Limitations of the Theory of Sampling with Kernelized Wasserstein Gradient Flows

Anna Korba
CREST, ENSAE, Institut Polytechnique de Paris

ICBINB seminar series

Outline

Sampling

Sampling problem: Sample (=generate new examples) from a target distribution π over $\mathbb{R}^d$, given some information on π.

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Two different settings:

1. π's density w.r.t. Lebesgue measure is known up to an intractable normalisation constant Z :

$$\pi(x) = \frac{\tilde{\pi}(x)}{Z}, \quad \tilde{\pi} \text{ known, } Z \text{ unknown.}$$

   Example: Bayesian inference.

2. one has access to a set of samples of π : $x_1, \ldots, x_n \sim \pi$.

   Example: (some) Neural networks, generative modelling (GANS...).

We'll focus on the first setting.

Bayesian inference

Let $\mathcal{D} = (w_i, y_i)_{i=1}^{m}$ a dataset of labelled examples $(w_i, y_i) \overset{i.i.d.}{\sim} P_{\text{data}}$.
Assume an underlying model parametrized by θ, e.g. :

$$y = g(w, \theta) + \epsilon, \quad \epsilon \sim \mathcal{N}(0, I)$$

Goal: learn the best distribution over θ to fit the data.

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1. Compute the Likelihood:

$$p(\mathcal{D}|\theta) = \prod_{i=1}^{m} p(y_i|\theta, w_i) \propto \exp\left(-\frac{1}{2}\sum_{i=1}^{m} \|y_i - g(w_i, \theta)\|^2\right).$$

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$$\theta \sim p, \quad \text{e.g. } p(\theta) \propto \exp\left(-\frac{\|\theta\|^2}{2}\right).$$
3. Bayes' rule yields:
$$\pi(\theta) := p(\theta|\mathcal{D}) = \frac{p(\mathcal{D}|\theta)p(\theta)}{Z} \quad Z = \int_{\mathbb{R}^d} p(\mathcal{D}|\theta)p(\theta)d\theta$$
i.e. $\pi(\theta) \propto \exp\left(-V(\theta)\right), \quad V(\theta) = \frac{1}{2}\sum_{i=1}^m \|y_i - g(w_i, \theta)\|^2 + \frac{\|\theta\|^2}{2}.$

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- prediction for a new input w:

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Given a discrete approximation $\mu_n = \frac{1}{n} \sum_{j=1}^{n} \delta_{\theta_j}$ of π:

$$y_{pred} \approx \frac{1}{n} \sum_{j=1}^{n} g(w, \theta_j).$$

Question: how can we build μ_n?

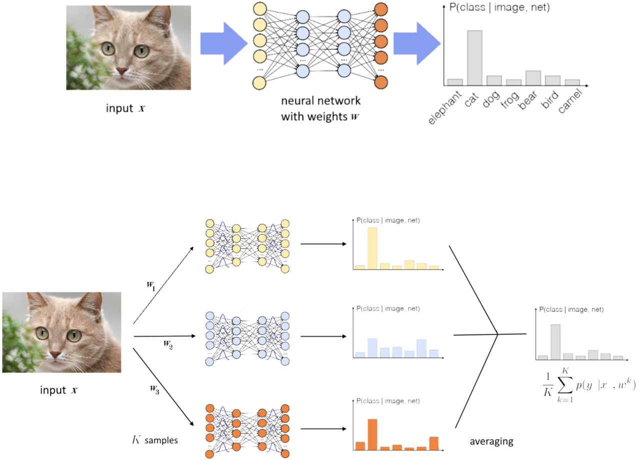

Figure: Ensembling on deep neural networks.

Sampling as optimisation

Notice that

$$\pi = \underset{\mu \in \mathcal{P}(\mathbb{R}^d)}{\operatorname{argmin}} \mathrm{KL}(\mu|\pi), \quad \mathrm{KL}(\mu|\pi) = \begin{cases} \int_{\mathbb{R}^d} \log\left(\frac{\mu}{\pi}(x)\right) d\mu(x) & \text{if } \mu \ll \pi \\ +\infty & \text{else.} \end{cases}$$

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Two ways to produce an approximation μ_n:

1. Markov Chain Monte Carlo (MCMC) methods: generate a Markov chain whose law converges to $\pi \propto \exp(-V)$

   Example: discretize an overdamped Langevin diffusion

   $$d\theta_t = -\nabla V(\theta_t) + \sqrt{2} dB_t \Longrightarrow \theta_{l+1} = \theta_l - \gamma \nabla V(\theta_l) + \sqrt{2\gamma}\epsilon_l, \ \epsilon_l \sim \mathcal{N}(0, I_d)$$

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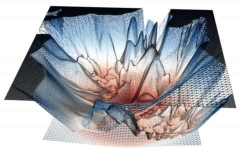
2. Interacting particle systems, e.g. by considering other metrics or functionals

Difficult cases (in practice and in theory)

Recall that

$$\pi(\theta) \propto \exp\left(-V(\theta)\right), \quad V(\theta) = \underbrace{\sum_{i=1}^{m} \|y_i - g(w_i, \theta)\|^2}_{\text{loss}} + \frac{\|\theta\|^2}{2}.$$

- if V is convex (e.g. $g(w, \theta) = \langle w, \theta \rangle$) many sampling methods are known to work quite well
- but if its not (e.g. $g(w, \theta)$ is a neural network), the situation is much more delicate



A highly nonconvex loss surface, as is common in deep neural nets. From `https://www.telesens.co/2019/01/16/neural-network-loss-visualization`.

Sampling as optimization over distributions

Assume that $\pi \in \mathcal{P}_2(\mathbb{R}^d) = \left\{\mu \in \mathcal{P}(\mathbb{R}^d), \int \|x\|^2 d\mu(x) < \infty\right\}$.

The sampling task can be recast as an optimization problem:

$$\pi = \operatorname*{argmin}_{\mu \in \mathcal{P}_2(\mathbb{R}^d)} D(\mu|\pi) := \mathcal{F}(\mu),$$

where D is a **dissimilarity functional.**

Starting from an initial distribution $\mu_0 \in \mathcal{P}_2(\mathbb{R}^d)$, one can then consider the **Wasserstein gradient flow** of $\mathcal{F}$ over $\mathcal{P}_2(\mathbb{R}^d)$ to transport μ_0 to π.

Outline

Euclidean gradient flow and continuity equation

Let $V : \mathbb{R}^d \to \mathbb{R}$. Consider the gradient flow

$$x'(t) = -\nabla V(x(t))$$

and assume $x(0)$ random with density μ_0. What is the dynamics of the density μ_t of $x(t)$? Let $\phi : \mathbb{R}^d \to \mathbb{R}$ a test function.

$$\frac{d}{dt}\mathbb{E}(\phi(x(t))) = -\int \langle \nabla\phi, \nabla V\rangle \mu_t(x)dx = \int \phi(x)\boldsymbol{\nabla}\cdot(\mu_t\nabla V)(x)dx,$$

and

$$\frac{d}{dt}\mathbb{E}(\phi(x(t))) = \int \phi(x)\frac{\partial\mu_t}{\partial t}(x)dx.$$

Therefore,

$$\frac{\partial\mu_t}{\partial t} = \boldsymbol{\nabla}\cdot(\mu_t\nabla V).$$

Setting - The Wasserstein space

Let $\mathcal{P}_2(\mathbb{R}^d)$ denote the space of probability measures on $\mathbb{R}^d$ with finite second moments, i.e.

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$\mathcal{P}_2(\mathbb{R}^d)$ is endowed with the Wasserstein-2 distance from **Optimal transport** :

$$W_2^2(\nu, \mu) = \inf_{s \in \Gamma(\nu,\mu)} \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x - y\|^2 \, ds(x, y) \qquad \forall \nu, \mu \in \mathcal{P}_2(\mathbb{R}^d)$$

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Can also be written:

$$W_2^2(\nu,\mu) = \inf_{(\rho_t, v_t)_{t\in[0,1]}} \left\{ \int_0^1 \|v_t(x)\|^2_{L^2(\rho_t)} dt(x) : \frac{\partial \rho_t}{\partial t} = \nabla \cdot (\rho_t v_t), \rho_0 = \nu, \rho_1 = \mu \right\}$$

Definition : Let $\mu \in \mathcal{P}_2(\mathbb{R}^d)$, $T : \mathbb{R}^d \to \mathbb{R}^d$. The pushforward measure $T_{\#}\mu$ is characterized by:

- $\forall$ B meas. set, $T_{\#}\mu(B) = \mu(T^{-1}(B))$
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(Brenier's theorem): Let $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$ s.t. $\mu \ll Leb$. Then, there exists $T_\mu^\nu : \mathbb{R}^d \to \mathbb{R}^d$ such that

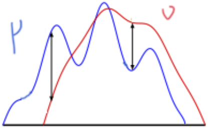
- $T^\nu_{\mu\#}\mu = \nu$
- $W_2^2(\mu, \nu) = \|I - T_\mu^\nu\|^2_{L_2(\mu)} = \int \|x - T_\mu^\nu(x)\|^2 d\mu(x)$

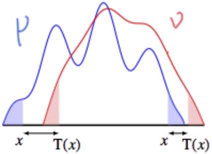
W_2 geodesics?

$\rho(0) = \mu, \rho(1) = \nu.$

$\rho(t) = ((1-t)I + tT_\mu^\nu)_\#\mu$

$\neq \rho(t) = \underbrace{(1-t)\mu + t\nu}_{\text{mixture}}$





Wasserstein gradient flows (WGF) [Ambrosio et al., 2008]

The first variation of $\mu \mapsto \mathcal{F}(\mu)$ evaluated at $\mu \in \mathcal{P}$, if it exists, is the unique function $\frac{\partial \mathcal{F}(\mu)}{\partial \mu} : \mathbb{R}^d \to \mathbb{R}$ s. t. for any $\mu, \mu' \in \mathcal{P}$:

$$\lim_{\epsilon \to 0} \frac{1}{\epsilon} \left[\mathcal{F}(\mu + \epsilon(\mu' - \mu)) - \mathcal{F}(\mu) \right] = \int_{\mathbb{R}^d} \frac{\partial \mathcal{F}(\mu)}{\partial \mu}(x)(d\mu' - d\mu)(x).$$

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The family $\mu : [0, \infty] \to \mathcal{P}, t \mapsto \mu_t$ satisfies a Wasserstein gradient flow of $\mathcal{F}$ if distributionally:

$$\boxed{\frac{\partial \mu_t}{\partial t} = \boldsymbol{\nabla} \cdot \left(\mu_t \nabla_{W_2} \mathcal{F}(\mu_t) \right),}$$

where $\nabla_{W_2} \mathcal{F}(\mu) := \nabla \frac{\partial \mathcal{F}(\mu)}{\partial \mu} \in L^2(\mu)$ denotes the Wasserstein gradient of $\mathcal{F}$.

WGF of Free energies

In particular, if the functional $\mathcal{F}$ is a free energy:

$$\mathcal{F}(\mu) = \underbrace{\int H(\mu(x))dx}_{\text{internal energy}} + \underbrace{\int V(x)d\mu(x)}_{\text{potential energy}} + \underbrace{\int W(x,y)d\mu(x)d\mu(y)}_{\text{interaction energy}}$$

$$\text{Then : } \frac{\partial \mu_t}{\partial t} = \boldsymbol{\nabla} \cdot \left(\mu_t \underbrace{\nabla (H'(\mu_t) + V + W * \mu_t)}_{\nabla_{W_2}\mathcal{F}(\mu)} \right). \qquad (1)$$

For instance, if $H = 0$ then (1) rules the density μ_t of particles $x_t \in \mathbb{R}^d$ driven by :

$$\frac{dx_t}{dt} = -\nabla V(x_t) - \int_{\mathbb{R}^d} \nabla W(x, x_t) d\mu_t(x)$$

$\mu_t = Law(x_t)$.

(Some) unbiased time discretizations

For a step-size $\gamma > 0$:

1. Backward (expensive) [Jordan et al., 1998] :

$$\mu_{l+1} = \mathsf{JKO}_{\gamma \mathcal{F}}(\mu_l)$$

$$\text{where } \mathsf{JKO}_{\gamma \mathcal{F}}(\mu_l) = \underset{\mu \in \mathcal{P}_2(\mathbb{R}^d)}{\mathrm{argmin}} \left\{ \mathcal{F}(\mu) + \frac{1}{2\gamma} W_2^2(\mu, \mu_l) \right\}.$$

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2. Forward (cheap) :

$$\mu_{l+1} = exp_{\mu_l}(-\gamma \nabla_{W_2}\mathcal{F}(\mu_l)) = \left(I - \gamma \nabla_{W_2}\mathcal{F}(\mu_l)\right)_{\#} \mu_l$$

where $exp_\mu : L^2(\mu) \to \mathcal{P}, \phi \mapsto (I + \phi)_{\#}\mu$,
and which corresponds in $\mathbb{R}^d$ to:

$$X_{l+1} = X_l - \gamma \nabla_{W_2}\mathcal{F}(\mu_l)(X_l) \sim \mu_{l+1}, \text{ if } X_l \sim \mu_l.$$

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Idea: replace it by the **empirical measure** of a system of n interacting particles:

$$X_0^1, \ldots, X_0^n \sim \mu_0$$

and for $j = 1, \ldots, n$:

$$\begin{aligned} X_{l+1}^j &= X_l^j - \gamma \nabla_{W_2} \mathcal{F}(\hat{\mu}_l)(X_l^j) \\ &= X_l^j - \frac{1}{\gamma} \left[\nabla V(X_l^j) + \frac{1}{n} \sum_{i=1}^n \nabla W(X_l^j, X_l^i) \right] \end{aligned}$$

where $\hat{\mu}_l = \frac{1}{n} \sum_{i=1}^n \delta_{X_l^i}$.

Outline

Goal: Sample from a target distribution π, whose density w.r.t. Lebesgue measure is known up to an intractable normalisation constant Z :

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Remember that

$$\pi = \operatorname{argmin} \mathrm{KL}(\mu|\pi), \quad \mathrm{KL}(\mu|\pi) = \int \log\Big(\frac{\mu}{\pi}\Big) d\mu \text{ if } \mu \ll \pi$$

and that we can consider the Forward time discretisation:

$$x_{l+1} = x_l - \gamma \nabla_{W_2} \mathrm{KL}(\mu_l|\pi)(x_l), \quad x_l \sim \mu_l,$$

where $\nabla_{W_2} \mathrm{KL}(\mu_l|\pi) = \nabla \frac{\partial \mathrm{KL}(\mu_l|\pi)}{\partial \mu} = \nabla \log\big(\frac{\mu_l}{\pi}(.)\big)$.

Problem: μ_l, hence $\nabla \log(\mu_l)$ is unknown and has to be estimated from a set of particles.

Background on kernels and RKHS [Steinwart and Christmann, 2008]

- Let $k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ a positive, semi-definite kernel
  $((k(x_i, x_j)_{i=1}^n)$ is a p.s.d. matrix for all $x_1, \ldots, x_n \in \mathbb{R}^d)$

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$$\mathcal{H}_k = \overline{\left\{ \sum_{i=1}^{m} \alpha_i k(\cdot, x_i);\ m \in \mathbb{N};\ \alpha_1, \ldots, \alpha_m \in \mathbb{R};\ x_1, \ldots, x_m \in \mathbb{R}^d \right\}}$$

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- assume $\int_{\mathbb{R}^d \times \mathbb{R}^d} k(x, x) d\mu(x) < \infty$ for any $\mu \in \mathcal{P}(\mathbb{R}^d)$,$\Longrightarrow \mathcal{H}_k \subset L^2(\mu)$.

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    $k(x, y) = (c + \|x - y\|)^{-\beta}$ with $\beta \in]0, 1[$
- $\mathcal{H}_k$ its corresponding RKHS (Reproducing Kernel Hilbert Space):

$$\mathcal{H}_k = \overline{\left\{ \sum_{i=1}^{m} \alpha_i k(\cdot, x_i);\ m \in \mathbb{N};\ \alpha_1, \dots, \alpha_m \in \mathbb{R};\ x_1, \dots, x_m \in \mathbb{R}^d \right\}}$$

- $\mathcal{H}_k$ is a Hilbert space with inner product $\langle ., . \rangle_{\mathcal{H}_k}$ and norm $\|.\|_{\mathcal{H}_k}$.
- assume $\int_{\mathbb{R}^d \times \mathbb{R}^d} k(x, x) d\mu(x) < \infty$ for any $\mu \in \mathcal{P}(\mathbb{R}^d)$,$\Longrightarrow \mathcal{H}_k \subset L^2(\mu)$.
- It satisfies the reproducing property:

$$\forall \quad f \in \mathcal{H}_k,\ x \in \mathbb{R}^d, \quad f(x) = \langle f, k(x, .) \rangle_{\mathcal{H}_k}.$$

Stein Variational Gradient Descent [Liu and Wang, 2016]

Consider the following metric depending on k

$$W_k^2(\mu_0, \mu_1) = \inf_{\mu, v} \left\{ \int_0^1 \|v_t(x)\|^2_{\mathcal{H}_k^d} dt(x) : \frac{\partial \mu_t}{\partial t} = \boldsymbol{\nabla} \cdot (\mu_t v_t) \right\}.$$

Then, the W_k gradient flow of the KL writes as the PDE [Liu, 2017], [Duncan et al., 2019]:

$$\frac{\partial \mu_t}{\partial t} + \boldsymbol{\nabla} \cdot \left(\mu_t P_{\mu_t} \nabla \log \left(\frac{\mu_t}{\pi} \right) \right) = 0, \quad P_\mu : f \mapsto \int k(x, .) f(x) d\mu(x).$$

It converges to $\pi \propto \exp(-V)$ under mild conditions on k and if V grows at most polynomially [Lu et al., 2019].

SVGD algorithm

SVGD trick: applying the kernel integral operator to the W_2 gradient of $\mathrm{KL}(\cdot|\pi)$ leads to

$$
\begin{aligned}
P_{\mu}\nabla\log\left(\frac{\mu}{\pi}\right)(\cdot) &= \int \nabla\log\left(\frac{\mu}{\pi}\right)(x)k(x,.)d\mu(x)\\
&= \int -\nabla\log(\pi(x))k(x,.)d\mu(x) + \int \nabla(\mu(x))k(x,.)dx\\
&\overset{I.P.P.}{=} -\int [\nabla\log\pi(x)k(x,\cdot) + \nabla_x k(x,\cdot)]d\mu(x),
\end{aligned}
$$

under appropriate boundary conditions on k and π, e.g. $\lim_{\|x\|\to\infty} k(x,\cdot)\pi(x) \to 0$.

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Algorithm : Starting from n i.i.d. samples $(X_0^i)_{i=1,\dots,n} \sim \mu_0$, SVGD algorithm updates the n particles as follows :

$$
\begin{aligned}
X_{l+1}^i &= X_l^i - \gamma \left[\frac{1}{n} \sum_{j=1}^n k(X_l^i, X_l^j) \nabla_{X_l^j} \log \pi(X_l^j) + \nabla_{X_l^j} k(X_l^j, X_l^i) \right] \\
&= X_l^i - \gamma P_{\mu_l^n} \nabla \log\left(\frac{\mu_l^n}{\pi}\right)(X_l^i), \quad \text{with } \mu_l^n = \frac{1}{n}\sum_{j=1}^n \delta_{X_l^j}
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SVGD in practice

- more than 600 citations for [Liu and Wang, 2016]
- Relative empirical success in Bayesian inference and more recently deep ensembles
- It can suffer for multimodal distributions [Wenliang and Kanagawa, 2020], underestimate the target variance [Ba et al., 2021], but still can be very efficient on difficult sampling problems.

		AUROC(H)	AUROC(MD)	Accuracy	H_o/H_t	MD_o/MD_t	ECE	NLL
FashionMNIST	**Deep ensemble [38]**	0.958±0.001	0.975±0.001	91.122±0.013	6.257±0.005	6.394±0.001	**0.012±0.001**	0.129±0.001
	SVGD [46]	0.960±0.001	0.973±0.001	91.134±0.024	6.315±0.019	6.395±0.018	0.014±0.001	0.127±0.001
	f-SVGD [67]	0.956±0.001	0.975±0.001	89.884±0.015	5.652±0.009	6.531±0.005	0.013±0.001	0.150±0.001
	kde-WGD (ours)	0.960±0.001	0.970±0.001	91.238±0.019	6.587±0.019	6.379±0.018	0.014±0.001	0.128±0.001
	sge-WGD (ours)	0.960±0.001	0.970±0.001	**91.312±0.016**	6.562±0.007	6.363±0.009	**0.012±0.001**	0.128±0.001
	ssge-WGD (ours)	0.968±0.001	0.979±0.001	91.198±0.024	6.522±0.009	6.610±0.012	**0.012±0.001**	0.130±0.001
	kde-fWGD (ours)	**0.971±0.001**	**0.980±0.001**	91.260±0.011	7.079±0.016	6.887±0.015	0.015±0.001	**0.125±0.001**
	sge-fWGD (ours)	0.969±0.001	0.978±0.001	91.192±0.013	7.076±0.004	6.900±0.005	0.015±0.001	**0.125±0.001**
	ssge-fWGD (ours)	**0.971±0.001**	**0.980±0.001**	91.240±0.022	**7.129±0.006**	**6.951±0.005**	0.016±0.001	**0.124±0.001**
CIFAR10	**Deep ensemble [38]**	**0.843±0.004**	0.736±0.005	85.552±0.076	**2.244±0.006**	1.667±0.008	0.049±0.001	0.277±0.001
	SVGD [46]	0.825±0.001	0.710±0.002	85.142±0.017	2.106±0.003	1.567±0.004	0.052±0.001	0.287±0.001
	fSVGD [67]	0.783±0.001	0.712±0.001	84.510±0.031	1.968±0.004	1.624±0.003	0.049±0.001	0.292±0.001
	kde-WGD (ours)	0.838±0.001	0.735±0.004	**85.904±0.030**	2.205±0.003	1.661±0.008	0.053±0.001	**0.276±0.001**
	sge-WGD (ours)	0.837±0.003	0.725±0.004	85.792±0.035	2.214±0.010	1.634±0.004	0.051±0.001	**0.275±0.001**
	ssge-WGD (ours)	0.832±0.003	0.731±0.005	85.638±0.038	2.182±0.015	1.655±0.001	0.049±0.001	**0.276±0.001**
	kde-fWGD (ours)	0.791±0.002	**0.758±0.002**	84.888±0.030	1.970±0.004	**1.749±0.005**	**0.044±0.001**	0.282±0.001
	sge-fWGD (ours)	0.795±0.001	0.754±0.002	84.766±0.060	1.984±0.003	1.729±0.002	0.047±0.001	0.288±0.001
	ssge-fWGD (ours)	0.792±0.002	0.752±0.002	84.762±0.034	1.970±0.006	1.723±0.005	0.046±0.001	0.286±0.001

From *Repulsive Deep Ensembles are Bayesian. F. D'angelo, V. Fortuin. Conference on Neural Information Processing Systems (NeurIPS 2021).*

Continuous-time dynamics of SVGD

$$\frac{\partial \mu_t}{\partial t} + \boldsymbol{\nabla} \cdot \left(\mu_t P_{\mu_t} \nabla \log \left(\frac{\mu_t}{\pi} \right) \right) = 0, \quad P_\mu : f \mapsto \int k(x,.) f(x) d\mu(x).$$

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How fast the KL decreases along SVGD dynamics? Apply the chain rule in the Wasserstein space:

$$\frac{d\, \mathrm{KL}(\mu_t|\pi)}{dt} = \left\langle V_t, \nabla \log \left(\frac{\mu_t}{\pi} \right) \right\rangle_{L^2(\mu_t)} = - \underbrace{\left\| P_{\mu_t} \nabla \log \left(\frac{\mu_t}{\pi} \right) \right\|^2_{\mathcal{H}_k}}_{\mathrm{KSD}^2(\mu_t|\pi)} \leq 0.$$

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On the r.h.s. we have the squared **Kernel Stein discrepancy (KSD)** [Chwialkowski et al., 2016] or **Stein Fisher information** of μ_t relative to π:

$$\begin{aligned} \left\| P_{\mu,k} \nabla \log\left(\frac{\mu}{\pi} \right) \right\|^2_{\mathcal{H}_k} &= \langle P_{\mu,k} \nabla \log\left(\frac{\mu}{\pi} \right), P_{\mu,k} \nabla \log\left(\frac{\mu}{\pi} \right) \rangle_{\mathcal{H}_k} \\ &= \iint \nabla \log\left(\frac{\mu}{\pi}(x) \right) \nabla \log\left(\frac{\mu}{\pi}(y) \right) k(x,y) d\mu(x) d\mu(y). \end{aligned}$$

Recall that the Fisher divergence is defined as $\|\nabla \log\left(\frac{\mu}{\pi}\right)\|^2_{L^2(\mu)}$.

Exponential decay?

Assume π satisfies the Stein log-Sobolev inequality [Duncan et al., 2019] with constant $\lambda > 0$ if for any μ:

$$\mathrm{KL}(\mu|\pi) \leq \frac{1}{2\lambda} \mathrm{KSD}^2(\mu|\pi).$$

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If it holds, we can conclude with Gronwall's lemma:

$$\frac{d\,\mathrm{KL}(\mu_t|\pi)}{dt} = -\,\mathrm{KSD}^2(\mu_t|\pi) \leq -2\lambda\,\mathrm{KL}(\mu_t|\pi) \Longrightarrow \mathrm{KL}(\mu_t|\pi) \leq e^{-2\lambda t}\,\mathrm{KL}(\mu_0|\pi).$$

When is Stein log-Sobolev satisfied? not so well understood [Duncan et al., 2019]:

- it fails to hold if k is too regular with respect to π (e.g. k bounded, π Gaussian)
- some working examples in dimension 1, open question in greater dimensions...

A descent lemma in discrete time for SVGD [Korba et al., 2020]

Idea: in optimisation, descent lemmas can be shown if the objective function has a bounded Hessian.

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Assume that $\pi \propto \exp(-V)$ where $\|H_V(x)\| \leq M$.
The Hessian of the KL at μ is an operator on $L^2(\mu)$:

$$\langle f, Hess_{\mathrm{KL}(.|\pi)}(\mu) f \rangle_{L^2(\mu)} = \mathbb{E}_{X\sim\mu}\left[\langle f(X), H_V(X) f(X)\rangle + \|Jf(X)\|^2_{HS}\right]$$

and yet, this operator **is not bounded** due to the Jacobian term.

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and yet, this operator **is not bounded** due to the Jacobian term.

However: In the case of SVGD, the descent directions f are restricted to $\mathcal{H}_k$ (bounded functions for bounded k).

Proposition: Assume (boundedness of k and ∇k, H_V and moments on the trajectory), then for γ small enough:

$$\mathrm{KL}(\mu_{l+1}|\pi) - \mathrm{KL}(\mu_l|\pi) \leq -c_\gamma \underbrace{\left\| P_{\mu_l} \nabla \log\left(\frac{\mu_l}{\pi}\right)\right\|^2_{\mathcal{H}_k}}_{\mathrm{KSD}^2(\mu_l|\pi)}.$$

Rates in KSD

Consequence of the descent lemma: for γ small enough,

$$\boxed{\min_{l=1,\dots,L} \mathrm{KSD}^2(\mu_l|\pi) \leq \frac{1}{L}\sum_{l=1}^{L} \mathrm{KSD}^2(\mu_l|\pi) \leq \frac{\mathrm{KL}(\mu_0|\pi)}{c_\gamma L}.}$$

This result does not rely on:

- convexity of V
- nor on Stein log Sobolev inequality
- only on smoothness of V.

in contrast with many convergence results on LMC.

The KSD metrizes convergence for instance when [Gorham and Mackey, 2017]:

- π is distantly dissipative (log concave at infinity, e.g. mixture of Gaussians)
- k is the IMQ kernel defined by $k(x, y) = (c^2 + \|x - y\|_2^2)^\beta$ for $c > 0$ and $\beta \in (-1, 0)$.

Open question 1: Rates in terms of the KL objective?

To obtain rates, one may combine a descent lemma (1) of the form

$$\mathrm{KL}(\mu_{l+1}|\pi) - \mathrm{KL}(\mu_l|\pi) \leq -c_\gamma \left\| S_{\mu_n} \nabla \log\left(\frac{\mu_l}{\pi}\right) \right\|^2_{\mathcal{H}_k}$$

and the Stein log-Sobolev inequality (2) with constant λ:

$$\mathrm{KL}(\mu_{l+1}|\pi) - \mathrm{KL}(\mu_l|\pi) \underbrace{\leq}_{(1)} -c_\gamma \left\| P_{\mu_l} \nabla \log\left(\frac{\mu_n}{\pi}\right) \right\|^2_{\mathcal{H}_k} \underbrace{\leq}_{(2)} -c_\gamma 2\lambda\, \mathrm{KL}(\mu_n|\pi).$$

Iterating this inequality yields $\mathrm{KL}(\mu_l|\pi) \leq (1 - 2c_\gamma \lambda)^l\, \mathrm{KL}(\mu_0|\pi)$.

"Classic" approach in optimization [Karimi et al., 2016] *or in the analysis of LMC.*

Problem: not possible to combine both.

First Experiments

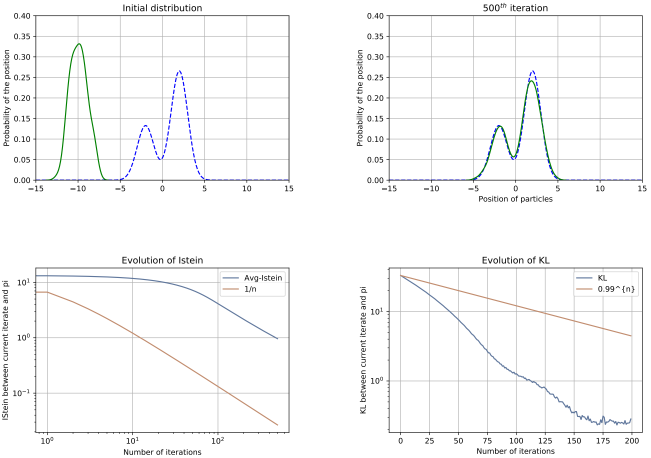

Figure: The particle implementation of the SVGD algorithm illustrates the convergence of $\mathrm{KSD}^2(k \star \mu_l^n|\pi), \mathrm{KL}(k \star \mu_l^n|\pi)$ to 0.

Not possible to combine both....

Given that both the kernel and its derivative are bounded, the equation

$$\int \sum_{i=1}^{d} [(\partial_i V(x))^2 k(x,x) \\ - \partial_i V(x)(\partial_i^1 k(x,x) + \partial_i^2 k(x,x)) + \partial_i^1 \partial_i^2 k(x,x)] d\pi(x) < \infty \quad (2)$$

reduces to a property on V which, as far as we can tell, always holds on $\mathbb{R}^d$...

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reduces to a property on V which, as far as we can tell, always holds on $\mathbb{R}^d$...

and this implies that Stein LSI does not hold [Duncan et al., 2019].

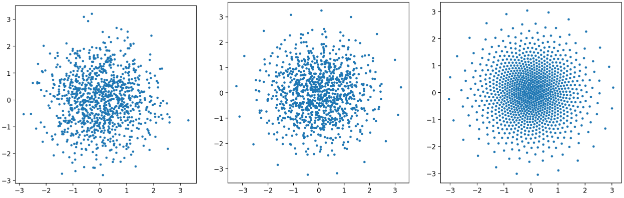
Remark : Equation (2) does not hold for :

- k polynomial of order ≥ 3, and
- π with exploding β moments with $\beta \geq 3$ (ex: a student distribution, which belongs to $\mathcal{P}_2$ the set of distributions with bounded second moment).

Open question 2: SVGD quantisation

The quality of a set of points $(x^1, \dots, x^n)$ can be measured by the integral approximation error:

$$E(x_1, \dots, x_n) = \left| \frac{1}{n} \sum_{i=1}^{n} f(x^i) - \int_{\mathbb{R}^d} f(x) d\pi(x) \right|. \qquad (3)$$



(a) i.i.d. (b) SVGD Gaussian k (c) SVGD Laplace k

For i.i.d. points or MCMC iterates, (3) is of order $n^{-\frac{1}{2}}$. Can we bound (3) for SVGD final states?

Ongoing work with L. Xu and D. Slepcev.

Outline

A lot of problems previously came from the fact that the KL is not defined for discrete measures μ_n. Can we consider functionals that are well-defined for μ_n?

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Remember the Kernel Stein discrepancy of μ relative to π:

$$\mathrm{KSD}^2(\mu|\pi) = \left\| P_{\mu,k} \nabla \log\left(\frac{\mu}{\pi}\right) \right\|^2_{\mathcal{H}_k}, \; P_{\mu,k} : f \mapsto \int f(x)k(x,.)d\mu(x).$$

With several integration by parts we have:

$$\begin{aligned}
&\mathrm{KSD}^2(\mu|\pi) = \left\| P_{\mu,k} \nabla \log\left(\frac{\mu}{\pi}\right) \right\|^2_{\mathcal{H}_k} \\
&= \int \int \nabla \log\left(\frac{\mu}{\pi}(x)\right) \nabla \log\left(\frac{\mu}{\pi}(y)\right) k(x,y) d\mu(x) d\mu(y) \\
&= \iint \nabla \log \pi(x)^T \nabla \log \pi(y) k(x,y) + \nabla \log \pi(x)^T \nabla_2 k(x,y) \\
&\quad + \nabla_1 k(x,y)^T \nabla \log \pi(y) + \boldsymbol{\nabla} \cdot_1 \nabla_2 k(x,y) d\mu(x) d\mu(y) \\
&:= \iint k_\pi(x,y) d\mu(x) d\mu(y).
\end{aligned}$$

can be written in closed-form for discrete measures μ.

KSD Descent - algorithms

We propose two ways to implement KSD Descent:

Algorithm 1 KSD Descent GD

Input: initial particles $(x_0^i)_{i=1}^N \sim \mu_0$, number of iterations M, step-size γ

for $n = 1$ **to** M **do**

$$[x_{n+1}^i]_{i=1}^N = [x_n^i]_{i=1}^N - \frac{2\gamma}{N^2} \sum_{j=1}^N [\nabla_2 k_\pi(x_n^j, x_n^i)]_{i=1}^N,$$

end for

Return: $[x_M^i]_{i=1}^N$.

Algorithm 2 KSD Descent L-BFGS

Input: initial particles $(x_0^i)_{i=1}^N \sim \mu_0$, tolerance tol

Return: $[x_*^i]_{i=1}^N = \text{L-BFGS}(L, \nabla L, [x_0^i]_{i=1}^N, \text{tol})$.

L-BFGS [Liu and Nocedal, 1989] is a quasi Newton algorithm that is faster and more robust than Gradient Descent, and **does not require the choice of step-size!**

L-BFGS

L-BFGS (Limited memory Broyden–Fletcher–Goldfarb–Shanno algorithm) is a quasi-Newton method:

$$x_{n+1} = x_n - \gamma_n B_n^{-1} \nabla L(x_n) := x_n + \gamma_n d_n \tag{4}$$

where B_n^{-1} is a p.s.d. matrix approximating the inverse Hessian at x_n.

Step1. (requires ∇L) It computes a cheap version of d_n based on BFGS recursion:

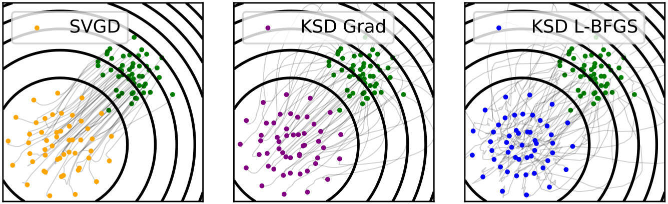
$$B_{n+1}^{-1} = \left(I - \frac{\Delta x_n y_n^T}{y_n^T \Delta x_n}\right) B_n^{-1} \left(I - \frac{y_n \Delta x_n^T}{y_n^T \Delta x_n}\right) + \frac{\Delta x_n \Delta x_n^T}{y_n^T \Delta x_n}$$

$$\text{where} \quad \begin{aligned} \Delta x_n &= x_{n+1} - x_n \\ y_n &= \nabla L(x_{n+1}) - \nabla L(x_n) \end{aligned}$$

Step2. (requires L and ∇L) A line-search is performed to find the best step-size in (4) :

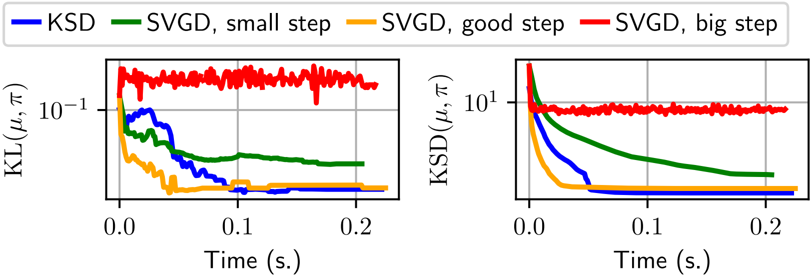
$$\begin{aligned} L(x_n + \gamma_n d_n) &\leq L(x_n) + c_1 \gamma_n \nabla L(x_n)^T d_n \\ \nabla L(x_n + \gamma_n d_n)^T d_n &\geq c_2 \nabla L(x_n)^T d_n \end{aligned}$$

Toy experiments - 2D standard gaussian



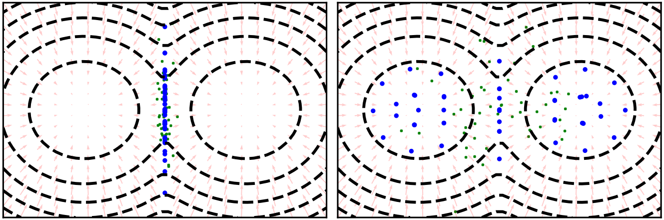
The green points represent the initial positions of the particles.
The light grey curves correspond to their trajectories.

SVGD vs KSD Descent - importance of the step-size



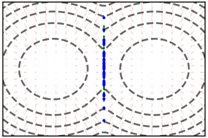
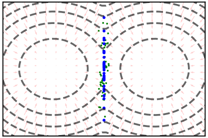
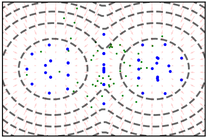
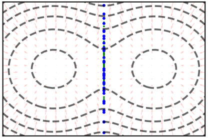
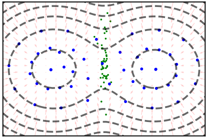
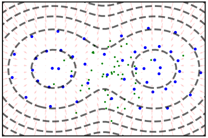
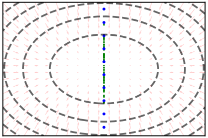
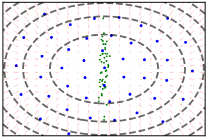
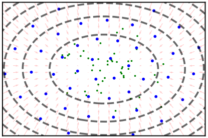
Convergence speed of KSD and SVGD on a Gaussian problem in 1D, with 30 particles.

2D mixture of (isolated) Gaussians - failure cases



The green crosses indicate the initial particle positions
the blue ones are the final positions
The light red arrows correspond to the score directions.

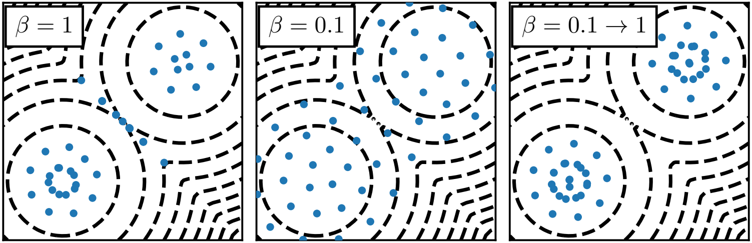
More initializations

Var\Init	on the s.a.	close to s.a.	Gaussian i.i.d. init
0.1			
0.3			
2			

Green crosses : initial particle positions
Blue crosses : final positions

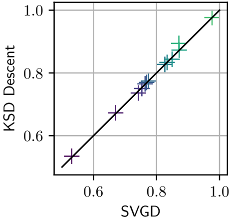
Isolated Gaussian mixture - annealing

Add an inverse temperature variable β : $\pi^{\beta}(x) \propto \exp(-\beta V(x))$, with $0 < \beta \leq 1$ (i.e. multiply the score by β.)

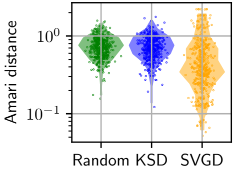


This is a hard problem, even for Langevin diffusions, where tempering strategies also have been proposed [Lee et al., 2018].

Real world experiments (10 particles)

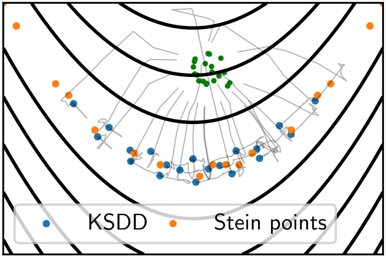


Bayesian logistic regression.
Accuracy of the KSD descent and SVGD for 13 datasets ($d \approx 50$).
Both methods yield similar results. KSD is better by 2% on one dataset.
Hint: convex likelihood.



Bayesian ICA.
Each dot is the Amari distance between an estimated matrix and the true unmixing matrix ($d \leq 8$).
KSD is not better than random.
Hint: highly non-convex likelihood.

So.. when does it work?



Comparison of KSD Descent and Stein points on a “banana” distribution. Green points are the initial points for KSD Descent. Both methods work successfully here, **even though it is not a log-concave distribution.**

We posit that KSD Descent succeeds because **there is no saddle point in the potential.**

Theoretical properties

Stationary measures:

- we show that if a stationary measure μ_∞ is full support, then $\mathcal{F}(\mu_\infty) = 0$.
- however, we also show that if *supp*$(\mu_0) \subset \mathcal{M}$, where $\mathcal{M}$ is a plane of symmetry of π, then for any time t it remains true for μ_t: *supp*$(\mu_t) \subset \mathcal{M}$.

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Explain convergence in the log-concave case? again an open question:

- the KSD is not geodesically convex
- it is not strongly geo convex near the global optimum π
- convergence of the continuous dynamics can be shown with a functional inequality, but which does not hold for discrete measures

First strategy : obtain a functional inequality

How fast $\mathcal{F}(\mu_t)$ decreases along its WGF ?

$$\frac{\partial \mu_t}{\partial t} = \boldsymbol{\nabla} \cdot (\mu_t V_t), \quad V_t = \nabla_{W_2} \mathcal{F}(\mu_t)$$

$$\begin{aligned}
\frac{d\mathcal{F}(\mu_t)}{dt} &= \left\langle V_t, \nabla_{W_2} \mathcal{F}(\mu_t) \right\rangle_{L^2(\mu_t)} \\
&= - \left\| \nabla_{W_2} \mathcal{F}(\mu_t) \right\|^2_{L^2(\mu_t)} \\
&= - \| \mathbb{E}_{x \sim \mu_t}[\nabla_2 k(x,y)] - \mathbb{E}_{x \sim \pi}[\nabla_2 k(x,y)] \|^2_{L^2(\mu_t)} \\
&= - \underbrace{\| \nabla f_{\mu_t,\pi} \|^2_{L_2(\mu_t)}}_{\| f_{\mu_t,\pi} \|_{\dot{H}^{-1}(\mu_t)}}
\end{aligned}$$

where $f_{\mu_t,\pi} = \mathbb{E}_{x \sim \mu_t}[k(x,.)] - \mathbb{E}_{x \sim \pi}[k(x,.)]$.

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&= -\underbrace{\|\nabla f_{\mu_t,\pi}\|^2_{L_2(\mu_t)}}_{\|f_{\mu_t,\pi}\|_{\dot{H}^{-1}(\mu_t)}}
\end{aligned}$$

where $f_{\mu_t,\pi} = \mathbb{E}_{x\sim\mu_t}[k(x,.)] - \mathbb{E}_{x\sim\pi}[k(x,.)]$.

It can be shown that:

$$\|f_{\mu_t,\pi}\|^2_{\mathcal{H}_k} \leq \|f_{\mu_t,\pi}\|_{\dot{H}(\mu_t)} \quad \underbrace{\|\mu_t - \pi\|_{\dot{H}^{-1}(\mu_t)}}_{\sup_{\|g\|^2_{\dot{H}(\mu_t)} \leq 1} |\int g d\mu_t - \int g d\pi|}$$

Hence, if $\|\mu_t - \pi\|_{\dot{H}^{-1}(\mu_t)} \leq C$ for all $t \geq 0$, we have

$$\frac{d\mathcal{F}(\nu_t)}{dt} \leq -C\mathcal{F}(\nu_t)^2, \text{ hence}$$

$$\mathcal{F}(\mu_t) \leq \frac{1}{\mathcal{F}(\mu_0) + 4C^{-1}t}$$

where $\mathcal{F}(\mu_0) = \frac{1}{2}\,\mathrm{MMD}^2(\mu_t, \pi)$.

Problems:

- depends on the whole sequence $(\mu_t)_{t\geq 0}$ (not only π)
- hard to verify in practice
- we observed convergence issues in practice (more for the MMD than the KSD)

Second strategy : geodesic convexity of the KSD?

Let $\psi \in C_c^\infty(\mathbb{R}^d)$ and the path $\rho_t = (I + t\nabla\psi)_\#\mu$ for $t \in [0,1]$.

Define the quadratic form $\operatorname{Hess}_\mu \mathcal{F}(\psi,\psi) := \frac{d^2}{dt^2}\Big|_{t=0} \mathcal{F}(\rho_t)$, which is related to the W_2 **Hessian of $\mathcal{F}$ at μ.**

For $\psi \in C_c^\infty(\mathbb{R}^d)$, we have

$$\begin{aligned}\operatorname{Hess}_\mu \mathcal{F}(\psi,\psi) = \mathbb{E}_{x,y\sim\mu}\left[\nabla\psi(x)^T \nabla_1\nabla_2 k_\pi(x,y)\nabla\psi(y)\right] \\ + \mathbb{E}_{x,y\sim\mu}\left[\nabla\psi(x)^T H_1 k_\pi(x,y)\nabla\psi(x)\right].\end{aligned}$$

The first term is always positive but not the second one.

$\Longrightarrow$ **the KSD is not convex w.r.t. W_2 geodesics.**

Third strategy : curvature near equilibrium?

What happens near equilibrium π? the second term vanishes due to the Stein property of k_π and :

$$\mathrm{Hess}_\pi\, \mathcal{F}(\psi,\psi) = \|S_{\pi,k_\pi}\mathcal{L}_\pi\psi\|^2_{\mathcal{H}_{k_\pi}} \geq 0$$

where

$$\mathcal{L}_\pi : f \mapsto -\Delta f - \langle \nabla \log \pi, \nabla f\rangle_{\mathbb{R}^d}$$

$$S_{\mu,k_\pi} : f \mapsto \int k_\pi(x,.)f(x)d\mu(x) \in \mathcal{H}_{k_\pi} = \overline{\left\{k_\pi(x,.), x \in \mathbb{R}^d\right\}}$$

Question: can we bound from below the Hessian at π by a quadratic form on the tangent space of $\mathcal{P}_2(\mathbb{R}^d)$ at π ($\subset L^2(\pi)$)?

$$\boxed{\|S_{\pi,k_\pi}\mathcal{L}_\pi\psi\|^2_{\mathcal{H}_{k_\pi}} = \mathrm{Hess}_\pi\, \mathcal{F}(\psi,\psi) \geq \lambda\|\nabla\psi\|^2_{L^2(\pi)} \text{ ?}}$$

That would imply exponential decay of $\mathcal{F}$ near π.

Curvature near equilibrium - negative result

The previous inequality

$$\boxed{\|S_{\pi,k_\pi}\mathcal{L}_\pi\psi\|^2_{\mathcal{H}_{k_\pi}} \geq \lambda\|\nabla\psi\|^2_{L^2(\pi)}}$$

- can be seen as a kernelized version of the Poincaré inequality for π :

$$\|\mathcal{L}_\pi\psi\|^2_{L_2(\pi)} \geq \lambda_\pi\|\nabla\psi\|^2_{L_2(\pi)}.$$

- can be written:

$$\langle\psi, P_{\pi,k_\pi}\psi\rangle_{L_2(\pi)} \geq \lambda\langle\psi, \mathcal{L}_\pi^{-1}\psi\rangle_{L_2(\pi)},$$

where $P_{\pi,k_\pi} : L^2(\pi) \to L^2(\pi), f \mapsto \int k_\pi(x,.)f(x)d\pi(x).$

Theorem : Let $\pi \propto e^{-V}$. Assume that $V \in C^2(\mathbb{R}^d)$, ∇V is Lipschitz and $\mathcal{L}_\pi$ has discrete spectrum. Then exponential decay near equilibium does not hold.

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Conclusion

- Mixing kernels and Wasserstein gradient flows enable to design deterministic interacting particle systems
- They can provide a better approximation of the target for a finite number of particles
- Theory does not match practice yet
- Numerics can be improved, via perturbed dynamics, change of geometry...
- Python package to try KSD descent:
  pip install ksddescent
  website: `pierreablin.github.io/ksddescent/`
  It also features pytorch/numpy code for SVGD.

```
>>> import torch
>>> from ksddescent import ksdd_lbfgs
>>> n, p = 50, 2
>>> x0 = torch.rand(n, p)  # start from uniform distribution
>>> score = lambda x: x  # simple score function
>>> x = ksdd_lbfgs(x0, score)  # run the algorithm
```

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