# Non-asymptotic analysis Stein Variational Gradient Descent

*Project report*

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## 1 Introduction

In this paper we will contextualize and describe the article Korba et al. [2020]. This paper brings theoretical results on the SVGD algorithm, where the goal is to approach an unknown probability distribution $\pi$ by iteratively transforming a arbitrary known distribution $\mu_0$. It was first introduced by Liu and Wang [2016]. Starting from an initial distribution $\mu_0$, this algorithm can be seen as a gradient descent in the Wasserstein space of distributions. On this work, our contributions were multiple: on one side, we provide proofs (see Annex) that were not given or very briefly in main papers (Korba et al. [2020], Liu and Wang [2016], and Liu [2017]), and on the other side, we re-implemented the given algorithm itself from scratch (the provided code was not reproducible) to understand better the contribution of the paper.
We will first present the necessary background to understand Korba et al. [2020], and present the original idea of SVGD from Liu and Wang [2016]. Then, we will focus on the contributions from Korba et al. [2020] before discussing on our experiments, and finishing by a more general discussion about the paper itself.

## 2 SVGD Context (Liu and Wang [2016])

We fix here $\pi$ an objective probability distribution, and an initial distribution $\mu_0$ over a set $\mathcal{X}$.
In all what follows, $\mathcal{X} = \mathbb{R}^d$, and both $\mu$ and $\pi$ admit a density that will also be denoted by $\mu$ and $\pi$ respectively.

### 2.1 Notations

We will denote by $\mathcal{P}_2(\mathcal{X})$ the set of probability measure on $\mathcal{X}$ with finite second order moment i.e. the set of distributions such that $\int ||x||^2 d\mu(x) < \infty$. We assume the objective distribution $\pi$ lives in $\mathcal{P}_2(\mathcal{X})$, and define the Kullback-Leibler divergence between $\pi_1$ and $\pi_2$ by

$$\mathrm{KL}(\pi_1||\pi_2) \triangleq \mathbb{E}_{\pi_1}[\log \pi_1(x)] - \mathbb{E}_{\pi_1}[\log \pi_2(x)]$$

Let $\mathcal{A}_\pi$ the Stein Operator defined by $\forall \phi \in \mathcal{H}, \forall x \in \mathcal{X}, \mathcal{A}_\pi \phi(x) = \nabla \log \pi(x) \phi(x)^\top + \nabla \cdot \phi(x)$, for some $\mathcal{H}$ we will precise later on.
We define the Stein class of $\pi$ the subset of functions $\phi$ such that $\lim_{||x|| \longrightarrow \infty} \phi(x)\pi(x) = 0$. Note that for every function in the Stein class of $\pi$, we have

$$\mathbb{E}_{x \sim \pi}[\mathcal{A}_\pi \phi(x)] = 0 \tag{1}$$

(see A.1 for the proof).

Also, we define the pushforward measure of $\mu$ by $T : \mathbb{R}^d \longrightarrow \mathbb{R}^d$ by $\int \phi(T(x))d\mu(x) = \int \phi(x)dT_{\#}\mu(x)$ for any bounded and measurable function $\phi$.
Finally, for $\phi : \mathbb{R}^d \longrightarrow \mathbb{R}^d$, we denote by $||\cdot||_{op}$ the operator norm.

### 2.2 Context

Let $\mu \in \mathcal{P}_2(\mathcal{X})$. Given a smooth function $\phi = [\phi_1, ..., \phi_d]^\top$, a small perturbation of $\mu$ in the direction of $\phi$ is given by

$$T_{\#}\mu \triangleq (I + \gamma\phi)_{\#}\mu, \tag{2}$$

for a small $\gamma > 0$.
Recall that $\mathbb{E}_{x\sim\mu}[\mathcal{A}_\pi\phi(x)] = \int_{\mathcal{X}} \big(\nabla \log \pi(x)^\top \phi(x) + \nabla \cdot \phi(x)\big)\mu(x)\,\mathrm{d}x$. As soon as $\mu$ is not in the Stein class of $\pi$, one can show that $|\mathbb{E}_{x\sim\mu}[\mathcal{A}_\pi\phi(x)] > 0|$, increasing w.r.t. the difference between $\mu$ and $\pi$. (proof in A.3).
Therefore, the problem we want to solve is to find

$$\mu^* = \arg\min_{\mu} \mathbb{S}(\mu, \pi) = \arg\min_{\mu} \max_{\phi\in\mathcal{H}} \{\mathbb{E}_{x\sim\mu}[\mathcal{A}_\pi\phi(x)]\}, \tag{3}$$

for a certain class $\mathcal{H}$ of functionals. Indeed, the above objective is equal to 0 if and only if $\mu = \pi$ and greater than 0 otherwise, with $\mathcal{H}$ sufficiently large. A question now raises: how to choose $\mathcal{H}$ to be rich enough and still tractable?

#### 2.2.1 Choice of $\mathcal{H}$

The idea of the original paper of SVGD (Liu and Wang [2016]) is too choose $\mathcal{H}$ a RKHS and to maximize $\mathbb{S}(\mu, \pi)$ in the unit ball of $\mathcal{H}$. This is called the Kernel Stein Discrepancy (KSD).
Let $\mathcal{H}_0$ be a RKHS with a kernel $k(x, x')$ in the Stein class of $\pi$. Let $\mathcal{H} = (\mathcal{H}_0^{(1)}, \ldots, \mathcal{H}_0^{(d)})$. The objective in (3) is then:

$$\mathbb{S}(\mu, \pi) = \max_{\phi\in\mathcal{H}} \{\mathbb{E}_{x\sim\mu}[\mathcal{A}_\pi\phi(x)],\ s.t.\ \|\phi\|_{\mathcal{H}} \leq 1\}. \tag{4}$$

Within this framework, one can show that the optimal solution of (4) is given by:

$$\phi(x) = \frac{\phi^*(x)}{\|\phi^*\|_{\mathcal{H}}}\text{ , where } \phi^*(.) = \mathbb{E}_{x\sim\mu}[\mathcal{A}_\pi \otimes k(x, \cdot)] = \int_{\mathcal{X}} (k(x, \cdot)\nabla \log \pi(x) + \nabla k(x, \cdot))\,\mathrm{d}\mu(x), \tag{5}$$

where $\mathcal{A}_\pi \otimes f(x) = f(x)\nabla \log \pi(x) + \nabla f(x)$, is a variant of Stein operator. We also know that $\phi^*$ is in the Stein class of $\pi$ as $k$ is. Moreover, $\mathbb{S}(\mu, \pi) = \|\phi^*\|_{\mathcal{H}}$ (complete proof in A.2). If we know how to sample from $\mu$, we can then approximate $\phi^*$ easily.

#### 2.2.2 Back to the problem

For $\gamma < \frac{1}{||\phi||_{op}}$, $(I + \gamma\phi)$ is locally one-to-one. We then have that:

$$\nabla_\gamma \mathrm{KL}(T_{\#}\mu||\pi)|_{\gamma=0} = -\mathbb{E}_{x\sim\pi}[\mathcal{A}_\pi\phi(x)].$$

Considering all descent directions on the ball $\{\phi \in \mathcal{H}, ||\phi||_{op}^2 \leq \mathbb{S}(\mu, \pi)\}$, the one we will keep for our gradient descent is the one minimizing the gradient of KL, which writes $\phi^*$ as showed just earlier.
The Stein Variational Gradient Descent (SVGD) algorithm consists in an iterative procedure where one apply successive transformations to an initial probability measure $\mu_0$ following the trajectory $\phi^*$ that minimizes the gradient of the Kullback-Leibler divergence:

$$\mu_{n+1} = (I + \gamma\phi^*)_{\#}\mu_n. \tag{6}$$

To be able to perform a SVGD iteration, the unknown distribution $\pi$ only appears in $\nabla \log \pi(x)$. This is very convenient as, in a Bayesian framework, $\pi$ could be a posterior distribution where the normalization constant is not known. However, $\nabla \log \pi(x) = \nabla \log \frac{\pi'}{Z} = \nabla \log \pi'$, where $\pi'$ is the unnormalized posterior and $Z$ is the normalization constant.

## 3 Non-asymptotic analysis of SVGD

In their paper (Korba et al. [2020]), under assumptions, the authors provided an exponential convergence rate for continuous time SVGD, and a convergence result between SVGD in the infinite particle setting and in the finite particle setting. This last result is very important as the latter setting is the one used in practice when implementing the SVGD algorithm and allows to make a link between the implementation and the theoretical results. They also reprove a descent lemma for discrete time SVGD, originally proved in 2017 (Liu [2017]), using the Wassertein gradient flow of the KL divergence.

### 3.1 Optimal transport reminders

Before going further, we will recall some notions of optimal transport that the authors used throughout their paper.

**Definition 1** (Wasserstein distance)**.** *Let $\mu$ and $\nu$ be two probability measures on $\mathcal{X}$ and*

$$\Gamma(\mu,\nu) = \left\{\gamma : \int_{\mathcal{X}} \gamma(x,y)\,\mathrm{d}y = \mu(x) \wedge \int_{\mathcal{X}} \gamma(x,y)\,\mathrm{d}x = \nu(y)\right\}.$$

*The $p$-Wasserstein distance between $\mu$ and $\nu$ is defined by*

$$\mathbb{W}_p(\mu,\nu) = \inf_{\gamma\in\Gamma(\mu,\nu)} \int_{\mathcal{X}}\int_{\mathcal{X}} \|x-y\|^p \gamma(x,y)\,\mathrm{d}x\,\mathrm{d}y.$$

*This define a distance on the space of probability measures as it is positive, symmetric, $0$ if and only if $\mu=\nu$ and satisfies the triangle inequality.*

**Definition 2** (Continuity equation Villani [2003])**.** *Let $\mathcal{X}$ be $\mathbb{R}^d$ and $(T_t)_{0\leq t}$ a measurable map from $\mathcal{X}$ to $\mathcal{X}$ such that $T_t(\cdot) = (I+\phi_t)(\cdot)$. Let $v_t$ be the velocity field associated with the trajectories $T_t$. Let $\mu_0 \in \mathcal{P}_2(\mathcal{X})$ and $\mu_{t+1} = T_t\#\mu_t$. Then, $\mu_t$ is the unique solution of the following continuity equation:*

$$\begin{cases} \frac{\partial \mu_t}{\partial t} + \nabla\cdot(v_t\mu_t) = 0 \\ v_t = \phi(t). \end{cases}$$

### 3.2 RKHS operators

In the entire paper, the authors let $\mathcal{X}$ be $\mathbb{R}^d$. They defined the RKHS $\mathcal{H}$ and $\mathcal{H}_0$ on real-valued function of $\mathcal{X}$ the same way as in Section 2.2.1

They start by defining operators on $\mathcal{H}$.

**Definition 3.** *Let $S_\mu : L_2(\mu) \to \mathcal{H}$ be the operator defined by:*

$$S_\mu f = \int_{\mathcal{X}} k(x,\cdot) f(x)\,\mathrm{d}\mu(x).$$

*Under the assumption that $\forall \mu \in \mathcal{P}_2(\mathcal{X})$, $\int_{\mathcal{X}} k(x,x)\,\mathrm{d}\mu(x) < \infty$, then, $\mathcal{H} \subset L^2(\mu)$ (proof in A.4).*

They also defined the inclusion $\iota : L^2(\mu) \to \mathcal{H}$ and its adjoint $\iota^* : \mathcal{H} \to L^2(\mu) = S_\mu$. Finally, they defined $P_\mu = \iota S_\mu$. Thanks to these operators, we now have that:

$$\langle f, \iota g\rangle_{L^2(\mu)} = \langle \iota^* f, g\rangle_{\mathcal{H}} = \langle S_\mu f, g\rangle_{\mathcal{H}},\ \forall f,g \in L^2(\mu)\times\mathcal{H}.$$

This allows to use proprieties of the scalar product of $\mathcal{H}$ for functions defined in $L^2(\mu)$ and to show that, if $k$ is also in the Stein class of $\mu$ (see A.5):

$$P_\mu \nabla \log\frac{\mu}{\pi}(\cdot) = -\phi^*(\cdot). \tag{7}$$

### 3.3 Convergence of rates for continuous time SVGD

In this setting, we consider the SVGD as a gradient flow, where $\mu_t$ is a function of time i.e. when $\gamma \to 0$ in the SVGD iteration (6).

**Definition 4** (Stein Fisher information)**.** *Let $\mu \in \mathcal{P}_2(\mathcal{X})$. The Stein Fisher information of $\mu$ relative to $\pi$ is defined as follows:*

$$I_{Stein}(\mu|\pi) = \left\| S_\mu \nabla \log \frac{\mu}{\pi} \right\|_{\mathcal{H}}^2.$$

*Note that $I_{Stein}(\mu|\pi)$ is the square of the optimum value of the Kernelized Stein Discrepancy defined in* (5)*.*

The authors proved the following proposition:

**Proposition 1.** *The time-derivative (or dissipation) of the* KL *divergence between $\mu_t$ and $\pi$ is*

$$\frac{\partial \mathrm{KL}(\mu_t||\pi)}{\partial t} = -I_{Stein}(\mu_t|\pi). \tag{8}$$

We provide a complete proof in A.6.

Using this proposition, the authors proved the following convergence rate for the average of $I_{Stein}(\mu|\pi)$ over time:

$$\forall t, \min_{0 \le s \le t} I_{Stein}(\mu_s|\pi) \le \frac{1}{t} \int_0^t I_{Stein}(\mu_s|\pi)\, \mathrm{d}s \le \frac{\mathrm{KL}(\mu_0||\pi)}{t}. \tag{9}$$

(It can be easily shown by integrating (8)). However, for the convergence of $I_{Stein}(\mu_t|\pi)$ to be fast, $\pi$ must satisfy the Stein log-Sobolev inequality:

**Definition 5** (Stein log-Sobolev inequality)**.** *Let $\lambda > 0$. We say $\pi$ satisfies the Stein log-Sobolev inequality if:*

$$\mathrm{KL}(\mu||\pi) \le \frac{1}{2\lambda} I_{Stein}(\mu|\pi).$$

This inequality holds if, for example, $\pi$ has exponential tails and the derivative of $k$ increases at most at a polynomial rate. E.g. $\pi$ is a Mixture of Gaussians and $k$ the RBF kernel.
Assuming this inequality holds for $\pi$, and by using Proposition 1 and the Gronwall's lemma, one can show that the KL divergence between $\mu_t$ and $\pi$ exponentially converges to zero (complete proof in A.7):

$$\mathrm{KL}(\mu_t||\pi) \le e^{-2\lambda t}\, \mathrm{KL}(\mu_0||\pi). \tag{10}$$

This last result is very interesting as it creates a direct link between the convergence of $\mathrm{KL}(\mu_t||\pi)$ and the convergence of $I_{Stein}(\mu_t|\pi)$, showing that the iterative process of SVGD minimizes the KL divergence between $\mu_t$ and $\pi$ exponentially fast, assuming $\pi$ satisfies the Stein log-Sobolev inequality.

### 3.4 SVGD in discrete time

We go back to the original setting of SVGD, where $\mu_n$ is a discrete time function, as defined in (6).

The authors defined the following mild assumptions:

- **(A1)**: $\exists B > 0$ such that $\forall x \in \mathcal{X}$:

$$\|k(x, \cdot)\|_{\mathcal{H}_0} \le B \text{ and } \|\nabla k(x, \cdot)\|_{\mathcal{H}} \le B;$$

- **(A2)** the Hessian $H_V$ of $V = \log \pi$ is well-defined and $\exists M > 0$ such that $\|H_V\|_{op} \le M$:
- **(A3)**: $\exists C > 0$ such that $I_{Stein}(\mu_n||\pi) < C$ for all $n$.

With these conditions satisfied, the authors were able to show the following descent lemma:

**Lemma 1** (Descent lemma for SVGD in discrete time)**.** *Let $\alpha > 1$ and $\gamma \leq \frac{\alpha-1}{\alpha B C^{\frac{1}{2}}}$. Then, for all $n \geq 0$:*

$$\mathrm{KL}(\mu_{n+1}||\pi) - \mathrm{KL}(\mu_n||\pi) \leq -\gamma\left(1 - \gamma\frac{(\alpha^2 + M)B^2}{2}\right) I_{Stein}(\mu_n||\pi).$$

A descent lemma has already been proved before (Liu [2017]), but the authors proved it using differential calculus in the Wasserstein space, showing a more direct link between the descent lemma and the Wasserstein gradient flow: $v_t \triangleq -P_{\mu_t}\nabla \log \frac{\mu_t}{\pi}$. This lemma also implies the convergence for the average of $I_{Stein}(\mu|\pi)$ defined in (9), but for discrete time (replacing the integral by a sum).

### 3.5 Finite particle setting

Finally, the authors proved a convergence bounds between $\mu_n$ and its equivalent in the finite particle setting. In practice, when implementing SVGD, one starts with $N$ particles such that $X_i \sim \mu_0$ for $i \in \{1, \dots, N\}$. Then, at each iteration $n$, SVGD computes the new particles $X_i^{n+1}$ as follows:

$$X_i^{n+1} = X_i^n - \gamma P_{\hat{\mu}_n} \nabla \log\left(\frac{\hat{\mu}_n}{\pi}\right)(X_i^n), \tag{11}$$

where $\hat{\mu}_n = \frac{1}{N}\sum_{i=1}^N \delta_{X_i^n}$ is the empirical distribution of the particles. Under some Lipschitz assumptions, the following proposition holds:

**Proposition 2.** *Let $n > 0$ and $T > 0$. Let $\mu_n$ and $\hat{\mu}_n$ defined in* (6) *and* (11) *respectively. Then, for any $0 \leq n \leq \frac{T}{\gamma}$:*

$$\mathbb{E}\big[\mathbb{W}_2^2(\mu_n, \hat{\mu}_n)\big] \leq \frac{1}{2}\left(\frac{1}{\sqrt{N}}\sqrt{var(\mu_0)}e^{LT}\right)\big(e^{2LT} - 1\big), \tag{12}$$

*where $L$ is a constant depending on $\pi$ and $k$.*

This last result connects the usual implementation of SVGD that is in the finite particle setting with the infinite setting. It allows to ensure that the theoretical results showed above asymptotically hold in practice, w.r.t. the number of particles $N$.
It is a first indication that, with enough particles, the implementation the SVGD algorithm should be able to minimize the KL divergence between $\mu_n$ and $\pi$.

## 4 Experiments

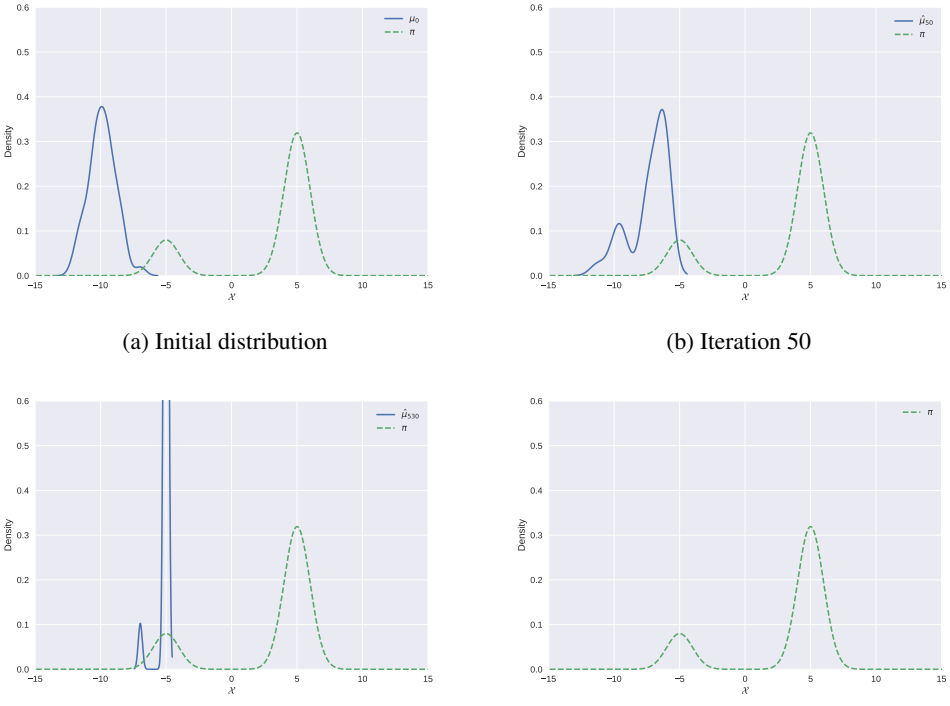
To assess the performance of the SVGD algorithm and the theoretical results, the authors performed an experiment on a 1D Gaussian mixture model. They initialized $100$ particles following a Gaussian distribution centered on $-10$ and with a variance of $1$. Then, they used the SVGD algorithm to minimize the KL divergence between the empirical distribution of the particles and a Gaussian mixture model with two modes. They also empirically verified that the inequality (9) holds, which seems to be the case in their example. They used the code provided in the original paper (Liu and Wang [2016]).

We decided to make a similar experiment but using our own code. Indeed, the original code is rather complex and implements many features that does not seem to be explicitly detailed in the paper. Therefore, we have implemented the SVGD algorithm only with the information provided in the studied paper (Korba et al. [2020]). We update the particles using (11) and we use PyTorch to compute the gradients of the kernel and $\log \pi$. We also wanted to verify that $\mathrm{KL}(\hat{\mu}_n||\pi)$ exponentially decreases, as shows (10). To do so, we made two experiments with different particles distributions. Both are Gaussian distributions, the first one is the same as the one used in the studied paper, and the second one is centered on $0$ and with a variance of $0.3$. $\pi$ is a Gaussian mixture model with two modes centered on $-5$ and $5$, with weights respectively $1/5$ and $4/5$, and with a variance of $1$. The others hyperparameters are detailed in Table 1.

For the first experiment, the empirical distribution does not succeed to imitate $\pi$. Indeed, the algorithm get stuck in a local minimum, making $\hat{\mu}_t$ only follow the first modes of $\pi$, until it

becomes a Dirac distribution centered on $-5$. This behavior is illustrated in Figure 1, where one can see that, at first, the particles are updated in order to get closer to $\pi$, as expected. But after a few iterations, as soon as the particles are close enough to the first mode of $\pi$, the algorithm does not foresee the second mode and get stuck in a local minimum (as one can see with Figure 2). However, the KL divergence decreases exponentially, until it reaches the local minimum. This is illustrated in Figure 3, where we empirically set $\lambda = 0.0008$. As (12) suggests, use more particles should solve the issue, but it would require too much of it to be computationally feasible in practice.

On the other hand, the second experiment is more successful. Indeed, the particules are distributed following a Gaussian distribution with a small variance around $0$, which allows the algorithm to take into account both mode of $\pi$. This is illustrated in Figure 4. The KL divergence also decreases exponentially, as shown in Figure 5, with $\lambda = 0.001$.




(a) Initial distribution

(b) Iteration 50

(c) Iteration 530

(d) Iteration 1000 ($\delta$ distribution not visible)

Figure 1: Initial distribution and several iterations of the SVGD algorithm of the first experiment. One can see that the algorithm get stuck in a local minimum, making $\hat{\mu}_t$ only follow the first modes of $\pi$, until it becomes a Dirac distribution centered on $-5$.

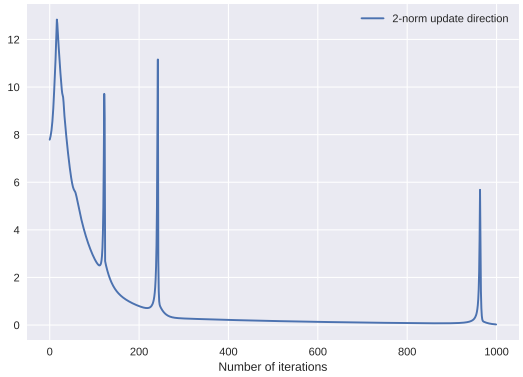



Figure 2: 2-norm of the update direction of the particles for the first experiment. It quickly converges to $0$, corroborating the fact that the algorithm get stuck in a local minimum. Spikes happen when particles "fall" in a mode.

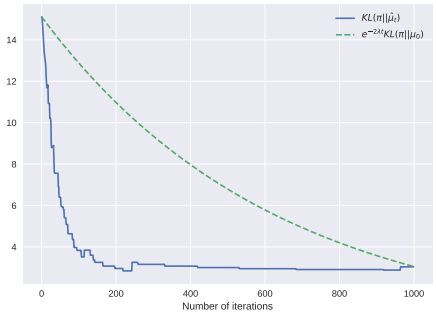
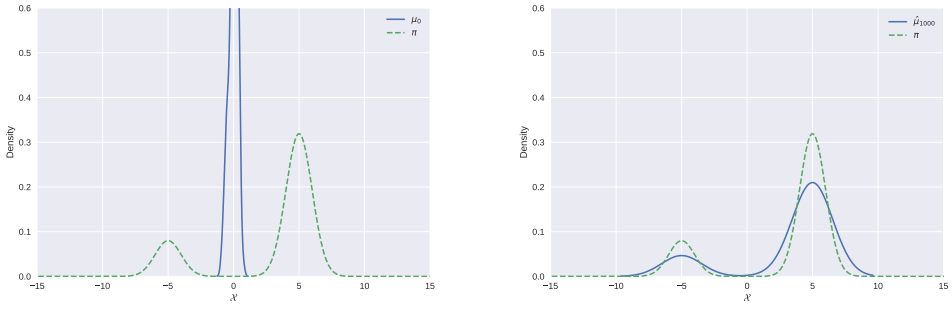



Figure 3: Exponential decrease of the KL divergence over time for the first experiment. $\lambda = 0.0008$.




(a) Initial distribution

(b) Iteration 1000

Figure 4: Initial distribution and last iteration of the SVGD algorithm of the second experiment. One can see that the algorithm is able to take into account both modes of $\pi$.

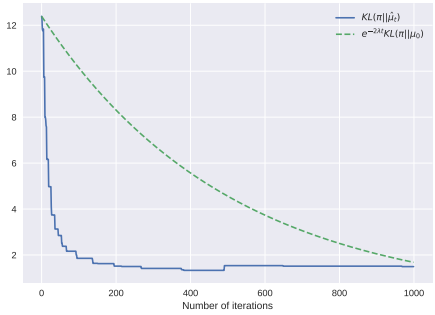



Figure 5: Exponential decrease of the KL divergence over time for the second experiment. $\lambda = 0.001$.

| | |
|---|---|
| $\pi$ | Mix Gaussian |
| N | 100 |
| $\gamma$ | 0.1 |
| $k$ | RBF kernel |
| # iter | 1000 |

Table 1: Hyperparameters used for the SVGD experiments.

## 5 Discussions

We will here discuss more about Korba et al. [2020] itself rather than on the SVGD. To us, a few problems appear which make the paper less understandable for non-expert reseachers on the subject. First of all, the necessary background on optimal transport and functional analysis (especially on the notations) can be a barrier to understanding the ideas of the paper. About the notations, there are many differences between Korba et al. [2020] and the original paper for SVGD Liu and Wang [2016]. Also, both papers base their background in optimal transport on books (Villani [2003] & Villani [2009]), which has even different notations. Thus, the workload to understand which notation correspond to which one is quite high.
Also, even though the abstract from Korba et al. [2020] tries to cover what the paper is about, we found it difficult to really understand where the authors want to bring us reading the paper, as the preliminaries and the necessary background on SVGD take in fact more than half of the paper. Yet, one absolutely needs to read Liu and Wang [2016] and Liu [2017] to fully understand the paper's contributions.
Some misleading typos took us a while to convince ourselves that they are actual errors and not just a misunderstanding of the paper, as we are not experts in the field. For example, in Equation (8), the authors wrote $\lim_{\|x\|\to\infty} k(x,x)\pi(x) = 0$ instead of $\lim_{\|x\|\to\infty} k(x,x)\mu(x) = 0$.
Finally, even though the experiments are given in annex, they link their it with a GitHub repository which is not easy to understand at all, and therefore is not reproducible. Also, it is based on the code from Liu and Wang [2016], which does not describe properly the steps in the code.
Overall, this is a nice theoretical paper giving useful insights of SVGD for the future. On the other hand, it is hard to understand for people with lighter background in state-of-the-art bayesian inference.

## 6 Conclusion

Overall, SVGD appears to be a competitive method for Bayesian inference. Korba et al. [2020] allows us to understand better the theory behind SVGD, providing new convergence rates and a first intuition on the convergence of the implementation of the SVGD. However, its properties are not as well known as Langevin Monte Carlo dynamics yet, which is its principal competitor. In the next few years, we can arguably suppose that SVGD dynamics will be understood even better,

and replacing Langevin-type algorithms in some research problems, such as black-box variational inference and GANs for instance (see Chu et al. [2020]).

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## A Proofs

### A.1 Proof of (1)

*Proof.*

$$
\begin{aligned}
\mathbb{E}_{x\sim\mu}[\mathcal{A}_\mu\phi(x)] &= \int_{\mathcal{X}} \big(\nabla \log \mu(\cdot)^\top \phi(\cdot) + \nabla\cdot\phi(\cdot)\big)\mu(x)\,\mathrm{d}x \\
&= \int_{\mathcal{X}} \nabla \log \mu(\cdot)^\top \phi(\cdot)\mu(x)\,\mathrm{d}x + \int_{\mathcal{X}} \nabla\cdot\phi(\cdot)\mu(x)\,\mathrm{d}x \\
&= \int_{\mathcal{X}} \nabla \log \mu(\cdot)^\top \phi(\cdot)\mu(x)\,\mathrm{d}x + \int_{\mathcal{X}} \sum_{k=1}^{d} \frac{\partial \phi_k}{\partial x_k}\mu(x)\,\mathrm{d}x \\
&= \int_{\mathcal{X}} \nabla \log \mu(\cdot)^\top \phi(\cdot)\mu(x)\,\mathrm{d}x + \sum_{k=1}^{d}\left(\int_{\partial X} (\pi(x)\phi_k(x))\cdot n\,\mathrm{d}n - \int_{\mathcal{X}} \frac{\partial \mu(x)}{\partial x_k}\phi_k(x)\,\mathrm{d}x\right) \\
&= \int_{\mathcal{X}} \nabla \log \mu(\cdot)^\top \phi(\cdot)\mu(x)\,\mathrm{d}x - \int_{\mathcal{X}} \sum_{k=1}^{d} \frac{\partial \mu(x)}{\partial x_k}\phi_k(x)\,\mathrm{d}x \\
&= \int_{\mathcal{X}} \mu(x)\sum_{k=1}^{d} \frac{\partial \log \mu(x)}{\partial x_k}\phi_k(x) - \mu(x)\sum_{k=1}^{d} \frac{\partial \log \mu(x)}{\partial x_k}\phi_k(x)\,\mathrm{d}x \quad \text{(log trick)} \\
&= 0.
\end{aligned}
$$

■

### A.2 Proof of (5)

*Proof.* We first need to prove that

$$\mathbb{E}_{x\sim\mu}[\mathcal{A}_\pi f(x)] = \langle f, \phi^* \rangle_{\mathcal{H}},\ \forall f \in \mathcal{H}:$$

$$\begin{aligned}
\langle f, \phi^* \rangle_{\mathcal{H}} &= \sum_{l=1}^{d} \Big\langle f^{(l)}, \mathbb{E}_{x\sim\mu}\Big[k(x,\cdot)\nabla \log \pi(x)^{(l)} + \nabla k(x,\cdot)^{(l)}\Big]\Big\rangle_{\mathcal{H}^0} \\
&= \mathbb{E}_{x\sim\mu}\left[\sum_{l=1}^{d} \Big\langle f^{(l)}, k(x,\cdot)\nabla \log \pi(x)^{(l)} + \nabla k(x,\cdot)^{(l)}\Big\rangle_{\mathcal{H}^0}\right] \\
&= \mathbb{E}_{x\sim\mu}\left[\sum_{l=1}^{d} \nabla \log \pi(x)^{(l)} \Big\langle f^{(l)}, k(x,\cdot)\Big\rangle_{\mathcal{H}^0} + \Big\langle f^{(l)}, \nabla k(x,\cdot)^{(l)}\Big\rangle_{\mathcal{H}^0}\right] \\
&= \mathbb{E}_{x\sim\mu}\left[\sum_{l=1}^{d} \nabla \log \pi(x)^{(l)} f^{(l)}(x) + \nabla_{x_l} f(x)^{(l)}\right] \text{ (see Zhou [2008])} \\
&= \mathbb{E}_{x\sim\mu}\big[\nabla \log \pi(x)^\top f(x) + \nabla \cdot f(x)\big] \\
&= \mathbb{E}_{x\sim\mu}[\mathcal{A}_\pi f(x)].
\end{aligned}$$

Moreover, $\langle f, \phi* \rangle_{\mathcal{H}} \leq \|f\|_{\mathcal{H}} \|\phi^*\|_{\mathcal{H}}$. Thus,

$$\mathbb{S}(\mu, \pi) = \max_{f\in\mathcal{H}} \{\mathbb{E}_{x\sim\mu}[\mathcal{A}_\pi f(x)] = \langle f, \phi^* \rangle_{\mathcal{H}},\ s.t.\ \|f\|_{\mathcal{H}} \leq 1\} \leq \|\phi^*\|_{\mathcal{H}}.$$

Let $f = \frac{\phi^*}{\|\phi^*\|_{\mathcal{H}}}$, then $\|f\|_{\mathcal{H}} = 1$ and

$$\mathbb{E}_{x\sim\mu}[\mathcal{A}_\pi \phi(x)] = \langle f, \phi^* \rangle_{\mathcal{H}} = \|\phi^*\|_{\mathcal{H}},$$

ending the proof. ■

### A.3 Proof that $\mathbb{E}_{x\sim\mu}[\mathcal{A}_\pi \phi(x)]$ measures the disperancy between $\mu$ and $\pi$

*Proof.*

$$\begin{aligned}
\mathbb{E}_{x\sim\mu}[\mathcal{A}_\pi \phi(x)] &= \int_{\mathcal{X}} \big(\nabla \log \pi(x)^\top \phi(x) + \nabla \cdot \phi(x)\big)\mu(x)\,\mathrm{d}x \\
&= \int_{\mathcal{X}} \nabla \log \pi(x)^\top \phi(x)\mu(x)\,\mathrm{d}x + \sum_{k=1}^{d}\left(\mathcal{R}_k - \int_{\mathcal{X}} \frac{\partial \mu(x)}{\partial x_k}\phi_k(x)\,\mathrm{d}x\right) \\
&= \sum_{k=1}^{d} \mathcal{R}_k + \int_{\mathcal{X}} \mu(x) \sum_{k=1}^{d} \frac{\partial \log \pi(x)}{\partial x_k}\phi_k(x) - \mu(x)\sum_{k=1}^{d}\frac{\partial \log \mu(x)}{\partial x_k}\phi_k(x)\,\mathrm{d}x \quad \text{(log trick)} \\
&= \sum_{k=1}^{d} \mathcal{R}_k + \sum_{k=1}^{d}[\mu(x)\phi_k(x)]_{\mathcal{X}} + \int_{\mathcal{X}} \mu(x)\left[\sum_{k=1}^{d}\phi_k(x)\left(\frac{\partial \log \pi(x)}{\partial x_k} - \frac{\partial \log \mu(x)}{\partial x_k}\right)\right]\mathrm{d}x \\
&= \sum_{k=1}^{d} \mathcal{R}_k + \sum_{k=1}^{d}[\mu(x)\phi_k(x)]_{\mathcal{X}} + \int_{\mathcal{X}} \mu(x)\left[\sum_{k=1}^{d}\phi_k(x)\left(\frac{\partial \log \frac{\pi(x)}{\mu(x)}}{\partial x_k}\right)\right]\mathrm{d}x.
\end{aligned}$$

■

### A.4 Proof of $\mathcal{H} \subset L^2(\mu)$ (Definition 3)

*Proof.* We want to prove that, $\forall f \in \mathcal{H}, \forall \mu \in \mathcal{P}_2(\mathcal{X})$, $\int_{\mathcal{X}} f(x)^2 \, \mathrm{d}\mu(x) < \infty$.

$$\begin{aligned}
\int_{\mathcal{X}} f(x)^2 \, \mathrm{d}\mu(x) &= \int_{\mathcal{X}} \sum_{l=1}^{d} \Big\langle f^{(l)}, k(x, \cdot) \Big\rangle_{\mathcal{H}_0}^2 \, \mathrm{d}\mu(x) \\
&\leq \sum_{l=1}^{d} \int_{\mathcal{X}} \left\| f^{(l)} \right\|_{\mathcal{H}_0}^2 \|k(x, \cdot)\|_{\mathcal{H}_0}^2 \, \mathrm{d}\mu(x) \text{ (by C.S)} \\
&= \sum_{l=1}^{d} \left\| f^{(l)} \right\|_{\mathcal{H}_0}^2 \int_{\mathcal{X}} \|k(x, \cdot)\|_{\mathcal{H}_0}^2 \, \mathrm{d}\mu(x) \\
&= \sum_{l=1}^{d} \left\| f^{(l)} \right\|_{\mathcal{H}_0}^2 \int_{\mathcal{X}} \langle k(x, \cdot), k(x, \cdot) \rangle_{\mathcal{H}_0} \, \mathrm{d}\mu(x) \\
&= \sum_{l=1}^{d} \left\| f^{(l)} \right\|_{\mathcal{H}_0}^2 \int_{\mathcal{X}} k(x, x) \, \mathrm{d}\mu(x) \text{ (by reproducing propriety)} \\
&< \infty, \text{ as } \int_{\mathcal{X}} k(x, x) \, \mathrm{d}\mu(x) < \infty.
\end{aligned}$$

■

### A.5 Proof of (7)

*Proof.* Let $k$ in the Stein class of $\mu$. Thus:

$$\begin{aligned}
P_\mu \nabla \log \frac{\mu}{\pi}(\cdot) &= \int_{\mathcal{X}} k(x, \cdot) \nabla \log \mu(x) \, \mathrm{d}\mu(x) - \int_{\mathcal{X}} k(x, \cdot) \nabla \log \pi(x) \, \mathrm{d}\mu(x) \\
&= \int_{\mathcal{X}} k(x, \cdot) \nabla \mu(x) \, \mathrm{d}x - \int_{\mathcal{X}} k(x, \cdot) \nabla \log \pi(x) \, \mathrm{d}\mu(x) \\
&= -\int_{\mathcal{X}} \nabla k(x, \cdot) \, \mathrm{d}\mu(x) - \int_{\mathcal{X}} k(x, \cdot) \nabla \log \pi(x) \, \mathrm{d}\mu(x) \\
&= -\int_{\mathcal{X}} k(x, \cdot) \nabla \log \pi(x) + \nabla k(x, \cdot) \, \mathrm{d}\mu(x) \\
&= -\phi^*(\cdot).
\end{aligned} \tag{13}$$

■

### A.6 Proof of Proposition 1

*Proof.* The time derivative of the KL writes:

$$\begin{aligned}
\frac{\partial KL(\mu_t \| \pi)}{\partial t} &= \frac{\partial}{\partial t} \int_{\mathcal{X}} \log \frac{\mu_t(x)}{\pi(x)} \, \mathrm{d}\mu_t(x) \\
&= \int_{\mathcal{X}} \frac{\partial \mu_t(x)}{\partial t} \log \frac{\mu_t(x)}{\pi(x)} \, \mathrm{d}x + \int_{\mathcal{X}} \mu_t(x) \frac{\partial \log \frac{\mu_t(x)}{\pi(x)}}{\partial t} \, \mathrm{d}x \\
&= \int_{\mathcal{X}} \frac{\partial \mu_t(x)}{\partial t} \log \frac{\mu_t(x)}{\pi(x)} \, \mathrm{d}x + \int_{\mathcal{X}} \mu_t(x) \frac{\partial \log \mu_t(x)}{\partial t} \, \mathrm{d}x \\
&= \int_{\mathcal{X}} \frac{\partial \mu_t(x)}{\partial t} \log \frac{\mu_t(x)}{\pi(x)} \, \mathrm{d}x + \int_{\mathcal{X}} \mu_t(x) \frac{\frac{\partial \mu_t(x)}{\partial t}}{\mu_t(x)} \, \mathrm{d}x \\
&= \int_{\mathcal{X}} \frac{\partial \mu_t(x)}{\partial t} \log \frac{\mu_t(x)}{\pi(x)} \, \mathrm{d}x + \int_{\mathcal{X}} \frac{\partial \mu_t(x)}{\partial t} \, \mathrm{d}x \\
&= \int_{\mathcal{X}} \frac{\partial \mu_t(x)}{\partial t} \log \frac{\mu_t(x)}{\pi(x)} \, \mathrm{d}x, \Big( \mu_t \text{ is a probability measure, so } \forall t, \int_{\mathcal{X}} \mathrm{d}\mu_t(x) = 1 \Big).
\end{aligned}$$

Furthermore, as $\mu_t$ satisfies the continuity equation (2) where $v_t = -P_{\mu_t} \nabla \log \frac{\mu}{\pi}$, we have:

$$\begin{aligned}
\frac{\partial KL(\mu_t \| \pi)}{\partial t} &= -\int_{\mathcal{X}} \nabla \cdot (\mu_t(x) v_t(x)) \log \frac{\mu_t(x)}{\pi(x)} \, \mathrm{d}x \\
&= -\sum_{l=1}^{d} \int_{\mathcal{X}} \frac{\partial \mu_t(x) v_t(x)}{\partial x_l} \log \frac{\mu_t(x)}{\pi(x)} \, \mathrm{d}x \\
&= -\int_{\partial X} \left( \mu_t(x) v_t(x) \log \frac{\mu_t(x)}{\pi(x)} \right) \cdot n \, \mathrm{d}n + \sum_{l=1}^{d} \int_{\mathcal{X}} \mu_t(x) v_t(x) \frac{\partial \log \frac{\mu_t(x)}{\pi(x)}}{\partial x_l} \, \mathrm{d}x
\end{aligned}$$

The first term cancels as probability densities tends to zero on the boundary.

$$\begin{aligned}
&= \int_{\mathcal{X}} v_t(x) \nabla \log \frac{\mu_t(x)}{\pi(x)} \, \mathrm{d}\mu_t(x) \\
&= \left\langle v_t, \nabla \log \frac{\mu_t}{\pi} \right\rangle_{L^2(\mu_t)} \\
&= \left\langle \iota^* v_t, \iota^* \nabla \log \frac{\mu_t}{\pi} \right\rangle_{\mathcal{H}} \\
&= \left\langle -\iota^* \iota S_{\mu_t} \nabla \log \frac{\mu_t}{\pi}, S_{\mu_t} \nabla \log \frac{\mu_t}{\pi} \right\rangle_{\mathcal{H}} \\
&= -\left\| S_{\mu_t} \nabla \log \frac{\mu_t}{\pi} \right\|_{\mathcal{H}}^2.
\end{aligned}$$

■

### A.7 Proof of (10)

*Proof.* Assume that $\pi$ satisfies the Stein log-Sobolev inequality. We have

$$\begin{aligned}
\mathrm{KL}(\mu_t || \pi) &\leq \frac{1}{2\lambda} I_{Stein}(\mu_t || \pi) \\
-I_{Stein}(\mu_t || \pi) &\leq -2\lambda \mathrm{KL}(\mu_t || \pi).
\end{aligned}$$

Now, using Proposition 1:

$$\begin{aligned}
\frac{\partial \mathrm{KL}(\mu_t || \pi)}{\partial t} &\leq -2\lambda \mathrm{KL}(\mu_t || \pi) \\
\mathrm{KL}(\mu_t || \pi) &\leq \mathrm{KL}(\mu_0 || \pi) \exp\left( \int_0^t -2\lambda \, \mathrm{d}s \right) \text{ (Gronwall's lemma)} \\
\mathrm{KL}(\mu_t || \pi) &\leq e^{-2\lambda t} \mathrm{KL}(\mu_0 || \pi).
\end{aligned}$$

■