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Stein Variational Gradient Descent: Main ideas

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1 Introduction

In this paper we will contextualize and describe the article Korba et al. [2020]. The goal is to be able to sample from an unknown distribution π thanks to an iterative procedure that is called Stein Variational Gradient Descent (SVGD). It was first introduced by Liu and Wang [2016]. Starting from an initial distribution μ_0, this algorithm can be seen as a gradient descent in the Wasserstein space of distributions $\mathcal{P}_2(\mathcal{X})$, with $\mathcal{X} \in \mathbb{R}^d$. **TODO METTRE NOS CONTRIBS**

2 SVGD Context (Liu and Wang [2016])

In all what follows, $\mathcal{X} = \mathbb{R}^d$.
We fix here π an objective distributions from which we want to sample, and an initial distribution from which we know how to sample μ_0.

2.1 Notations

We will denote as earlier by $\mathcal{P}_2(\mathcal{X})$ the Wasserstein space of distributions i.e. the set of distributions such that $\int ||x||^2 d\mu(x) < \infty$. We assume the objective distribution π lives in $\mathcal{P}_2(\mathcal{X})$, and define the Kullback-Liebler divergence between π_1 and π_2 by

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

Let $\mathcal{A}_\pi$ the Stein Operator defined by $\forall \phi \in \mathcal{H}, \forall x \in \mathcal{X}, \mathcal{A}_\pi \phi(x) = \nabla \log \pi(x)\phi(x)^T + \nabla \cdot \phi(x)$, for some $\mathcal{H}$ we will precise later on.
We define the Stein class of π the subset of functions ϕ such that $\lim_{||x|| \longrightarrow \infty} \phi(x)\pi(x) = 0$. Note that for every function in the Stein class of π, 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 μ 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 ϕ.
The gradient of $\mathrm{KL}(\cdot||\pi)$ at μ in $\mathcal{P}_2(\mathcal{X})$ is given by $\nabla_{W_2}\mathrm{KL}(\mu||\pi) = \nabla \log(\frac{\mu}{\pi})$. The idea behind SVGD is to iteratively follow the descent direction given by $\nabla_{W_2}\mathrm{KL}(\cdot||\pi)$.
Finally, for $\phi : \mathbb{R}^d \longrightarrow \mathbb{R}^d$, we denote by $||\phi||_{op}$ the operator norm.

2.2 Context

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

$$\mu_{[T]} = \mu_\#(I + \gamma\phi) \tag{2}$$

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 μ is not in the Stein class of π, one can show that $\mathbb{E}_{x\sim\mu}[\mathcal{A}_\pi \phi(x)] > 0$, increasing w.r.t. the difference between μ and π (Proof here: 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. A question now raises: how to choose $\mathcal{H}$?

Choice of $\mathcal{H}$ In all papers, $\mathcal{H}$ is chosen as the product RKHS of $\mathcal{X}$. We will quickly explain here why so.
Let $\mathcal{H}_0$ be a RKHS with a kernel $k(x,x')$ in the Stein class of π. Let $\mathcal{H} = (\mathcal{H}_0^{(1)}, \dots, \mathcal{H}_0^{(d)})$. The KSD maximizes ϕ in the unit ball of $\mathcal{H}$. 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 ϕ^* is in the Stein class of π as k is. Moreover, $\mathbb{S}(\mu,\pi) = \|\phi^*\|_{\mathcal{H}}$. (Complete proof in A.2)

Return 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 $\{\phi \in \mathcal{H}, ||\phi||^2_{op} \leq \mathbb{S}(\mu,\pi)\}$, the one we will keep for our gradient descent is the one minimizing the gradient of KL, which writes ϕ^* as showed just earlier.
The Stein Variational Gradient Descent (SVGD) algorithm consists in an iterative procedure where one apply successive transformations to an initial density μ_0 following the trajectory ϕ^* that minimizes the gradient of the Kullback-Leibler divergence:

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

3 Non-asymptotic analysis of SVGD

In their paper (Korba et al. [2020]), under assumptions, the authors provide 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 μ and ν 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 μ and ν is defined by

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

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 $T_t = I + \phi(t)$. 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, μ_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
They start by defining operators on the RKHS.

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

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

They also make the assumption that $\int_{\mathcal{X}} k(x,x)\, \mathrm{d}\mu(x) < \infty$, $\forall \mu \in \mathcal{P}_2(\mathcal{X})$, which implies $\mathcal{H} \subset L^2(\mu)$ (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 μ (see A.5):

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

3.3 Convergence of rates for continuous time SVGD

Definition 4 (Stein Fisher information). *Let $\mu \in \mathcal{P}_2(\mathcal{X})$. The Stein Fisher information of μ relative to π 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 μ_t and π is*

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

We provide a more 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:

$$\forall t, \min_{0 \le s \le t} I_{Stein}(\mu_s|\pi) \le \frac{1}{t}\int_0^t I_{Stein}(\mu_s|\pi)\, \mathrm{d}s \le \frac{\mathrm{KL}(\mu_0||\pi)}{t}. \tag{8}$$

(It can be easily shown by integrating A.6). However, for the convergence of $I_{Stein}(\mu_t|\pi)$ to be fast, π must satisfy the Stein log-Sobolev inequality:

Definition 5 (Stein log-Sobolev inequality). *Let $\lambda > 0$. We say π 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, π has exponential tails and the derivative of k increases at most at a polynomial rate. E.g. π is a Mixture of Gaussians and k the RBF kernel.
Assuming this inequality holds for π, and by using Proposition 1 and the Gronwall's lemma, one can show that the KL divergence between μ_t and π exponentially converges to zero (complete proof in A.7):

$$\mathrm{KL}(\mu_t||\pi) \le e^{-2\lambda t}\, \mathrm{KL}(\mu_0||\pi). \tag{9}$$

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 μ_t and π exponentially fast, assuming π satisfies the Stein log-Sobolev inequality.

3.4 SVGD in discrete time

The authors defined the following mild assumptions:

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

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

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

With these condition 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: $v_t = -P_{\mu_t}\nabla \log \frac{\mu_t}{\pi}$. This lemma also implies the convergence for the average of $I_{Stein}(\mu|\pi)$ defined in (8), but for discrete time (replacing the integral by a sum).

4 Experiences

5 Discussions

Bibliography

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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

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

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

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 μ and π

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 $\mathcal{H} \subset L^2(\mu)$ (3)

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

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

∎

A.5 Proof of 7

Proof. Let k in the Stein class of μ. Thus:

$$\begin{aligned}
P_\mu \nabla \log \frac{\mu}{\pi}(\cdot) &= \int_{\mathcal{X}} k(x,\cdot)\nabla \log \mu(x)\,\mathrm{d}\mu(x) - \int_{\mathcal{X}} k(x,\cdot)\nabla \log \pi(x)\,\mathrm{d}\mu(x) \\
&= \int_{\mathcal{X}} k(x,\cdot)\nabla \mu(x)\,\mathrm{d}x - \int_{\mathcal{X}} k(x,\cdot)\nabla \log \pi(x)\,\mathrm{d}\mu(x) \\
&= -\int_{\mathcal{X}} \nabla k(x,\cdot)\,\mathrm{d}\mu(x) - \int_{\mathcal{X}} k(x,\cdot)\nabla \log \pi(x)\,\mathrm{d}\mu(x) \\
&= -\int_{\mathcal{X}} k(x,\cdot)\nabla \log \pi(x) + \nabla k(x,\cdot)\,\mathrm{d}\mu(x) \\
&= -\phi^*(\cdot).
\end{aligned} \tag{10}$$

■

A.6 Proof of Proposition 1

Proof. The time derivative of the KL writes:

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

Furthermore, as μ_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.

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

■

A.7 Proof of 9

Proof. Assume that π 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:

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

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