\frac{\partial \mu_t}{\partial t} + \text{div}(\mu_t v_t) = 0
\end{equation}
holds in the distributional sense. A family $(\mu_t)_t$ satisfying a continuity equation with \(\|v_t\|_{L^2(\mu_t)}\) integrable over $(0, T)$ is said absolutely continuous. Among the possible processes $(v_t)_t$, one has a minimal $L^2(\mu_t)$ norm and is called the velocity field of $(\mu_t)_t$. In a Riemannian interpretation of the Wasserstein space Otto (2001), this minimality condition can be characterized by $v_t$ belonging to the tangent space to $P_2(\mathcal{X})$ at $\mu_t$ denoted $T_{\mu_t}P_2(\mathcal{X})$, which is a subset of $L^2(\mu_t)$.

### 2.2 A functional defined over the Wasserstein space

Consider $\pi \propto \exp(-V)$ where $V : \mathcal{X} \to \mathbb{R}$ is a smooth function, i.e. $V \in C^2(\mathcal{X})$ and its Hessian $H_V$ is bounded above. For any $\mu, \pi \in P_2(\mathcal{X})$, the Kullback-Leibler divergence of $\mu$ w.r.t. $\pi$ is defined by
\begin{equation}
\text{KL}(\mu|\pi) = \int \log \left( \frac{d\mu}{d\pi}(x) \right) d\mu(x)
\end{equation}
if $\mu$ is absolutely continuous w.r.t. $\pi$ with Radon-Nikodym density $d\mu/d\pi$, and $\text{KL}(\mu|\pi) = +\infty$ otherwise. Consider the functional $\text{KL}(\cdot|\pi) : P_2(\mathcal{X}) \to (-\infty, +\infty)$, $\mu \mapsto \text{KL}(\mu|\pi)$ defined over the Wasserstein space. We shall perform differential calculus over this space for such a functional, which is a "powerful way of computing" (Villani 2003, Section 8.2). If $\mu \in P_2(\mathcal{X})$ satisfies some mild regularity conditions, the (Wasserstein) gradient of $\text{KL}(\cdot|\pi)$ at $\mu$ is denoted by $\nabla_W \text{KL}(\mu|\pi) \in L^2(\mu)$ and defined by $\nabla \log \left( \frac{d\mu}{d\pi} \right)$. Moreover, the (Wasserstein) Hessian of $\text{KL}(\cdot|\pi)$ at $\mu$ is an operator over $T_{\mu}P_2(\mathcal{X})$ defined by
\begin{equation}
(v, H_{\text{KL}(\cdot|\pi)}(\mu)v)_{L^2(\mu)} = \mathbb{E}_{X \sim \mu} \left[ \left( \langle v(X), H_V(X)v(X) \rangle \right) + \|J_v(X)\|_{H^2_S} \right]
\end{equation}
for any tangent vector $v \in T_{\mu}P_2(\mathcal{X})$. Note that the Hessian of $\text{KL}(\cdot|\pi)$ is not bounded above. An important property of the Wasserstein gradient is that it satisfies a chain rule. Let $(\mu_t)_t$ be an absolutely continuous curve s. t. $\mu_t$ has a density. Denote $(v_t)$ the velocity field of $(\mu_t)_t$. If $\phi(t) = \text{KL}(\mu_t|\pi)$, then under mild technical assumptions $\phi'(t) = \langle v_t, \nabla_W \text{KL}(\mu_t|\pi)\rangle_{L^2(\mu_t)}$, see Ambrosio et al. (2008).

### 3 Presentation of Stein Variational Gradient Descent (SVGD)

In this section, we present our point of view on SVGD in the infinite number of particles regime.

#### 3.1 Kernel integral operator

Consider a positive semi-definite kernel $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ and $\mathcal{H}_0$ its corresponding RKHS of real-valued functions on $\mathcal{X}$. The space $\mathcal{H}_0$ is a Hilbert space with inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}_0}$ and norm $\| \cdot \|_{\mathcal{H}_0}$ (see Smola and Schölkopf (1998)). Moreover, $k$ satisfies the reproducing property: $\forall f \in \mathcal{H}_0$, $f(x) = \langle f, k(x, :) \rangle_{\mathcal{H}_0}$. Denote by $\mathcal{H}$ the product RKHS consisting of elements $f = (f_1, \ldots, f_d)$ with $f_i \in \mathcal{H}_0$, and with a standard inner product $\langle f, g \rangle_{\mathcal{H}} = \sum_{i=1}^d \langle f_i, g_i \rangle_{\mathcal{H}_0}$. Let $\mu \in P_2(\mathcal{X})$; the integral operator associated to kernel $k$ and measure $\mu$ denoted $S_\mu : L^2(\mu) \to \mathcal{H}$ is
\begin{equation}
S_\mu f = \int k(x, \cdot) f(x) d\mu(x).
\end{equation}
Consider functions $f, g \in L^2(\mu) \times \mathcal{H}$ and denote the inclusion $\iota : \mathcal{H} \to L^2(\mu)$, with $\iota^* = S_\mu$ its adjoint. Then following e.g. Steinwart and Christmann (2008, Chapter 4),
\begin{equation}
\langle f, \iota g \rangle_{L^2(\mu)} = \langle \iota^* f, g \rangle_{\mathcal{H}} = \langle S_\mu f, g \rangle_{\mathcal{H}}.
\end{equation}
When the kernel is integrally strictly positive definite, then $\mathcal{H}$ is dense in $L^2(\mu)$ for any probability measure $\mu$. Sriperumbudur et al. (2011). We also define $P_\mu : L^2(\mu) \to L^2(\mu)$ the operator $P_\mu = \iota S_\mu$; notice that it differs from $S_\mu$ only from its range.
### 3.2 Stein Variational Gradient Descent

We can now present the Stein Variational Gradient Descent (SVGD) algorithm [Liu and Wang (2016)]. The goal of this algorithm is to provide samples from a target distribution \( \pi \propto \exp(-V) \) with positive density w.r.t. Lebesgue measure and known up to a normalization constant. Several points of views on SVGD have been adopted in the literature. In this paper, we view SVGD as an optimization algorithm [Liu (2017)] to minimize the Kullback-Leibler (KL) divergence w.r.t. \( \pi \), see Problem (1).

Denote \( \mathcal{KL}(\cdot|\pi) : \mathcal{P}_2(\mathcal{X}) \to (-\infty, +\infty] \) the functional \( \mu \mapsto \mathcal{KL}(\mu|\pi) \). More precisely, in order to obtain samples from \( \pi \), SVGD applies a gradient descent-like algorithm to the functional \( \mathcal{KL}(\cdot|\pi) \).

The standard gradient descent algorithm in the Wasserstein space applied to \( \mathcal{KL}(\cdot|\pi) \), at each iteration \( n \geq 0 \), is

\[
\mu_{n+1} = \left( I - \gamma \nabla \log \left( \frac{\mu_n}{\pi} \right) \right) \mu_n, \tag{6}
\]

where \( \mu_{n+1} = \left( I - \gamma \nabla \log \left( \frac{\pi}{\mu_n} \right) \right) \mu_n, \tag{7}\)

Instead of using \( \nabla_{W_2} \mathcal{KL}(\mu_n|\pi) \) as the gradient, SVGD uses \( \mu_n \nabla_{W_2} \mathcal{KL}(\mu_n|\pi) \). This can be seen as the gradient of \( \mathcal{KL}(\cdot|\pi) \) under the inner product of \( \mathcal{H} \), since \( \langle S \mu \nabla_{W_2} \mathcal{KL}(\mu|\pi), v \rangle_{\mathcal{H}} = \langle \nabla_{W_2} \mathcal{KL}(\mu|\pi), \mu \rangle_{L^2(\mu)} \) for any \( v \in \mathcal{H} \). The important fact is that given samples of \( \mu \), the evaluation of \( \mu \nabla_{W_2} \mathcal{KL}(\mu|\pi) \) is simple. Indeed under appropriate conditions on \( k \) and \( \pi \), see Liu (2017),

\[
P_\mu \nabla \log \left( \frac{\mu}{\pi} \right) (\cdot) = - \int \left[ \nabla \log \pi(x) k(x, \cdot) + \nabla_x k(x, \cdot) \right] d\mu(x),
\]

using an integration by parts.

**Remark 1.** An alternative sampling algorithm which does not imply to compute the exact gradient of the KL is the Unadjusted Langevin Algorithm (ULA). It is an implementable algorithm that computes a gradient step with \( \nabla \log \pi \), and a flow step adding a Gaussian noise to the particles. However, it is not a gradient descent discretization; it is rather performing a Forward-Flow (FFl) discretization, which is biased (Wibisono, 2018, Section 2.2.2).

### 3.3 Stein Fisher Information

The squared RKHS norm of the gradient \( S_\mu \nabla \log(\frac{\mu}{\pi}) \) is defined as the Stein Fisher Information:

**Definition 1.** Let \( \mu \in \mathcal{P}_2(\mathcal{X}) \). The Stein Fisher Information of \( \mu \) relative to \( \pi \) [Duncan et al. (2019)] is defined by:

\[
I_{\text{Stein}}(\mu|\pi) = \| S_\mu \nabla \log \left( \frac{\mu}{\pi} \right) \|^2_{\mathcal{H}}. \tag{9}
\]

**Remark 2.** Notice that since \( P_\mu = \iota S_\mu \) with \( \iota^* = S_\mu \), we can write \( I_{\text{Stein}}(\mu|\pi) = \langle \nabla \log(\frac{\mu}{\pi}), P_\mu \nabla \log(\frac{\mu}{\pi}) \rangle_{L^2(\mu)} \).

The quantity (9) is also referred to in the literature as the squared Kernel Stein Discrepancy (KSD), used in nonparametric statistical tests for goodness-of-fit [Liu et al. (2016), Chwialkowski et al. (2016), Gorham and Mackey (2017)]. The KSD provides a discrepancy between probability distributions, which depends on \( \pi \) only through the score function \( \nabla \log \pi \) which can be calculated without knowing the normalization constant of \( \pi \). Whether the convergence of the KSD to zero, i.e. \( I_{\text{Stein}}(\mu_n|\pi) \to 0 \) when \( n \to \infty \) implies the weak convergence of \( (\mu_n)_n \) to \( \pi \) (denoted \( \mu_n \to \pi \)) depends on the choice of the kernel relatively to the target. This question has been treated in Gorham and Mackey (2017).

Sufficient conditions include \( \pi \) being distantly dissipative\(^1\) and the kernel being translation invariant with a non-vanishing Fourier transform, or \( k \) being the inverse multi-quadratic kernel defined by \( k(x, .) = 0 \) \( \forall x \in \partial \mathcal{X} \) when \( \mathcal{X} \) is compact, or \( \lim_{\|x\| \to \infty} k(x, .) \pi(x) = 0 \) when \( \mathcal{X} = \mathbb{R}^d \).

\(^1\)this includes finite Gaussian mixtures with common covariance and all distributions strongly log-concave outside of a compact set, including Bayesian linear, logistic, and Huber regression posteriors with Gaussian priors.
\[ k(x, y) = (c^2 + \|x - y\|^2_2)^\beta \] for \( c > 0 \) and \( \beta \in [-1, 0]. \] In these cases, \( I_{\text{stein}}(\mu_n | \pi) \to 0 \) implies \( \mu_n \to \pi. \)

In order to study the continuous time dynamics of SVGD, Duncan et al. (2019) introduced a kernel version of a log-Sobolev inequality (which usually upper bounds the KL by the Fisher divergence) into the Stein setting.

\[ I_{\text{stein}}(\mu | \pi) \leq \frac{1}{2\lambda} I_{\text{stein}}(\mu | \pi). \] (10)

The functional inequality (10) is not as well known and understood as the classical log-Sobolev inequality. Duncan et al. (2019) provided a first investigation into when this condition might hold. They show that it fails to hold if the kernel is too regular w.r.t. \( \pi \), more precisely for \( k \in C^3,1(X \times X) \), and if \( \sum_{i=1}^d (|\partial_i V(x)|^2 k(x, x) - \partial_i V(x)(\partial_i^1 k(x, x) + \partial_i^2 k(x, x)) + \partial_i^1 \partial_i^2 k(x, x)|d\pi(x) < \infty \), where \( \partial_i^1 \) and \( \partial_i^2 \) denote derivatives with respect to the first and second argument of \( k \), respectively (Duncan et al., 2019 Lemma 36). This holds for instance in the case where \( \pi \) has exponential tails and the derivatives of \( k \) and \( V \) grow at most at a polynomial rate. However, they provide interesting cases in dimension 1 where (10) holds, depending on \( k \) and \( \pi \). For instance, by choosing a nondifferentiable kernel that is adapted to the tails of the target \( k(x, y) = \pi(x)^{-1/2}e^{-|x-y|/\beta}\pi(y)^{-1/2} \), and if \( V''(x) + V'(x)^2/2 \geq \lambda > 0 \) for any \( x \in \mathbb{R} \), then (10) holds with \( \lambda = \min(1, \lambda) \) (Duncan et al., 2019 Example 40). Another case where it holds is for a quadratic potential \( V(x) = \frac{\alpha}{2}x^2 \), \( \alpha > 0 \) and a linear kernel \( k(x, y) = xy \), then \( \lambda = 2\alpha \int x^2 d\pi(x) \) (Duncan et al., 2019 Lemma 43). Conditions where (10) holds in higher dimensions are more challenging to establish, and are a topic of current research.

### 3.4 Related work

SVGD was originally introduced by Liu and Wang (2016), and was shown empirically to be competitive with state-of-the-art methods in Bayesian inference. Liu (2017) developed the first theoretical analysis and studied the weak convergence properties of SVGD. They showed that for any iteration, the empirical distribution of the SVGD samples (i.e., for a finite number of particles) weakly converges to the target distribution when the number of particles goes to infinity. In the infinite particle regime, they provided a descent lemma showing that the KL objective decreases at each iteration (see Remark 4). Finally, they derived the non-linear partial differential PDE equation that governs continuous time dynamics of SVGD, and provided a geometric intuition that interprets SVGD as a gradient flow of the KL divergence under a new Riemannian metric structure (the Stein geometry) induced by the kernel. Liu and Wang (2018) studied the fixed point properties of the algorithm for a finite number of particles, and showed that it exactly estimates expectations under the target distribution, for a set of functions called the Stein matching set, that are determined by the Stein operator (depending on the target distribution) and the kernel. In particular, they showed that by choosing linear kernels, SVGD can exactly estimate the mean and variance of Gaussian distributions when the number of particles is greater than the dimension. They further derived high probability bounds that bound the Kernel Stein Discrepancy between the empirical distribution and the target measure when the kernel is approximated with random features. Lu et al. (2019), studied the continuous time dynamics of SVGD in the infinite number of particles regime. They showed that the PDE governing continuous-time, infinite sample SVGD dynamics is well-posed, and that the law of the particle system (for a finite number of particles) is a weak solution of the equation, under appropriate growth conditions on the score function \( \nabla \log \pi \), and they studied the regularity of the PDE. Finally, Duncan et al. (2019) investigated the contraction and equilibration properties of this PDE. In particular, they proposed conditions that induce exponential convergence to the equilibrium in continuous time, notably as the Stein log-Sobolev inequality, which relates the convexity of the KL objective to the Stein geometry (see Section 4). By contrast with (Lu et al., 2019), we develop a theoretical understanding of SVGD in discrete time, where to our knowledge rates of convergence have yet to be established.

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1. i.e. \( \text{KL}(\mu | \pi) \leq 1/2\lambda \| \nabla \log (\pi) \|_{L^2(\mu)}^2 \), which holds for instance as soon as \( V \) is \( \lambda \)-strongly convex.
4 Continuous-time dynamics of SVGD

This section defines and describes the SVGD dynamics in continuous time. Some of the results are already stated in [Liu (2017)] and [Duncan et al. (2019)] but are necessary to understand the discrete time analysis. We provide intuitive sketches of the proof ideas in the main document, which exploit the differential calculus over the Wasserstein space. Detailed proofs are given in the Appendix.

The SVGD gradient flow is defined as the flow induced by the continuity equation [Liu (2017)]:

\[ \frac{\partial \mu_t}{\partial t} + \text{div}(\mu_t v_t) = 0, \quad v_t := -P_{\mu_t} \nabla \log \left( \frac{\mu_t}{\pi} \right) \]  \hspace{1cm} (11)

Equation (11) was shown to admit an unique and well defined solution (given an initial condition \( \mu_0 \in \mathcal{P}(\mathcal{X}) \)) provided some smoothness and growth assumptions on both kernel and target density \( \pi \) are satisfied ([Lu et al. (2019)]). Notice that the SVGD update (7) is a forward Euler discretization of (11). We propose to study the dissipation of the KL along the trajectory of the SVGD gradient flow.

The Stein Fisher Information turns out to be the quantity that quantifies this dissipation, as stated in Proposition 1. Let \( \mu_t \) be a solution of (11). Then

\[ \frac{d\text{KL}(\mu_t|\pi)}{dt} = -I_{\text{Stein}}(\mu_t|\pi). \]  \hspace{1cm} (12)

**Proof.** Recall that \( \nabla W_2 \text{KL}(\mu|\pi) = \nabla \log(\frac{\mu}{\pi}) \), using differential calculus in the Wasserstein space and the chain rule we have:

\[ \frac{d\text{KL}(\mu_t|\pi)}{dt} = \left\langle v_t, \nabla \log \left( \frac{\mu_t}{\pi} \right) \right\rangle_{L^2(\mu_t)} = -\left\| S_{\mu_t} \nabla \log \left( \frac{\mu_t}{\pi} \right) \right\|^2_{\mathcal{H}}. \]

Since \( I_{\text{Stein}}(\mu_t|\pi) \) is nonnegative, Proposition 1 shows that the KL divergence with respect to \( \pi \) decreases along the SVGD dynamics, i.e. the KL is a Lyapunov functional for the PDE (11). It can actually be proven that \( I_{\text{Stein}}(\mu_t|\pi) \to 0 \), as stated in the following proposition. Its proof is deferred to Section 5.

**Proposition 2.** Let \( \mu_t \) be a solution of (11). Then \( I_{\text{Stein}}(\mu_t|\pi) \to 0 \).

**Remark 3.** In the proof of [Lu et al. (2019) Theorem 2.8], the authors show that \( \mu_t \) converges weakly towards \( \pi \) when \( V \) grows at most polynomially. However, they implicitly assumed that \( I_{\text{Stein}}(\mu_t|\pi) \to 0 \) which does not need to be true in general ([Lesigne, 2010]). It can actually be proven that \( I_{\text{Stein}}(\mu_t|\pi) \to 0 \) by controlling the oscillation of the \( I_{\text{Stein}}(\mu_t|\pi) \) in time, using a semi-convexity result on the KL.

A second consequence of Proposition 1 is the following continuous time convergence rate for the average of \( I_{\text{Stein}}(\mu_t|\pi) \). It is obtained immediately by integrating (12) and using the positivity of the KL.

**Proposition 3.** For any \( t \geq 0 \),

\[ \min_{0 \leq s \leq t} I_{\text{Stein}}(\mu_s|\pi) \leq \frac{1}{t} \int_0^t I_{\text{Stein}}(\mu_s|\pi) ds \leq \frac{\text{KL}(\mu_0|\pi)}{t}. \]  \hspace{1cm} (13)

The convergence of \( I_{\text{Stein}}(\mu_t|\pi) \) itself can be arbitrarily slow, however. To guarantee faster convergence rates of the SVGD dynamics, further properties are needed, such as convexity properties of the KL-divergence with respect to the Stein geometry. This is the purpose of the inequality (10) which implies exponential convergence of the SVGD gradient flow near equilibrium. Indeed, if \( \pi \) satisfies the Stein log-Sobolev inequality, the Kullback-Leibler divergence converges exponentially fast along the SVGD dynamics.

**Proposition 4.** Assume \( \pi \) satisfies the Stein log-Sobolev inequality with \( \lambda > 0 \). Then

\[ \text{KL}(\mu_t|\pi) \leq e^{-2\lambda t} \text{KL}(\mu_0|\pi). \]

**Proof.** Combining (12) and (10) yields \( \frac{d\text{KL}(\mu_t|\pi)}{dt} \leq -2\lambda \text{KL}(\mu_t|\pi) \). We conclude by applying Gronwall’s lemma. \( \square \)

In the next section, we provide a non-asymptotic analysis for SVGD. Our first results holds without any convexity assumptions on the KL, but mainly under a smoothness assumption on \( \pi \), while our second result leverages (10) to obtain rates of convergence.
5 Non-asymptotic analysis for SVGD

This section studies the SVGD dynamics in discrete time. Although one of the results echoes (Liu [2017] Theorem 3.3), we provide new convergence rates for the discrete time SVGD under mild conditions, and using different techniques: we return to this point in detail in Remark [4] below. Moreover, our proof technique is different. As in the previous section, we provide intuitive sketch of the proofs exploiting the differential calculus over the Wasserstein space. Each step of the proofs is rigorously justified in the Supplementary material.

Recall that the SVGD update is defined as (7). Let \( \mu_0 \in \mathcal{P}_2(\mathcal{X}) \) and assume that it admits a density. For every \( n \geq 0 \), \( \mu_n \) is the distribution of \( x_n \), where
\[
x_{n+1} = x_n - \gamma P_{\mu_n} \nabla \log \left( \frac{\mu_n}{\pi} \right) (x_n), \quad x_0 \sim \mu_0.
\]
(14)

This particle update leads to the finite particles implementation of SVGD, analyzed in Section [9].

In this section, we analyze SVGD in discrete time, in the infinite number of particles regime (7). We propose to study the dissipation of the KL along the SVGD algorithm. The Stein Fisher Information once again quantifies this dissipation, as in the continuous time case. Before going further, note that discrete time analyses often require more assumptions that continuous time analyses. In optimization, these assumptions typically require some smoothness of the objective function. Here, we assume the following.

(A1) Assume that \( \exists B > 0 \) s.t. for all \( x \in \mathcal{X} \),
\[
\|k(x, .)\|_{H_0} \leq B \text{ and } \|\nabla_x k(x, .)\|_{H} = \left( \sum_{i=1}^d \|\partial_{x_i} k(x, .)\|_{H_0}^2 \right)^{1/2} \leq B.
\]

(A2) The Hessian of \( V = -\log \pi \), \( H_V \) is well-defined and \( \exists M > 0 \) s.t. \( \|H_V\|_{op} \leq M \).

(A3) Assume that \( \exists C > 0 \) s.t. : \( I_{Stein}(\mu_n|\pi) < C \) for all \( n \).

Under Assumptions (A1) and (A2), a sufficient condition for Assumption (A3) is \( \sup_n \int \|x\|\mu_n(x)dx < \infty \). Bounded moment assumption such as these are commonly used in stochastic optimization, for instance in some analysis of the stochastic gradient descent [Moulines and Bach [2011]]. Given our assumptions, we quantify the decreasing of the KL along the SVGD algorithm, also called a descent lemma in optimization.

Proposition 5. Assume that Assumptions (A1) to (A3) hold and that \( \int \|x\|\mu_n(x)dx \) remains bounded for all \( n \). Let \( \alpha > 1 \) and choose \( \gamma \leq \frac{\alpha - 1}{\alpha BC^2} \). Then:
\[
KL(\mu_{n+1}|\pi) - KL(\mu_n|\pi) \leq -\gamma \left( 1 - \gamma \frac{(\alpha^2 + M)B^2}{2} \right) I_{Stein}(\mu_n|\pi).
\]
(15)

Proof. Our goal is to prove a discrete dissipation of the form \( (KL(\mu_{n+1}|\pi) - KL(\mu_n|\pi))/\gamma \leq -I_{Stein}(\mu_n|\pi) + \text{error term} \). Our assumptions will control the error term. Fix \( n \geq 0 \) and denote \( g = P_{\mu_n} \nabla \log \left( \frac{\mu_n}{\pi} \right), \phi_t = I - tg \) for \( t \in [0, \gamma] \) and \( \rho_t = (\phi_t)_\# \mu_n \). Note that \( \rho_0 = \mu_n \) and \( \rho_\gamma = \mu_{n+1} \).

Under our assumptions, one can show that for any \( x \in \mathcal{X} \), \( \|g(x)\|^2 \leq B^2 I_{Stein}(\mu_n|\pi) \) and \( \|Jg(x)\|^2_{H} \leq B^2 I_{Stein}(\mu_n|\pi) \), using the reproducing property and Cauchy-Schwartz in \( H \). Hence, \( \|tg(x)\|_{op} \leq 1 \) and \( \phi_t \) is a diffeomorphism for every \( t \in [0, \gamma] \). Moreover, \( \|J(\phi_t)^{-1}(x)\|_{op} \leq \alpha \).

Using [Villani [2003] Theorem 5.34], the velocity field ruling the time evolution of \( \rho_t \) is \( w_t \) \( L^2(\rho_t) \) defined by \( w_t(x) = -g(\phi_t^{-1}(x)) \).

Denote \( \varphi(t) = KL(\rho_t|\pi) \). Using a Taylor expansion, \( \varphi(\gamma) = \varphi(0) + \gamma \varphi'(0) + \int_0^\gamma (\gamma - t) \varphi''(t)dt \).

We now identify each term. First,
\[
\varphi(0) = KL(\mu_n|\pi) \quad \text{and} \quad \varphi(\gamma) = KL(\mu_{n+1}|\pi).
\]

Then, using the chain rule [Villani [2003] Section 8.2],
\[
\varphi'(t) = (\nabla w_t, KL(\rho_t|\pi))_{L^2(\rho_t)} \quad \text{and} \quad \varphi''(t) = (w_t, Hess_{KL(\cdot|\pi)}(\rho_t)w_t)_{L^2(\rho_t)}.
\]

Therefore, \( \varphi'(0) = -\langle \nabla \log \left( \frac{\mu_n}{\pi} \right), g \rangle_{L^2(\mu_n)} = -I_{Stein}(\mu_n|\pi) \). Moreover, \( \varphi''(t) = \psi_1(t) + \psi_2(t) \), where
\[
\psi_1(t) = \mathbb{E}_{x \sim \rho_t}\left[ (w_t(x), H_V(x)w_t(x)) \right] \quad \text{and} \quad \psi_2(t) = \mathbb{E}_{x \sim \rho_t}\left[ \|Jw_t(x)\|_{HS}^2 \right].
\]
We illustrate the validity of the rates of Corollary 6 with simple experiments provided Section 11. To we can easily obtain convergence rates, which were not previously known.

Although the Hessian of $KL(\cdot | \pi)$ is not bounded over the whole tangent space, our proof relies on controlling the Hessian when restricted to $H$. Since $I_{\text{Stein}}(\mu_n | \pi)$ is nonnegative, Proposition 5 shows that the KL divergence w.r.t. $\pi$ decreases along the SVGD algorithm, i.e. the KL is a Lyapunov functional for SVGD. A first consequence of Proposition 5 is the convergence of $I_{\text{Stein}}(\mu_n | \pi)$ to zero, similarly to the continous time case, see Proposition 2. Indeed, the descent lemma implies that the sequence $I_{\text{Stein}}(\mu_n | \pi)$ is summable and hence converges to zero. A second consequence of the descent lemma is the following discrete time convergence rate for the average of the sequence $I_{\text{Stein}}(\mu_n | \pi)$.

**Corollary 6.** Let $\alpha > 1$ and $\gamma \leq \min \left( \frac{\alpha-1}{\alpha BC^2}, \frac{2}{(\alpha+M)B^2} \right)$ and $c_\gamma = \gamma \left( 1 - \gamma \frac{(\alpha^2+M)B^2}{2} \right)$. Then,

$$
\min_{k=1, \ldots, n} I_{\text{Stein}}(\mu_n | \pi) \leq \frac{1}{n} \sum_{k=1}^n I_{\text{Stein}}(\mu_k | \pi) \leq \frac{KL(\mu_0 | \pi)}{c_\gamma n}.
$$

We illustrate the validity of the rates of Corollary 6 with simple experiments provided Section 11. To guarantee convergence rates of the SVGD algorithm in terms of the KL objective, further properties are needed. Similarly to the continous time case, if $\pi$ satisfies the Stein log-Sobolev inequality, the Kullback-Leibler divergence converges exponentially fast along the SVGD algorithm.

**Theorem 7.** Let $\alpha > 1$ and $\gamma \leq \min \left( \frac{\alpha-1}{\alpha BC^2}, \frac{2}{(\alpha+M)B^2} \right)$. Under the assumptions of Proposition 5 if $\pi$ satisfies the Stein log Sobolev inequality (10) with $\lambda > 0$ at all iterations $n \geq 0$, then with $c_\gamma = \gamma \left( 1 - \gamma \frac{(\alpha^2+M)B^2}{2} \right)$,

$$
KL(\mu_{n+1} | \pi) \leq (1 - 2c_\gamma \lambda)^n KL(\mu_0 | \pi).
$$

Hence, if $2c_\gamma \lambda < 1$, we obtain exponential convergence.

**Proof.** Using the descent Proposition 5 and the Stein log Sobolev inequality (10), it holds that:

$$
KL(\mu_{n+1} | \pi) - KL(\mu_n | \pi) \leq -c_\gamma I_{\text{Stein}}(\mu_n | \pi) \leq -2c_\gamma \lambda KL(\mu_n | \pi).
$$

It follows that $KL(\mu_{n+1} | \pi) \leq (1 - 2c_\gamma \lambda) KL(\mu_n | \pi)$, which gives the result by iterating. 

**Remark 4.** A descent lemma was also obtained for SVGD in [Liu, 2017] Theorem 3.3) under a boundedness condition of the KSD and the kernel. While we obtain similar conditions on the step size, our approach, shown in the proof sketch (and, in greater detail, the Appendix), gives clearer connections with Wasserstein gradient flows. More precisely, we prove Proposition 5 by performing differential calculus over the Wasserstein space. We are able to replace the boundedness condition on the KSD by a simple boundedness condition of the first moment of $\mu_n$ at each iteration, which echoes analyses of some optimization algorithms like Stochastic Gradient Descent [Moulines and Bach, 2011]. Our construction also brings with it a simple yet informative perspective, arising from the optimization literature, into why SVGD actually satisfies a descent lemma. In optimization, it is well known that descent lemmas can be obtained under a boundedness condition on the Hessian matrix. Here, the Hessian operator of the KL at $\mu$ is an operator on $L^2(\mu)$; and yet, this operator is not bounded [Wibisono, 2018, Section 3.1.1]. By restricting the Hessian operator to the RKHS however, and then using the reproducing property and our assumptions, the resulting Hessian operator is provably bounded under simple conditions on the kernel and $\pi$. A next insight deriving from the optimization perspective is that linear rates can be obtained by combining a descent result and a Polyak-Lojasiewicz condition on the objective function [Karimi et al., 2016]. In our case, the latter condition corresponds to the Stein log Sobolev inequality from [Duncan et al., 2019]. When this holds, we can easily obtain convergence rates, which were not previously known.

**Remark 5.** SVGD implements a variant of a Forward discretization of the gradient flow of the KL whereas ULA implements a Forward-flow discretization. Hence, the techniques to obtain rates of convergence are very different, and we leverage techniques from the study of gradient descent in Hilbert spaces.
6 Conclusion

In this paper, we provide a non-asymptotic analysis for the SVGD algorithm. Our results build upon the connection of SVGD with gradient descent on the Wasserstein space [Liu 2017]. In establishing these results, we draw on perspectives and techniques used to establish convergence in optimization, and on recent results on the Stein geometry induced by the kernel characterizing the convexity of the objective (depending on the target π) with respect to this geometry.

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7 Background

7.1 Dissipation of the KL

The time derivative, or the dissipation of the KL divergence along any flow is given by:

\[
\frac{d}{dt} \text{KL}(\mu_t | \pi) = \frac{d}{dt} \int \mu_t \log \left( \frac{\mu_t}{\pi} \right) dx = \int \frac{\partial \mu_t}{\partial t} \log \left( \frac{\mu_t}{\pi} \right) dx
\]

(17)

since the second part of the chain rule is null:

\[
\int \mu_t \frac{\partial}{\partial t} \log \left( \frac{\mu_t}{\pi} \right) dx = \int \frac{\partial \mu_t}{\partial t} \log \left( \frac{\mu_t}{\pi} \right) dx = \frac{d}{dt} \int \mu_t dx = 0.
\]

Moreover, if \( \mu_t \) satisfies a continuity equation of the form:

\[
\frac{\partial \mu_t}{\partial t} + \text{div}(\mu_t v_t) = 0
\]

where \( v_t \) is called the velocity field, then by an integration by parts:

\[
\frac{d}{dt} \text{KL}(\mu_t | \pi) = - \int \text{div}(\mu_t(x)v_t(x)) \log \left( \frac{\mu_t}{\pi} \right) dx
\]

\[
= \int v_t(x) \nabla \log \left( \frac{\mu_t}{\pi} \right) \mu_t(x) dx = \langle v_t, \nabla \log \left( \frac{\mu_t}{\pi} \right) \rangle_{L^2(\mu_t)}.
\]

(18)

7.2 Descent lemma for Gradient Descent in \( \mathbb{R}^d \)

In this section we show how to obtain a descent lemma for the gradient descent algorithm. We do not claim any generality here, the goal of this section is to provide an intuition behind the proof of Proposition 5 for SVGD.

Consider \( F: \mathbb{R}^d \to \mathbb{R} \) a \( C^2(\mathbb{R}^d) \) function with Hessian \( H_F \), and the gradient descent algorithm written at iteration \( n + 1 \):

\[
x_{n+1} = x_n - \gamma \nabla F(x_n).
\]

(19)

Consider \( n \geq 0 \) fixed. For every \( t \geq 0 \), denote \( x(t) = x_n - t \nabla F(x_n) \). Then, \( x(0) = x_n \) and \( x(\gamma) = x_{n+1} \). We assume that there exists \( M \geq 0 \) such that for every \( t \geq 0 \), \( \|H_F(x(t))\| \leq M \).

Denote \( \varphi(t) = F(x(t)) \). Using Taylor expansion,

\[
\varphi(\gamma) = \varphi(0) + \gamma \varphi'(0) + \int_0^\gamma (\gamma - t) \varphi''(t) dt.
\]

(20)

Denote by \( \dot{x} \) the derivative of \( x \). We now identify each term. First, \( \varphi(0) = F(x_n) \) and \( \varphi(\gamma) = F(x_{n+1}) \). Second, \( \varphi'(0) = \langle \nabla F(x(0)), \dot{x}(0) \rangle = \langle \nabla F(x_n), -\nabla F(x_n) \rangle = -\|\nabla F(x_n)\|^2 \). Finally, since \( \dot{x} = 0 \),

\[
\varphi''(t) = \langle \dot{x}(t), H_F(x(t)) \dot{x}(t) \rangle \leq M \|\dot{x}(t)\|^2 = M \|\nabla F(x_n)\|^2.
\]

(21)

Therefore

\[
F(x_{n+1}) \leq F(x_n) - \gamma \|\nabla F(x_n)\|^2 + M \int_0^\gamma (\gamma - t) \|\nabla F(x_n)\|^2 dt
\]

\[
\leq F(x_n) - \gamma \|\nabla F(x_n)\|^2 + \frac{M \gamma^2}{2} \|\nabla F(x_n)\|^2.
\]

(22)

8 Proofs

8.1 Proof of Proposition 5

Proposition 8. Under Assumption \([A_1],[A_2]\) and assuming \( \exists C > 0 \) such that \( \int \|x\| d\mu_t(x) < C \) for all \( t \geq 0 \), there exists \( \lambda \in \mathbb{R}^+ \) such that:

\[
\frac{dI_{\text{Stein}}(\mu_t | \pi)}{dt} \leq \lambda I_{\text{Stein}}(\mu_t | \pi).
\]

(23)

Proof. We first need to compute \( D_t = \frac{dI_{\text{Stein}}(\mu_t | \pi)}{dt} \). We denote by \( v_t = S_{\mu_t} \nabla \log (\frac{\mu_t}{\pi}) \). Recalling that \( I_{\text{Stein}}(\mu_t | \pi) = \sum_{i=1}^d \|v_t^i\|_{\mathcal{H}_0}^2 \), we have by differentiation that:

\[
D_t = 2 \sum_{i=1}^d \langle v_t^i, \frac{dv_t^i}{dt} \rangle_{\mathcal{H}_0}
\]

(24)
We recall that by assumption

We need to show that the

We thus need to compute each component

We finally get:

where the second line uses an integration by parts. Hence by using the reproducing property,

where

We will use the reproducing property recalling that each component \( v_i^t \) is an element of the RKHS \( \mathcal{H}_0 \), i.e:

We thus have:

Indeed, if \( \|A_{i,j}\|_{HS} \leq R \) for some \( R > 0 \), then we directly conclude that:

By assumptions on the kernel and Hessian of \( \log \pi \) we have that:

We recall that by assumption \( \|k(x,.)\|_{\mathcal{H}_0} \leq B \), \( \|\partial_i k(x,.)\|_{\mathcal{H}_0} \leq B \) and \( \|H \log \pi(x)\|_{op} \leq M \). Hence, we have:

It remains to control \( \partial_i \log \pi(x) \). This can be done under the additional assumption:

for some positive constant \( C \). Hence, we have:

We finally get:

Denoting \( \lambda = dB^2(M + 1 + MC + |\partial_i \log \pi(0)|) \) gives the desired result.
Recall, from the dissipation (Proposition 1) that \( \text{KL}(\mu_t | \pi) \leq \text{KL}(\mu_0 | \pi) \). Since \( \rho \mapsto \text{KL}(\rho | \pi) \) is weakly coercive (i.e., has compact sub-level sets in the weak topology, (van Erven and Harremoes 2014 Theorem 20)), the family \( \{\mu_t\} \) is weakly relatively compact. Besides, \( I_{\text{Stein}}(\rho | \pi) \) is weakly continuous, therefore its supremum over the weakly relatively compact set \( \{\mu_t\} \) is finite: \( \sup_t I_{\text{Stein}}(\mu_t | \pi) < \infty \). Therefore, there exists \( L \geq 0 \) such that \( \|I_{\text{Stein}}(\mu_t | \pi)\| \leq L \).

We can now show that \( I_{\text{Stein}}(\mu_t | \pi) \) converges to 0. Indeed, otherwise we would have a sequence \( t_k \to \infty \) such that \( I_{\text{Stein}}(\mu_{t_k} | \pi) > \varepsilon > 0 \). Moreover, since \( I_{\text{Stein}}(\mu_t | \pi) \) has bounded time derivative, it is uniformly \( L \)-Lipschitz. There exists a sequence of intervals \( I_k \) of length \( \frac{\varepsilon}{L} \) centered at \( t_k \) (that we can assume disjoints without loss of generality since \( t_k \to \infty \)), such that \( I_{\text{Stein}}(\mu_{t_k} | \pi) \geq \frac{\varepsilon}{2} \) for every \( t \in I_k \). Now, integrating the dissipation (see Proposition 1) over \( \mathbb{R}^+ \) we get:

\[
\text{KL}(\mu_0 | \pi) - \text{KL}(\mu_t | \pi) = \int_0^t I_{\text{Stein}}(\mu_s | \pi)ds \geq \sum_{k, t_k \leq t} \frac{\varepsilon^2}{2L}.
\]

The above sum diverges as \( t \) goes to infinity since \( t_k \to \infty \). This is in contradiction with \( \text{KL}(\mu_0 | \pi) < \infty \). Hence, \( I_{\text{Stein}}(\mu_t | \pi) \to 0 \).

### 8.2 Proof of Proposition 5

We justify each step of the sketch of the proof of Section 7.2.

Consider \( n \geq 0 \) fixed and \( \gamma \leq \frac{\alpha^{-1}}{\alpha + BC^2} \). Denote \( g = P_{\mu_n} \triangledown \log \left( \frac{\mu_0}{\pi} \right) \) and for every \( t \in [0, \gamma] \), \( \phi_t = (I - tg) \).

Denote \( \rho_0 = \phi_{\#} \mu_n \). Then, \( \rho_0 = \mu_n \) and \( \rho_\gamma = \mu_{n+1} \).

**Lemma 9.** Suppose Assumption \([A_1]\) holds, i.e. the kernel and its gradient are bounded by some positive constant \( B \). Then for any \( x \in \mathcal{X} \):

\[
\|g(x)\| \leq BI_{\text{Stein}}(\mu_n | \pi)^{\frac{1}{2}} \tag{32}
\]

\[
\|Jg(x)\|_{HS} \leq BI_{\text{Stein}}(\mu_n | \pi)^{\frac{1}{2}} \tag{33}
\]

**Proof.** This is a consequence of the reproducing property and Cauchy-Schwarz inequality in the RKHS space.

Let \( g' = S_{\mu_n} \triangledown \log \left( \frac{\mu_0}{\pi} \right) \), hence for any \( x \in \mathcal{X} \), \( g(x) = g'(x) \) and:

\[
\|g(x)\|^2 = \sum_{i=1}^d (k(x, .), g'_i \pi_0) \leq \|k(x, .)\|_{HS} \|g'\|_{HS} \leq B^2 I_{\text{Stein}}(\mu_n | \pi).
\]

Similarly:

\[
\|Jg(x)\|^2_{HS} = \sum_{i,j=1}^d \left| \frac{\partial g_j(x)}{\partial x_i} \right|^2 = \sum_{i,j=1}^d (\partial_{x_j} k(x, .), g'_i \pi_0) \leq \sum_{i,j=1}^d \|\partial_{x_j} k(x, .)\|_{HS} \|g'_i\|_{HS} \leq B^2 I_{\text{Stein}}(\mu_n | \pi).
\]

**Lemma 10.** Suppose that Assumption \([A_2]\) and Assumption \([A_3]\) hold. Then, for any \( x \in \mathcal{X} \), \( \|tJg(x)\|_{op} \leq tB\sqrt{C} \) and for every \( t < \frac{1}{B\sqrt{C}} \), \( \phi_t \) is a diffeomorphism. Moreover, \( \|(J\phi_t(x))^{-1}\|_{op} \leq \alpha \).

**Proof.** First, by Lemma 9 and Assumption \([A_3]\) we have \( \|Jg(x)\|_{op} \leq \|Jg(x)\|_{HS} \leq B\sqrt{C} \). If \( t < \frac{1}{B\sqrt{C}} \), then \( \|tJg(x)\|_{op} < 1 \). Therefore, \( J(\phi_t(x)) = I - tJg(x) \) is regular for every \( x \) and \( \phi_t \) is a diffeomorphism. Moreover,

\[
\|(J\phi_t(x))^{-1}\|_{op} \leq \sum_{k=0}^\infty \|tJg(x)\|^k_{op} \leq \sum_{k=0}^\infty \|tJg(x)\|^k_{HS} \leq \sum_{k=0}^\infty (tB\sqrt{C})^k \leq \alpha,
\]

where we used \( \gamma \leq \frac{\alpha^{-1}}{\alpha + BC^2} \).

Denote \( \varphi(t) = \text{KL}(\rho_t | \pi) \). Using Taylor expansion,

\[
\varphi(\gamma) = \varphi(0) + \gamma \varphi'(0) + \int_0^\gamma (\gamma - t) \varphi''(t) dt.
\]

We now identify each term. First, \( \varphi(0) = \text{KL}(\mu_n | \pi) \) and \( \varphi(\gamma) = \text{KL}(\mu_{n+1} | \pi) \).
To compute $\varphi'(t)$ and $\varphi''(t)$ we have two options. Either we check the assumptions of the optimal transport theorems allowing to apply the chain rule [Villani (2003); Ambrosio et al. (2008)], or we do a direct computation. The latter is preferred, although differential calculus over the Wasserstein space is a powerful way to guess the formulas.

**Lemma 11.** Denote $w_t(x) = -g(\phi_t^{-1}(x))$. Then,

$$\varphi'(0) = \langle \nabla W_2(\rho_0, \pi), w_0 \rangle_{L^2(\mu_n)} = -I_{Stein}(\mu_n|\pi),$$

and,

$$\varphi''(t) = \langle w_t, Hess_{KL}(\rho_t)w_t \rangle_{L^2(\rho_t)} = \int \left[ \|Jg(x)(J\phi_t(x))^{-1}\|_{H^2}^2 + \langle g(x), H_V(\phi_t(x))g(x) \rangle \right] \mu_n(x) dx.$$ 

**Proof.** We know by Lemma [10] that $\phi_t$ is a diffeomorphism, therefore, $\rho_t$ admits a density given by the change of variables formula:

$$\rho_t(x) = |J\phi_t(\phi_t^{-1}(x))|^{-1/2} \mu_n(\phi_t^{-1}(x)).$$

Using the transfer lemma with $\rho_t = \phi_t^*\mu_n$, $\varphi(t)$ is given by:

$$\varphi(t) = \int \log \left( \frac{\rho_t(y)}{\pi(y)} \right) \rho_t(y) dy = \int \log \left( \frac{\mu_n(x)}{J\phi_t(x)} \right) \mu_n(x) dx.$$ 

We can now take the time derivative of $\varphi(t)$ which gives:

$$\varphi'(t) = -\int tr \left( J\phi_t(x)^{-1} \frac{dJ\phi_t(x)}{dt} \right) \mu_n(x) dx - \int \langle \nabla \log \pi(\phi_t(x)), \frac{d\rho_t(x)}{dt} \rangle \mu_n(x) dx.$$ 

Hence, we can use the explicit expression of $\phi_t$ to write:

$$\varphi'(t) = \int tr(J\phi_t(x)^{-1}Jg(x))\mu_n(x) dx + \int \langle \nabla \log \pi(\phi_t(x)), g(x) \rangle \mu_n(x) dx.$$ 

The Jacobian at time $t = 0$ is simply equal to the identity since $\phi_0 = I$. It follows that $tr(J\phi_0(x)^{-1}Jg(x)) = tr(Jg(x)) = div(g(x))$ by definition of the divergence operator. Using an integration by parts:

$$\varphi'(0) = -\int \left[ -div(g(x)) - \langle \nabla \log \pi(x), g(x) \rangle \right] \mu_n(x) dx$$

$$= -\int \langle \nabla \log \left( \frac{\mu_n}{\pi} \right), g(x) \rangle \mu_n(x) dx = -I_{Stein}(\mu_n|\pi).$$ 

Now, we prove the second statement. First,

$$\varphi''(t) = \int \left[ tr((Jg(x)(J\phi_t(x))^{-1})^2) + \langle g(x), H_V(\phi_t(x))g(x) \rangle \right] \mu_n(x) dx.$$ 

Since $Jg(x)$ and $J\phi_t(x)$ commutes, $tr((Jg(x)(J\phi_t(x))^{-1})^2) = \|Jg(x)(J\phi_t(x))^{-1}\|_{H^2}^2$. Moreover, using the chain rule,

$$-Jw_t(x) = J(g \circ \phi_t^{-1})(x) = Jg(\phi_t^{-1}(x))J(\phi_t^{-1})(x) = Jg(\phi_t^{-1})(J\phi_t^{-1})(\phi_t^{-1}(x)).$$

Therefore, $\|Jg(x)(J\phi_t(x))^{-1}\|_{H^2}^2 = \|Jw_t(\phi_t(x))\|_{H^2}^2$, which proves the second part of the second statement. Using the transfer lemma,

$$\varphi''(t) = \int \left[ \|Jw_t(y)\|_{H^2}^2 + \langle w_t(y), H_V(y)w_t(y) \rangle \right] \rho_t(y) dy$$

$$= \langle w_t, Hess_{KL}(\rho_t)w_t \rangle_{L^2(\rho_t)}.$$ 

which concludes the proof. 

Denote

$$\psi_1(t) = \int \left[ \|Jg(x)(J\phi_t(x))^{-1}\|_{H^2}^2 \right] \mu_n(x) dx \quad \text{and} \quad \psi_2(t) = \int \langle g(x), H_V(\phi_t(x))g(x) \rangle \mu_n(x) dx.$$ 

Then, $\varphi''(t) = \psi_1(t) + \psi_2(t)$. We bound $\psi_1$ and $\psi_2$ separately. First, since the potential $V$ is $M$-smooth,

$$\psi_2(t) \leq M \int \|g(x)\|^2 \mu_n(x) dx \leq MB^2I_{Stein}(\mu_n|\pi),$$

by using Lemma [9]. Now, we bound $\psi_1(t)$ using Lemma [10] and [9]:

$$\|Jg(x)(J\phi_t(x))^{-1}\|_{H^2}^2 \leq \|Jg(x)\|_{H^2}^2 \|J\phi_t(x)^{-1}\|_{Lip}^2 \leq \alpha^2 B^2 I_{Stein}(\mu_n|\pi).$$

Finally, $\varphi''(t) \leq (\alpha^2 + M)B^2I_{Stein}(\mu_n|\pi)$. Plugging into (35) gives the result.
9 Finite number of particles regime

In this section, we investigate the deviation of the discrete distributions generated by the SVGD algorithm for a finite number of particles, to its population version. In practice, starting from \( N \) i.i.d. samples \( X_0 \sim \mu_0 \), SVGD algorithm updates the \( N \) particles as follows:

\[
X_{n+1}^i = X_n^i - \gamma P_{\hat{\mu}_n} \nabla \log \left( \frac{\hat{\mu}_n}{\pi} \right) (X_n^i), \quad \hat{\mu}_n = \frac{1}{N} \sum_{j=1}^{N} \delta_{X_n^j}, \tag{39}
\]

where \( \hat{\mu}_n \) denotes the empirical distribution of the interacting particles. Recall that \( P_{\hat{\mu}_n} \nabla \log \left( \frac{\hat{\mu}_n}{\pi} \right) \) is well defined even if \( \hat{\mu}_n \) is discrete.

In Liu (2017), the authors show that the empirical distribution of the SVGD samples weakly converge to its population limit for any iteration. More precisely, under the assumptions that \( b(x, y) = \nabla \log \pi(x)k(x, y) + \nabla_x k(x, y) \) is jointly Lipschitz and that \( \mu_n \) converges weakly to \( \mu_0 \) as \( N \to \infty \) (which happens by drawing \( N \) i.i.d. samples of \( \mu_0 \)), for any \( n \geq 0 \), they show that \( \hat{\mu}_n \) converges weakly to \( \mu_n \). This happens as soon as Assumptions \( (A_1), (A_2), (B_1), (B_2) \) are satisfied (since the product of bounded Lipschitz functions is a Lipschitz function):

\begin{itemize}
  \item \((B_1)\) Assume that \( \exists C_V \) s.t. for all \( x \in \mathcal{X}, \|V(x)\| \leq C_V \).
  \item \((B_2)\) Assume \( \exists D > 0, k \) is continuous on \( \mathcal{X} \) and D-Lipschitz:
      \[ |k(x, x') - k(y, y')| \leq D(\|x - y\| + \|x' - y'\|) \]
      for all \( x, x', y, y' \in \mathcal{X} \),

      and \( k \) is continuously differentiable on \( \mathcal{X} \) with D-Lipschitz gradient:
      \[ \|\nabla k(x, x') - \nabla k(y, y')\| \leq D(\|x - y\| + \|x' - y'\|) \]
      for all \( x, x', y, y' \in \mathcal{X} \).
\end{itemize}

Under these assumptions, we quantify the dependency in the number of particles in the following proposition.

**Proposition 12.** Let \( n \geq 0 \) and \( T > 0 \). Let \( \mu_n \) and \( \hat{\mu}_n \) be defined by (7) and (39) respectively. Under Assumptions \( (A_1), (A_2), (B_1), (B_2) \) for any \( 0 \leq n \leq \frac{T}{\gamma} \):

\[
E[W_2^2(\mu_n, \hat{\mu}_n)] \leq \frac{1}{2} \left( \frac{1}{\sqrt{N}} \sqrt{\text{var}(\mu_n)e^{LT}} \right) (e^{2LT} - 1)
\]

where \( L \) is a constant depending on \( k \) and \( \pi \).

Proposition 12, whose proof is provided below, controls the *propagation the chaos* at each iteration, and uses techniques from Jourdain et al. (2007). The time growing constant is common in this interacting particle system literature: obtaining uniform in time bounds for the propagation of chaos require substantial further work and assumptions on the potential Durmus et al. (2018a).

9.1 Proof of Proposition 12

Introduce the system of \( N \) independent particles:

\[
\tilde{X}_{n+1}^i = \tilde{X}_n^i - \gamma P_{\hat{\mu}_n} \nabla \log \left( \frac{\hat{\mu}_n}{\pi} \right) (\tilde{X}_n^i), \quad \tilde{X}_0^i \sim \mu_0. \tag{40}
\]

By definition, \( (\tilde{X}_n^i)_{i=1}^{N} \) are i.i.d. samples from \( \mu_n \). Let \( c_n = \left( \frac{1}{N} \sum_{i=1}^{N} \mathbb{E}[\tilde{X}_n^i - X_n^i]^2 \right)^{\frac{1}{2}} \). Notice that \( c_n \geq W_2(\mu_n, \hat{\mu}_n) \) since the 2-Wasserstein is the infimum over the couplings between \( \mu_n \) and \( \hat{\mu}_n \). At time \( n + 1 \), we have:

\[
c_{n+1} = \frac{1}{\sqrt{N}} \left( \sum_{i=1}^{N} \mathbb{E}[\|\tilde{X}_{n+1}^i - X_{n+1}^i\|^2] \right)^{\frac{1}{2}}
\]

\[
= \frac{1}{\sqrt{N}} \left( \sum_{i=1}^{N} \mathbb{E}[\|\tilde{X}_n^i - X_n^i - \gamma (P_{\hat{\mu}_n} \nabla \log(\frac{\hat{\mu}_n}{\pi}))(X_n^i) - P_{\mu_n} \nabla \log(\frac{\mu_n}{\pi})(X_n^i)]\|^2] \right)^{\frac{1}{2}}
\]

\[
\leq c_n + \frac{\gamma}{\sqrt{N}} \left( \sum_{i=1}^{N} \mathbb{E}[\|P_{\hat{\mu}_n} \nabla \log(\frac{\hat{\mu}_n}{\pi})(X_n^i) - P_{\mu_n} \nabla \log(\frac{\mu_n}{\pi})(X_n^i)]\|^2] \right)^{\frac{1}{2}}
\]
By introducing $\bar{\mu}_n$, the empirical distribution of the particles $(X^i_n)_{i=1}^N$, the second term on the right hand side can be decomposed as the square root of the sum of two terms $A$ and $B$ defined as:

$$A = \sum_{i=1}^N \mathbb{E}[[P_{\bar{\mu}_n} \nabla \log(\frac{\bar{\mu}_n}{\pi})(X^i_n) - P_{\bar{\mu}_n} \nabla \log(\frac{\bar{\mu}_n}{\pi})(\bar{X}^i_n)]^2]$$

$$B = \sum_{i=1}^N \mathbb{E}[[P_{\bar{\mu}_n} \nabla \log(\frac{\bar{\mu}_n}{\pi})(\bar{X}^i_n) - P_{\bar{\mu}_n} \nabla \log(\frac{\bar{\mu}_n}{\pi})(\bar{X}^i_n)]^2]$$

By using Lemma 15 the map $(z, \mu) \mapsto P_{\mu} \nabla \log(\frac{\mu}{\pi})(z)$ is $L$-Lipschitz and we can bound the first term as follows:

$$A \leq \sum_{i=1}^N \mathbb{E}||P_{\bar{\mu}_n} \nabla \log(\frac{\bar{\mu}_n}{\pi})(X^i_n) - P_{\bar{\mu}_n} \nabla \log(\frac{\bar{\mu}_n}{\pi})(\bar{X}^i_n)||^2 + \sum_{i=1}^N \mathbb{E}||P_{\bar{\mu}_n} \nabla \log(\frac{\bar{\mu}_n}{\pi})(\bar{X}^i_n) - P_{\bar{\mu}_n} \nabla \log(\frac{\bar{\mu}_n}{\pi})(\bar{X}^i_n)||^2$$

$$\leq \sum_{i=1}^N 2L^2\mathbb{E}||X^i_n - \bar{X}^i_n||^2 + \sum_{i=1}^N 2L^2\mathbb{E}[W^2_2(\bar{\mu}_n, \bar{\mu}_n)]$$

$$= NL^2c_n^2 + NL^2\mathbb{E}[W^2_2(\bar{\mu}_n, \bar{\mu}_n)].$$

Hence,

$$A^{\frac{1}{2}} \leq L\sqrt{N}(c_n + \mathbb{E}[W^2_2(\bar{\mu}_n, \bar{\mu}_n)])^{\frac{1}{2}} \leq 2L\sqrt{N}c_n.$$ 

The second term can be bounded as:

$$B = \sum_{i=1}^N \mathbb{E}\left[ \frac{1}{N} \sum_{i=1}^N [b(\bar{X}^i_n, \bar{X}^i_n) - \int b(x, \bar{X}^i_n)d\mu_n(x)]^2 \right]$$

$$= \sum_{i=1}^N \frac{1}{N^2} \sum_{j=1}^N \mathbb{E}[||b(\bar{X}^i_n, \bar{X}^j_n) - \int b(x, \bar{X}^i_n)d\mu_n(x)||^2]$$

$$\leq \sum_{i=1}^N \frac{1}{N^2} \sum_{j=1}^N L^2\mathbb{E}[||\bar{X}^i_n - \int xd\mu_n(x)||^2]$$

$$\leq L^2\text{var}(\mu_n)$$

by using Corollary 16. Hence,

$$B^{\frac{1}{2}} \leq L\sqrt{\text{var}(\mu_n)},$$

and we get the recurrence relation for $c_n$:

$$c_{n+1} \leq c_n + \frac{\gamma}{\sqrt{N}}(A + B)^{\frac{1}{2}}$$

$$\leq c_n + \frac{\gamma}{\sqrt{N}}(2L\sqrt{N}c_n + L\sqrt{\text{var}(\mu_n)})$$

$$\leq c_n(1 + 2\gamma L) + \frac{\gamma L}{\sqrt{N}}\sqrt{\text{var}(\mu_n)}$$

$$\leq \frac{1}{2}\left(\frac{1}{\sqrt{N}}\sqrt{\text{var}(\mu_0)e^{LT}}\right)(e^{2LT} - 1)$$

where the last line uses Lemma 13.

**Lemma 13.** Consider an initial distribution $\mu_0$ with finite variance. Define the sequence of probability distributions $\mu_{n+1} = (1 - \gamma P_{\bar{\mu}_n} \nabla \log(\frac{\mu_n}{\pi}))\#\mu_n$. Under Assumption $[A_2](\underline{A}_2), [B_1], [B_2]$, the variance of $\mu_n$ satisfies for all $T > 0$ and $n \leq \frac{T}{\gamma}$ the following inequality:

$$\text{var}(\mu_n)^{\frac{1}{2}} \leq \text{var}(\mu_0)^{\frac{1}{2}}e^{LT}$$

for $L$ a constant depending on $k$ and $\pi$. 

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Proof. Denote by $x$ and $x'$ two independent samples from $\mu_n$. We have:

$$\text{var}(\mu_{n+1})^{1/2} = \left( \mathbb{E} \left[ x - \mathbb{E}[x'] - \gamma \nabla \log \left( \frac{\mu_n}{\pi} \right)(x) + \gamma \mathbb{E} \left[ \nabla \log \left( \frac{\mu_n}{\pi} \right)(x') \right] \right]^2 \right)^{1/2} \leq \text{var}(\mu_n)^{1/2} + \gamma \left( \mathbb{E} \left[ \nabla \log \left( \frac{\mu_n}{\pi} \right)(x) - \mathbb{E} \left[ \nabla \log \left( \frac{\mu_n}{\pi} \right)(x') \right] \right]^2 \right)^{1/2} \leq \text{var}(\mu_n)^{1/2} + \gamma \frac{L}{n} \mathbb{E} \left[ ||x - x'||^2 \right]^{1/2} \leq \text{var}(\mu_n)^{1/2} + \gamma \frac{L}{n} \text{var}(\mu_n)^{1/2} .$$

The second and last lines are obtained using a triangular inequality while the third line uses that $P_{\mu_n} \nabla \log (\frac{\mu_n}{\pi})(x)$ is $L$-Lipschitz by Lemma 15. We then conclude using Lemma 14.

Lemma 14. [Discrete Gronwall lemma] Let $a_{n+1} \leq (1 + \gamma A)a_n + b$ with $\gamma > 0$, $A > 0$, $b > 0$ and $a_0 = 0$, then:

$$a_n \leq \frac{b}{\gamma A} (e^{n\gamma A} - 1).$$

Proof. Using the recursion, it is easy to see that for any $n > 0$:

$$a_n \leq (1 + \gamma A)^n a_0 + b \left( \sum_{i=0}^{n-1} (1 + \gamma A)^k \right)$$

One concludes using the identity $\sum_{i=0}^{n-1} (1 + \gamma A)^k = \frac{1}{\gamma A} ((1 + \gamma A)^n - 1)$ and recalling that $(1 + \gamma A)^n \leq e^{n\gamma A}$.

## 10 Auxiliary results

Lemma 15. Under Assumption \([A_1],[A_2],[B_1],[B_2]\) the map $(z, \mu) \mapsto P_{\mu} \nabla \log (\frac{\mu}{\pi})(z)$ is $L$-Lipschitz with:

$$\|P_{\mu} \nabla \log (\frac{\mu}{\pi})(z) - P_{\mu'} \nabla \log (\frac{\mu'}{\pi})(z')\| \leq L(\|z - z'\| + W_2(\mu, \mu'))$$

where $L$ depends on $k$ and $\pi$.

Proof. We will consider an optimal coupling $s$ with marginals $\mu$ and $\mu'$:

$$\|P_{\mu} \nabla \log (\frac{\mu}{\pi})(z) - P_{\mu'} \nabla \log (\frac{\mu'}{\pi})(z')\| = \mathbb{E}_s \left[ \nabla \log \pi(x) k(x, z) - \nabla \log \pi(x') k(x', z') \right]$$

$$\leq B \mathbb{E}_s \left[ \left\| \nabla \log \pi(x) - \nabla \log \pi(x') \right\| \right] + C_V \mathbb{E}_s \left[ \left\| k(x, z) - k(x', z') \right\| \right] + \mathbb{E}_s \left[ \left\| \nabla_1 k(x, z) - \nabla_1 k(x', z') \right\| \right]$$

$$\leq B M \mathbb{E}_s \left[ \left\| x - x' \right\| \right] + C_V D \left( \left\| z - z' \right\| + \mathbb{E}_s \left[ \left\| x - x' \right\| \right] \right) + \mathbb{E}_s \left[ \left\| x - x' \right\| \right] + \mathbb{E}_s \left[ \left\| x - x' \right\| \right]$$

$$\leq L(\| z - z' \| + W_2(\mu, \mu')).$$

The second line is obtained by convexity while the third one uses Assumption \([B_1],[A_2]\) and \([A_2]\). The penultimate line uses Assumption \([A_2]\) and \([B_2]\) finally the last line relies on $s$ being optimal and setting $L = C_V (D + 1) + BM$.

Corollary 16. Let $b$ the function defined by $b(x, z) = \nabla \log \pi(x) k(x, z) + \nabla k(x, z)$. Under the assumptions of Lemma 15 $b$ is $L$-Lipschitz in its first variable.

Proof. Notice that $P_{\mu} \nabla \log (\frac{\mu}{\pi})(y) = \mathbb{E}_{x \sim \mu} [b(x, z)]$ for any $\mu \in \mathcal{P}_2(\mathcal{X})$ and $z \in \mathcal{X}$. Hence, for any $y, y' \in \mathcal{X}$, $|b(y, \cdot) - b(y', \cdot)| \leq L W_2(\delta_y, \delta_{y'}) = L \| y - y' \|$.

Lemma 17. Suppose Assumption \([A_1]\) holds, i.e. the kernel and its gradient are bounded by some positive constant $B$. Moreover, assume that $\nabla \log (\pi)$ is $M$-Lipschitz and that $\| x \| \pi_n(x) dx$ is uniformly bounded on $n$. Then $I_{\text{Stein}}(\mu_n, \pi)$ remains bounded by some $C > 0$, i.e. Assumption \([A_3]\) holds.
Proof. For any $\mu$, we have:

$$I_{\text{Stein}}(\mu | \pi) = \langle \int \nabla \log \pi(x)k(x,. )d\mu(x), \int \nabla \log \pi(y)k(y,. )d\mu(y) \rangle_{\mathcal{H}}$$

Using the reproducing property and integration by parts it is possible to write $I_{\text{Stein}}(\mu | \pi)$ as:

$$I_{\text{Stein}}(\mu | \pi) = \int \nabla_1 \nabla_2 k(x,y)d\mu(x)d\mu(y) + \int \langle \nabla \log \pi(y)k(x,. )k(x,y)d\mu(x)d\mu(y) + \int \langle \nabla \log \pi(y), \nabla_1 k(y, x) \rangle d\mu(x)d\mu(y).$$

The terms involving the kernel are easily bounded since the kernel is bounded with bounded derivatives. Using that $\nabla \log \pi$ is $M$-Lipschitz, it is easy to see that

$$\|\nabla \log \pi(x)\| \leq \|\nabla \log \pi(0)\| + M\|x\|.$$  \hspace{1cm} (42)

Using the above inequality, one can directly conclude that $\int \|x\|\mu_n(x)dx$ remains bounded.

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11 Experiments

We downloaded and reused the code (in Python) from Liu and Wang (2016) available at https://github.com/dilinwang820/Stein-Variational-Gradient-Descent for our experiments. It implements a toy example with a 1-D Gaussian mixture and a gaussian kernel. In the upper figures, the blue dashed lines are the target density function and the solid green lines are the densities of the (200) particles at different iterations of our algorithm (estimated using kernel density estimator). The lower figures represent the evolution of $I_{\text{Stein}}(\hat{\mu}_n | \pi)$ and $\hat{\text{KL}}(\hat{\mu}_n | \pi)$ along iterations $n \geq 0$. One can see on the upper figures that the particles recover the target distribution. On the lower left figure (in log-log scale), one can see that the average $I_{\text{Stein}}$ over $n$ iterations (i.e. $1/n \sum_{k=1}^{n} I_{\text{Stein}}(\hat{\mu}_k | \pi)$) decreases at rate $1/n$ as predicted in Corollary 6. On the lower right figure (in log scale for the $y$-axis only), one can see that the KL decreases at linear rate as predicted in Theorem 7. The flattening of the KL around 200 iterations arises because we use an estimator for this quantity, which becomes visible when it is small.

\footnote{where the KL($\hat{\mu}_n | \pi$) is estimated with scipy.stats.entropy.}
Figure 1: The particle implementation of the SVGD algorithm illustrates the convergence of $I_{\text{Stein}}(\mu_n|\pi)$ and $\text{KL}(\mu_n|\pi)$ to 0.