

Sampling with Kernelized Wasserstein Gradient Flows

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Frontiers in kinetic equations for plasmas and collective
behaviour

Outline

Problem and Motivation

Wasserstein Gradient Flows

Part I - Stein Variational Gradient Descent

Part II : Sampling as optimization of the KSD/MMD

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 $\pi : x_1, \dots, x_n \sim \pi$.

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 $(w_i, y_i) \stackrel{i.i.d.}{\sim} P_{\text{data}}$.
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:

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

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3. Bayes' rule yields:

$$\pi(\theta) := p(\theta|\mathcal{D}) = \frac{p(\mathcal{D}|\theta)p(\theta)}{Z} \quad Z = \int_{\mathbb{R}^d} p(\mathcal{D}|\theta)p(\theta)d\theta$$

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

π is needed both for

- ▶ 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 ?

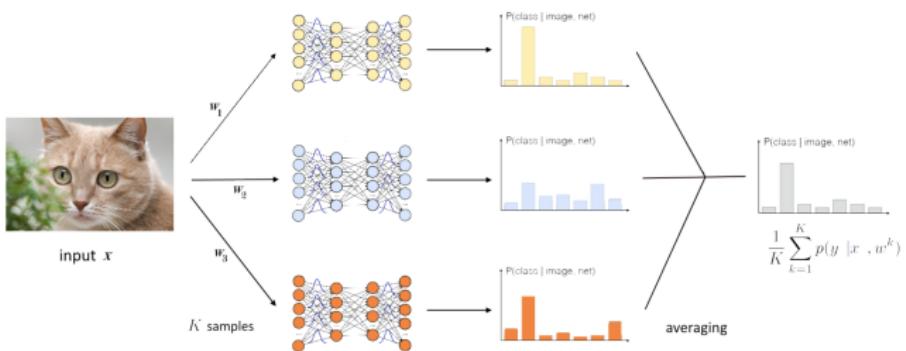
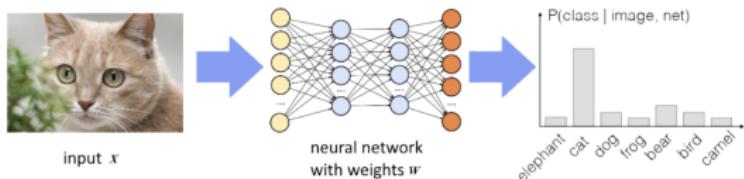


Figure: Ensembling on deep neural networks.

Sampling as optimisation

Notice that

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

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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

$$d\theta_t = -\nabla V(\theta_t) + \sqrt{2}dB_t \implies \theta_{t+1} = \theta_t - \gamma \nabla V(\theta_t) + \sqrt{2\gamma}\epsilon_t, \quad \epsilon_t \sim \mathcal{N}(0, I_d)$$

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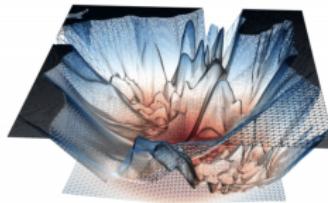
2. Interacting particle systems, e.g. by considering other metrics or functionals

Difficult cases (in practice and in theory)

Recall that

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

- ▶ 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](https://www.telesens.co/2019/01/16/neural-network-loss-visualization).

Sampling as optimization over distributions

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

The sampling task can be recast as an optimization problem:

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

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 .

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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 :

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

where $\Gamma(\nu, \mu)$ is the set of possible couplings between ν and μ .

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

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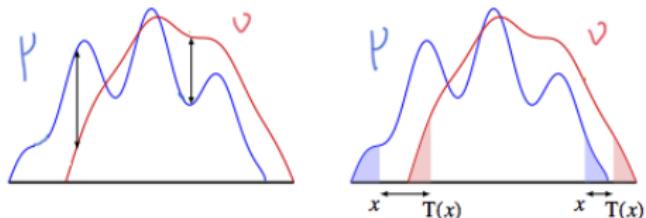
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(Brenier's theorem): Let $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$ s.t. $\mu \ll Leb$. Then, there exists $T_{\mu}^{\nu} : \mathbb{R}^d \rightarrow \mathbb{R}^d$ such that

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

W_2 geodesics?

$$\begin{aligned} \rho(0) &= \mu, \rho(1) = \nu. \\ \rho(t) &= ((1-t)I + tT_{\mu}^{\nu})_{\#}\mu \\ &\neq \rho(t) = \underbrace{(1-t)\mu + t\nu}_{\text{mixture}} \end{aligned}$$



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

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

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

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} .

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

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

WGF of Free energies

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

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

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

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) :

$$\mu_{I+1} = \text{JKO}_{\gamma\mathcal{F}}(\mu_I)$$

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

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2. Forward (cheap) :

$$\mu_{I+1} = \exp_{\mu_I}(-\gamma \nabla_{W_2} \mathcal{F}(\mu_I)) = (I - \gamma \nabla_{W_2} \mathcal{F}(\mu_I)) \# \mu_I$$

where $\exp_\mu : L^2(\mu) \rightarrow \mathcal{P}, \phi \mapsto (I + \phi)_\# \mu,$

and which corresponds in \mathbb{R}^d to:

$$X_{I+1} = X_I - \gamma \nabla_{W_2} \mathcal{F}(\mu_I)(X_I) \sim \mu_{I+1}, \text{ if } X_I \sim \mu_I.$$

Space discretization - Interacting particle system

If the vector field depends on the density of the particles at time I , replace μ_I by the empirical measure of a system of n interacting particles:

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

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

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

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

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

Remember that

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

and that we can consider the Forward time discretisation:

$$x_{I+1} = x_I - \gamma \nabla_{W_2} \text{KL}(\mu_I|\pi)(x_I), \quad x_I \sim \mu_I,$$

$$\text{where } \nabla_{W_2} \text{KL}(\mu_I|\pi) = \nabla \frac{\partial \text{KL}(\mu_I|\pi)}{\partial \mu} = \nabla \log\left(\frac{\mu_I}{\pi}(\cdot)\right).$$

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

Background on kernels and RKHS

[Steinwart and Christmann, 2008]

- ▶ Let $k : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ a positive, semi-definite kernel
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- ▶ \mathcal{H}_k its corresponding RKHS (Reproducing Kernel Hilbert Space):

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- ▶ It satisfies the reproducing property:

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

Stein Variational Gradient Descent [Liu and Wang, 2016]

Consider the following metric depending on k

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

Then, the W_k gradient flow of the KL writes as the PDE

[Liu, 2017], [Duncan et al., 2019]:

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

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 $\text{KL}(\cdot|\pi)$ leads to

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

under appropriate boundary conditions on k and π , e.g.

$$\lim_{\|x\| \rightarrow \infty} k(x, \cdot) \pi(x) \rightarrow 0.$$

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

under appropriate boundary conditions on k and π , e.g.

$$\lim_{\|x\| \rightarrow \infty} k(x, \cdot) \pi(x) \rightarrow 0.$$

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 :

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

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SVGD in practice

- ▶ Relative empirical success in Bayesian inference, but other machine learning tasks e.g. reinforcement learning
- ▶ It can suffer for multimodal distributions , underestimate the target variance, 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
	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
	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
	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
	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
	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
	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
	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
CIFAR10	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
	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
	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
	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
	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
	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
	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
	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
	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
	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

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

Continuous-time dynamics of SVGD

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

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

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

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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 :

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

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

Exponential decay?

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

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

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

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 $L^2(\mu)$:

$$\langle f, \text{Hess}_{\text{KL}(\cdot|\pi)}(\mu)f \rangle_{L^2(\mu)} = \mathbb{E}_{X \sim \mu} [\langle f(X), H_V(X)f(X) \rangle + \|Jf(X)\|_{HS}^2]$$

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

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

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

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

Proof of a descent lemma for GD of a smooth function

Gradient descent for $V : \mathbb{R}^d \rightarrow \mathbb{R}$ a $C^2(\mathbb{R}^d)$ s.t. $\|H_V(x)\| \leq M$ for any x .

$$x_{n+1} = x_n - \gamma \nabla V(x_n).$$

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Denote $x(t) = x_n - t \nabla V(x_n)$ and $\varphi(t) = V(x(t))$. Using Taylor expansion :

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

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Since $(\ddot{x}(t) = 0)$:

$$\varphi'(0) = \langle \nabla V(x(0)), \dot{x}(0) \rangle = \langle \nabla V(x(0)), -\nabla V(x_n) \rangle = -\|\nabla V(x_n)\|^2,$$

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we have

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

$$V(x_{n+1}) - V(x_n) \leq -\gamma \left(1 - \frac{M\gamma}{2}\right) \|\nabla V(x_n)\|^2.$$

Sketch of proof - 1

Fix $n \geq 0$. Denote $g = P_{\mu_n} \nabla \log\left(\frac{\mu_n}{\pi}\right)$, $\phi_t = I - tg$ for $t \in [0, \gamma]$ and $\rho_t = (\phi_t)_\# \mu_n$. We have $\frac{\partial \rho_t}{\partial t} = \nabla \cdot (\rho_t w_t)$ with $w_t = -g \circ \phi_t^{-1}$.

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

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

Step 1. $\varphi(0) = \text{KL}(\mu_n | \pi)$ and $\varphi(\gamma) = \text{KL}(\mu_{n+1} | \pi)$.

Step 2. Using the chain rule,

$$\varphi'(t) = \langle \nabla_{w_t} \text{KL}(\rho_t | \pi), w_t \rangle_{L^2(\rho_t)}.$$

Hence :

$$\varphi'(0) = -\langle \nabla \log\left(\frac{\mu_n}{\pi}\right), g \rangle_{L^2(\mu_n)} = -\left\| S_{\mu_n} \nabla \log\left(\frac{\mu_n}{\pi}\right) \right\|_{\mathcal{H}}^2.$$

Sketch of proof - 2

Step 3.

$$\varphi''(t) = \langle w_t, \text{Hess}_{\text{KL}(\cdot|\pi)}(\rho_t) w_t \rangle_{L^2(\rho_t)} := \psi_1(t) + \psi_2(t),$$

$$\psi_1(t) = \mathbb{E}_{x \sim \rho_t} [\langle w_t(x), H_V(x) w_t(x) \rangle] \quad \text{and} \quad \psi_2(t) = \mathbb{E}_{x \sim \rho_t} [\|Jw_t(x)\|_{HS}^2]$$

where $\rho_t = (\phi_t)_\# \mu_n$, $w_t = -g \circ (\phi_t)^{-1}$.

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Step 3.a. Assuming $\|H_V\| \leq M$ and $k(\cdot, \cdot) \leq B$:

$$\psi_1(t) \leq M \|g\|_{L^2(\mu_n)}^2 \leq MB^2 \left\| S_{\mu_n} \nabla \log \left(\frac{\mu_n}{\pi} \right) \right\|_{\mathcal{H}}^2.$$

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Step 3.b. Since $\rho_t = (\phi_t)_\# \mu_n$, $w_t = -g \circ (\phi_t)^{-1}$,

$$\begin{aligned} \psi_2(t) &= \mathbb{E}_{x \sim \mu_n} [\|Jw_t \circ \phi_t(x)\|_{HS}^2] \leq \|Jg(x)\|_{HS}^2 \|(J\phi_t)^{-1}(x)\|_{op}^2 \\ &\leq B^2 \left\| S_{\mu_n} \nabla \log \left(\frac{\mu_n}{\pi} \right) \right\|_{\mathcal{H}}^2 \alpha^2, \end{aligned}$$

assuming $\|\nabla k(\cdot, \cdot)\| \leq B$ and choosing $\gamma \leq f(\alpha)$ with $\alpha > 1$.

From:

$$\varphi(\gamma) = \varphi(0) + \gamma\varphi'(0) + \int_0^\gamma (\gamma - t)\varphi''(t)dt$$

we have:

$$\begin{aligned} \text{KL}(\mu_{n+1}|\pi) - \text{KL}(\mu_n|\pi) &\leq -\gamma \|S_{\mu_n} \nabla \log \left(\frac{\mu_n}{\pi} \right)\|_{\mathcal{H}}^2 \\ &\quad + \frac{\gamma^2}{2} (\alpha^2 + M) B^2 \|S_{\mu_n} \nabla \log \left(\frac{\mu_n}{\pi} \right)\|_{\mathcal{H}}^2. \end{aligned}$$

Choosing γ small enough yields a descent lemma :

$$\text{KL}(\mu_{n+1}|\pi) - \text{KL}(\mu_n|\pi) \leq -c_\gamma \underbrace{\left\| S_{\mu_n} \nabla \log \left(\frac{\mu_n}{\pi} \right) \right\|_{\mathcal{H}}^2}_{\text{KSD}^2(\mu_n|\pi)}.$$

Rates in KSD

Consequence of the descent lemma: for γ small enough,

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

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

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

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

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

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

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

Problem: not possible to combine both.

Not possible to combine both....

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

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

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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).

Experiments

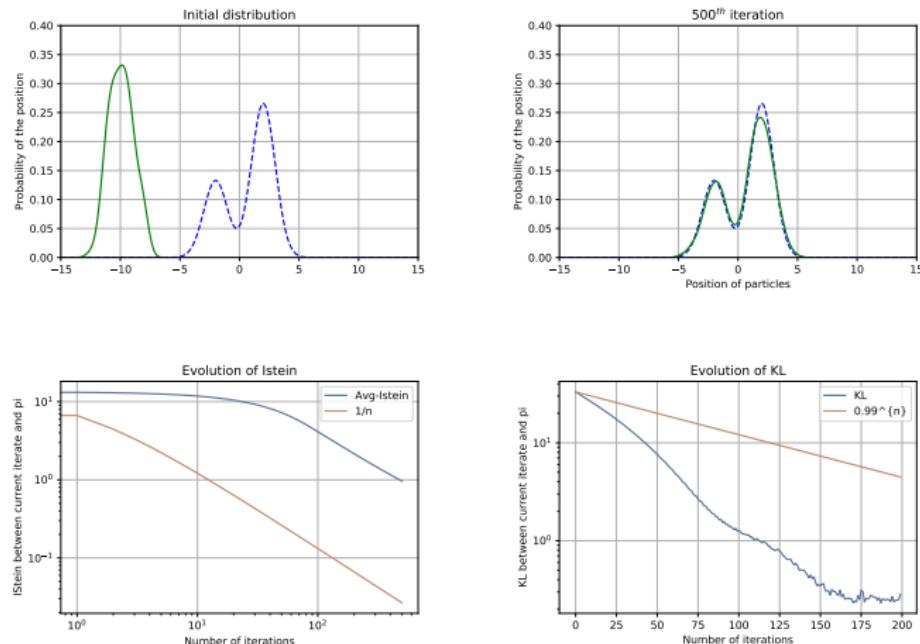
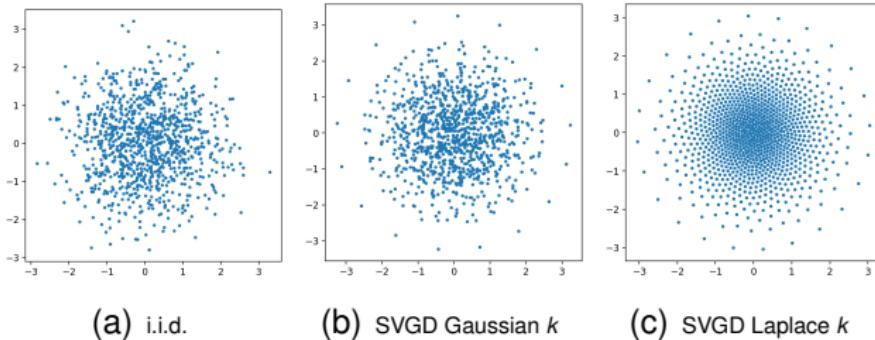


Figure: The particle implementation of the SVGD algorithm illustrates the convergence of $\text{KSD}^2(k \star \mu_i^n | \pi)$ to 0.

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:

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



For i.i.d. points, (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

Problem and Motivation

Wasserstein Gradient Flows

Part I - Stein Variational Gradient Descent

Part II : Sampling as optimization of the KSD/MMD

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 :

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

With several integration by parts we have:

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

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:

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

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:

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

$$\text{where } \Delta x_n = x_{n+1} - x_n$$

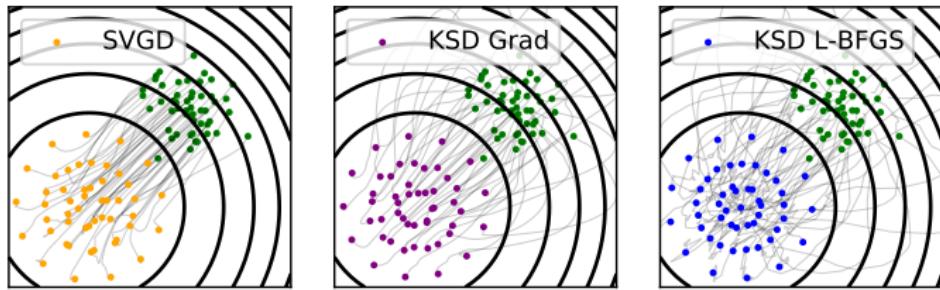
$$y_n = \nabla L(x_{n+1}) - \nabla L(x_n)$$

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

$$L(x_n + \gamma_n d_n) \leq L(x_n) + c_1 \gamma_n \nabla L(x_n)^T d_n$$

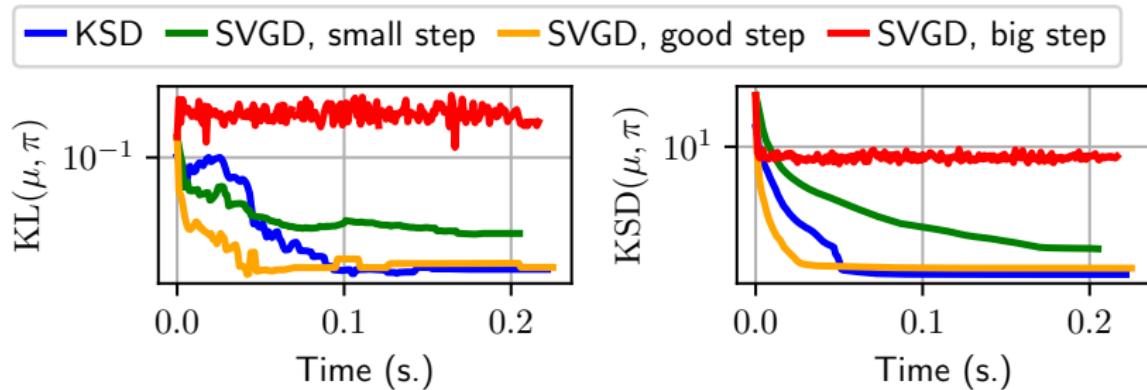
$$\nabla L(x_n + \gamma_n d_n)^T d_n \geq c_2 \nabla L(x_n)^T d_n$$

Toy experiments - 2D standard gaussian



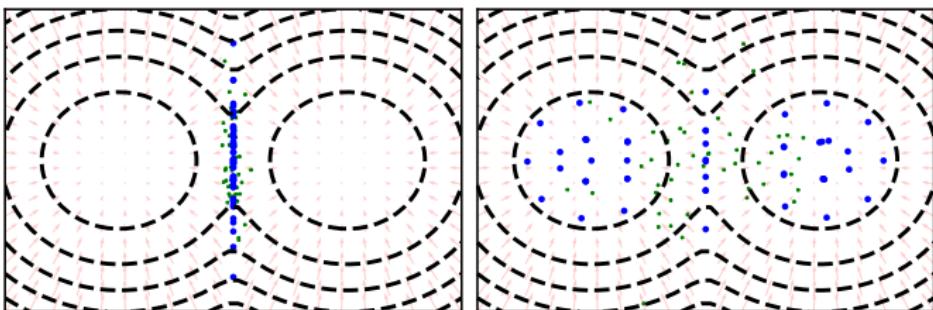
The green points represent the initial positions of the particles.
The light grey curves correspond to their trajectories.

SVGD vs KSD Descent - importance of the step-size



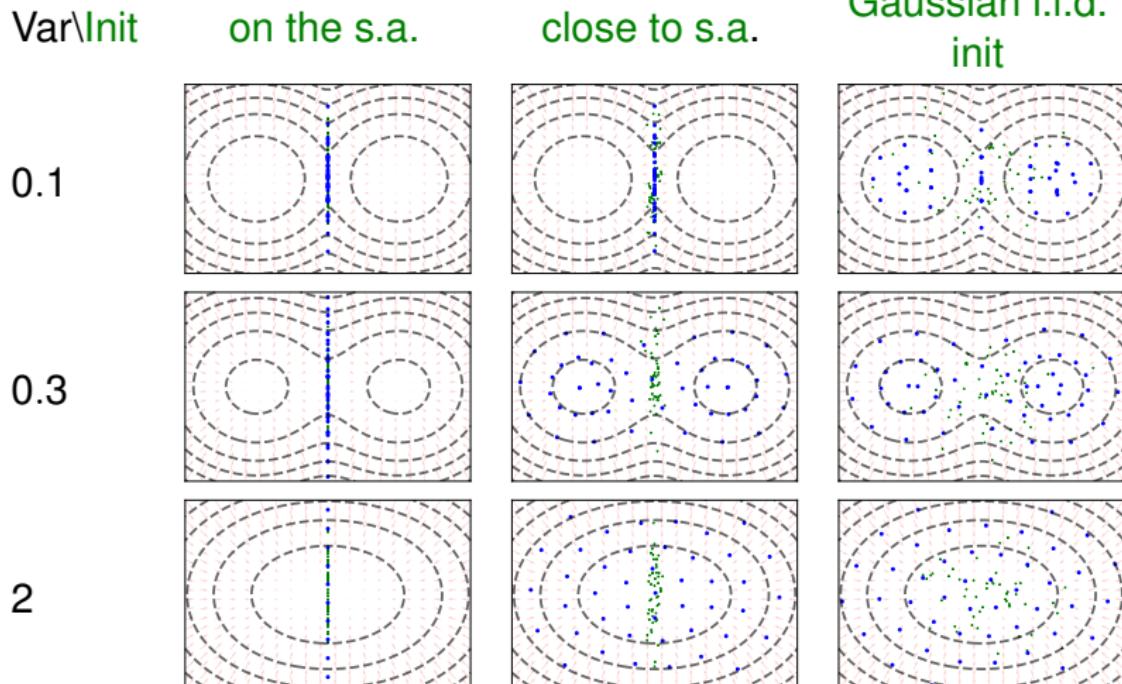
Convergence speed of KSD and SVGD on a Gaussian problem in 1D, with 30 particles.

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.

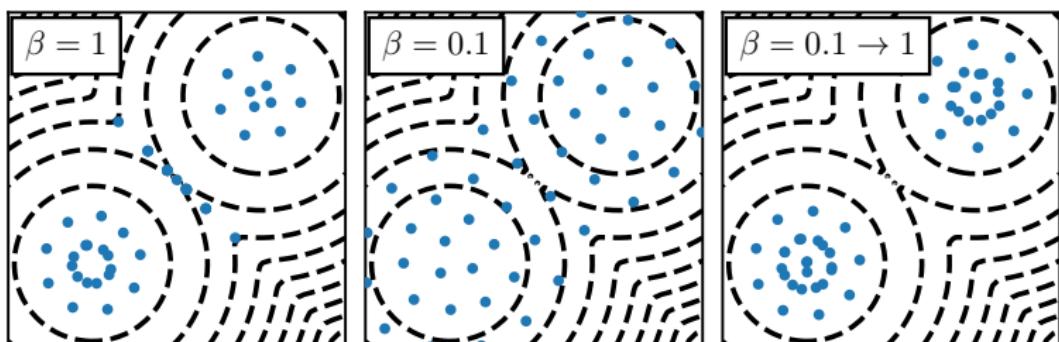
More initializations



Green crosses : initial particle positions
Blue crosses : final positions

Isolated Gaussian mixture - annealing

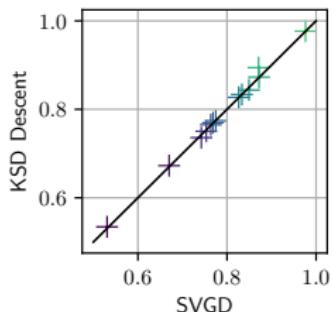
Add an inverse temperature variable $\beta : \pi^\beta(x) \propto \exp(-\beta V(x))$, with $0 < \beta \leq 1$ (i.e. multiply the score by β .)



This is a hard problem, even for Langevin diffusions, where tempering strategies also have been proposed.

Beyond Log-concavity: Provable Guarantees for Sampling Multi-modal Distributions using Simulated Tempering Langevin Monte Carlo. Rong Ge, Holden Lee, Andrej Risteski. 2017.

Real world experiments (10 particles)

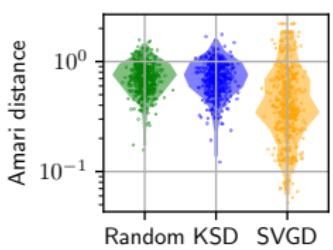


Bayesian logistic regression.

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.



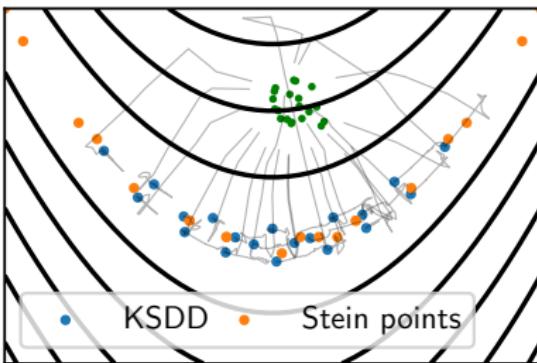
Bayesian ICA.

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

Conclusion

- ▶ Mixing kernels and Wasserstein gradient flows enable to design deterministic interacting particle systems

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

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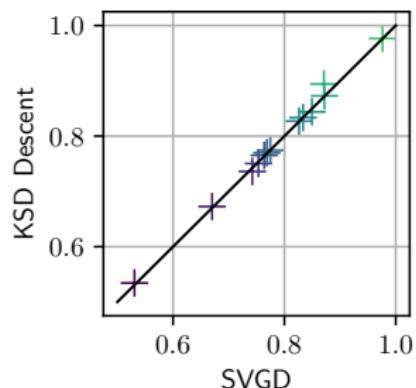
1 - Bayesian Logistic regression

Datapoints $d_1, \dots, d_q \in \mathbb{R}^p$, and labels $y_1, \dots, y_q \in \{\pm 1\}$.

Labels y_i are modelled as $p(y_i = 1 | d_i, w) = (1 + \exp(-w^\top d_i))^{-1}$ for some $w \in \mathbb{R}^p$.

The parameters w follow the law $p(w|\alpha) = \mathcal{N}(0, \alpha^{-1} I_p)$, and $\alpha > 0$ is drawn from an exponential law $p(\alpha) = \text{Exp}(0.01)$.

The parameter vector is then $x = [w, \log(\alpha)] \in \mathbb{R}^{p+1}$, and we use KSD-LBFGS to obtain samples from $p(x | (d_i, y_i)_{i=1}^q)$ for 13 datasets, with $N = 10$ particles for each.



Accuracy of the KSD descent and SVGD on bayesian logistic regression for 13 datasets.

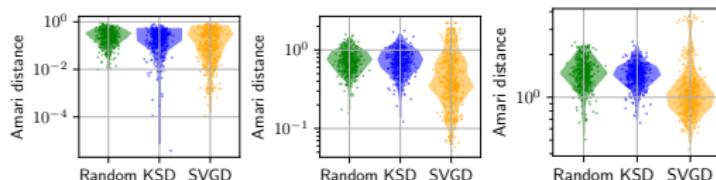
**Both methods yield similar results.
KSD is better by 2% on one dataset.**

2 - Bayesian Independent Component Analysis

ICA: $x = W^{-1}s$, where x is an observed sample in \mathbb{R}^p , $W \in \mathbb{R}^{p \times p}$ is the unknown square unmixing matrix, and $s \in \mathbb{R}^p$ are the independent sources.

- 1) Assume that each component has the same density $s_i \sim p_s$.
- 2) The likelihood of the model is $p(x|W) = \log |W| + \sum_{i=1}^p p_s([Wx]_i)$.
- 3) Prior: W has i.i.d. entries, of law $\mathcal{N}(0, 1)$.

The posterior is $p(W|x) \propto p(x|W)p(W)$, and the score is given by $s(W) = W^{-\top} - \psi(Wx)x^\top - W$, where $\psi = -\frac{p'_s}{p_s}$. In practice, we choose p_s such that $\psi(\cdot) = \tanh(\cdot)$. We then use the presented algorithms to draw 10 particles $W \sim p(W|x)$ on 50 experiments.



Left: $p = 2$. Middle: $p = 4$. Right: $p = 8$.

Each dot = Amari distance between an estimated matrix and the true unmixing matrix.

KSD Descent is not better than random. Explanation: ICA likelihood is highly non-convex.

(descent lemma for SVGD) Sketch of proof - 1

Fix $n \geq 0$. Denote $g = P_{\mu_n} \nabla \log\left(\frac{\mu_n}{\pi}\right)$, $\phi_t = I - tg$ for $t \in [0, \gamma]$ and $\rho_t = (\phi_t)_\# \mu_n$. We have $\frac{\partial \rho_t}{\partial t} = \nabla \cdot (\rho_t w_t)$ with $w_t = -g \circ \phi_t^{-1}$.

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

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

Step 1. $\varphi(0) = \text{KL}(\mu_n | \pi)$ and $\varphi(\gamma) = \text{KL}(\mu_{n+1} | \pi)$.

Step 2. Using the chain rule,

$$\varphi'(t) = \langle \nabla_{w_t} \text{KL}(\rho_t | \pi), w_t \rangle_{L^2(\rho_t)}.$$

Hence :

$$\varphi'(0) = -\langle \nabla \log\left(\frac{\mu_n}{\pi}\right), g \rangle_{L^2(\mu_n)} = -\left\| S_{\mu_n} \nabla \log\left(\frac{\mu_n}{\pi}\right) \right\|_{\mathcal{H}}^2.$$

Sketch of proof - 2

Step 3.

$$\varphi''(t) = \langle w_t, \text{Hess}_{\text{KL}(\cdot|\pi)}(\rho_t) w_t \rangle_{L^2(\rho_t)} := \psi_1(t) + \psi_2(t),$$

$$\psi_1(t) = \mathbb{E}_{x \sim \rho_t} [\langle w_t(x), H_V(x) w_t(x) \rangle] \quad \text{and} \quad \psi_2(t) = \mathbb{E}_{x \sim \rho_t} [\|Jw_t(x)\|_{HS}^2]$$

where $\rho_t = (\phi_t)_\# \mu_n$, $w_t = -g \circ (\phi_t)^{-1}$.

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where $\rho_t = (\phi_t)_\# \mu_n$, $w_t = -g \circ (\phi_t)^{-1}$.

Step 3.a. Assuming $\|H_V\| \leq M$ and $k(\cdot, \cdot) \leq B$:

$$\psi_1(t) \leq M \|g\|_{L^2(\mu_n)}^2 \leq MB^2 \left\| S_{\mu_n} \nabla \log \left(\frac{\mu_n}{\pi} \right) \right\|_{\mathcal{H}}^2.$$

Sketch of proof - 2

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Step 3.a. Assuming $\|H_V\| \leq M$ and $k(\cdot, \cdot) \leq B$:

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Step 3.b. Since $\rho_t = (\phi_t)_\# \mu_n$, $w_t = -g \circ (\phi_t)^{-1}$,

$$\begin{aligned} \psi_2(t) &= \mathbb{E}_{x \sim \mu_n} [\|Jw_t \circ \phi_t(x)\|_{HS}^2] \leq \|Jg(x)\|_{HS}^2 \|(J\phi_t)^{-1}(x)\|_{op}^2 \\ &\leq B^2 \left\| S_{\mu_n} \nabla \log \left(\frac{\mu_n}{\pi} \right) \right\|_{\mathcal{H}}^2 \alpha^2, \end{aligned}$$

assuming $\|\nabla k(\cdot, \cdot)\| \leq B$ and choosing $\gamma \leq f(\alpha)$ with $\alpha > 1$.

From:

$$\varphi(\gamma) = \varphi(0) + \gamma\varphi'(0) + \int_0^\gamma (\gamma - t)\varphi''(t)dt$$

we have:

$$\begin{aligned} \text{KL}(\mu_{n+1}|\pi) - \text{KL}(\mu_n|\pi) &\leq -\gamma \|S_{\mu_n} \nabla \log \left(\frac{\mu_n}{\pi} \right)\|_{\mathcal{H}}^2 \\ &\quad + \frac{\gamma^2}{2} (\alpha^2 + M) B^2 \|S_{\mu_n} \nabla \log \left(\frac{\mu_n}{\pi} \right)\|_{\mathcal{H}}^2. \end{aligned}$$

Choosing γ small enough yields a descent lemma :

$$\text{KL}(\mu_{n+1}|\pi) - \text{KL}(\mu_n|\pi) \leq -c_\gamma \underbrace{\left\| S_{\mu_n} \nabla \log \left(\frac{\mu_n}{\pi} \right) \right\|_{\mathcal{H}}^2}_{\text{KSD}^2(\mu_n|\pi)}.$$

Forward method for the KL

Problem: $\nabla_{W_2} \text{KL}(\mu_n | \pi) = \nabla \log\left(\frac{\mu_n}{\pi}\right)$ where μ_n is unknown.

While $\nabla \log \pi$ is known, $\nabla \log \mu_n$ has to be estimated from N particles X_n^1, \dots, X_n^N , e.g. with¹:

1. Kernel Density Estimation (KDE):

$$\mu_n(\cdot) \approx \frac{1}{N} \sum_{i=1}^N k(X_n^i - \cdot)$$

Then,

$$-\nabla_{W_2} \text{KL}(\mu_n | \pi)(\cdot) \approx - \left(\nabla V(\cdot) + \frac{\sum_{i=1}^N \nabla k(\cdot - X_n^i)}{\sum_{i=1}^N k(\cdot - X_n^i)} \right)$$

Remark: it is not the W_2 gradient of some functional (see the next slide)

¹assume a symmetric, translation invariant kernel

2. Blob Method [Carrillo et al., 2019]:

Instead of

$$\mathcal{U}(\mu) = \int \log(\mu(x)) d\mu(x),$$

consider

$$\mathcal{U}_k(\mu) = \int \log(k * \mu(x)) d\mu(x), \text{ where } k * \mu(x) = \int k(x-y) d\mu(y).$$

Then,

$$\frac{\partial \mathcal{U}_k(\mu)}{\partial \mu}(.) = k * \left(\frac{\mu}{k * \mu} \right) + \log(k * \mu)$$

$$\implies \nabla_{W_2} \mathcal{U}_k(\mu) = \nabla k * \left(\frac{\mu}{k * \mu} \right) + \underbrace{\nabla \log(k * \mu)}_{\frac{\nabla k * \mu}{k * \mu}}$$

$$\implies \nabla_{W_2} \text{KL}(\mu_n | \pi)(.) \approx - (\nabla V(.)) +$$

$$\sum_{i=1}^N \frac{\nabla k(. - X_n^i)}{\sum_{m=1}^N k(X_n^i - X_n^m)} + \frac{\sum_{i=1}^N \nabla k(. - X_n^i)}{\sum_{i=1}^N k(. - X_n^i)}$$

SVGD trick and the kernel integral operator

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

For instance assume $\|k(x, \cdot)\|_{\mathcal{H}_k}^2 = k(x, x) \leq B^2$, then for $f \in \mathcal{H}_k$

$$\begin{aligned}\|f\|_{L^2(\mu)}^2 &= \int \|f(x)\|^2 d\mu(x) = \int \langle f, k(x, \cdot) \rangle_{\mathcal{H}_k}^2 d\mu(x) \\ &\leq \|f\|_{\mathcal{H}_k}^2 \int k(x, x) d\mu(x) \leq B^2 \|f\|_{\mathcal{H}_k}^2\end{aligned}$$

Then, the injection from $\iota : \mathcal{H} \rightarrow L^2(\mu)$ admits an adjoint $\iota^* = S_\mu$,
where $S_\mu : L^2(\mu) \rightarrow \mathcal{H}$ is defined by:

$$S_\mu f(\cdot) = \int k(x, \cdot) f(x) d\mu(x), \quad f \in L^2(\mu).$$

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$$\begin{aligned}\|f\|_{L^2(\mu)}^2 &= \int \|f(x)\|^2 d\mu(x) = \int \langle f, k(x, \cdot) \rangle_{\mathcal{H}_k}^2 d\mu(x) \\ &\leq \|f\|_{\mathcal{H}_k}^2 \int k(x, x) d\mu(x) \leq B^2 \|f\|_{\mathcal{H}_k}^2\end{aligned}$$

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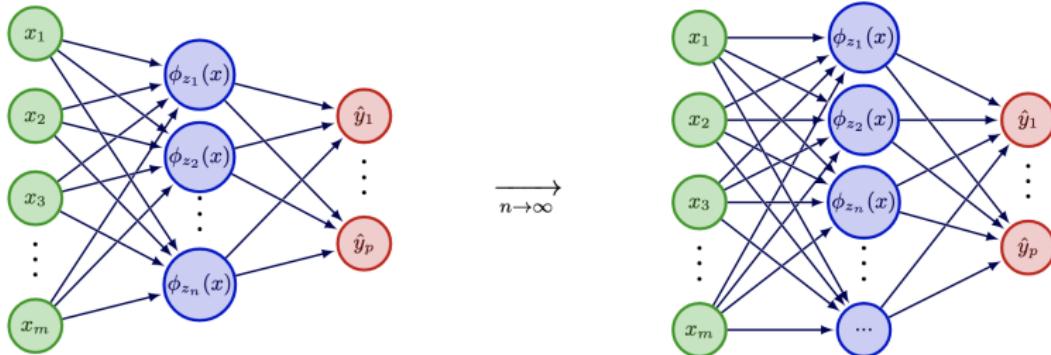
$$S_\mu f(\cdot) = \int k(x, \cdot) f(x) d\mu(x), \quad f \in L^2(\mu).$$

We have for any $f, g \in L_2(\mu) \times \mathcal{H}$:

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

We will denote $P_\mu = \iota \circ S_\mu$.

Example 2 : Regression with infinite width NN



$$\min_{(z_i)_{i=1}^n \in \mathbb{R}^d} \mathbb{E}_{(x,y) \sim P_{data}} \left[\underbrace{\left\| y - \frac{1}{n} \sum_{i=1}^n \phi_{z_i}(x) \right\|^2}_{\hat{y}} \right] \xrightarrow{n \rightarrow \infty} \min_{\mu \in \mathcal{P}(\mathbb{R}^d)} \underbrace{\mathbb{E}_{(x,y) \sim P_{data}} \left[\left\| y - \int_{\mathbb{R}^d} \phi_z(x) d\mu(z) \right\|^2 \right]}_{\mathcal{F}(\mu)}$$

Define the target distribution $\pi \in \operatorname{argmin} \mathcal{F}(\mu)$.

Optimising the neural network is equivalent to approximating π .

Assume $\exists \pi \in \mathcal{P}$, $\mathbb{E}[y|X=x] = \mathbb{E}_{Z \sim \pi}[\phi_Z(x)]$, then the above problem corresponds to

$$\min_{\nu \in \mathcal{P}} \text{MMD}^2(\nu, \pi) := \iint_{\mathbb{R}^d} k(z, z') d(\mu - \pi)(z) d(\mu - \pi)(z'),$$

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Example of Student-Teacher networks:

- ▶ The output of the Teacher network is deterministic and given by

$$y = \int \phi_Z(x) d\pi(Z) \text{ where } \pi = \frac{1}{M} \sum_{m=1}^M \delta_{U^m}.$$

- ▶ Student network parametrized by $\mu = \frac{1}{N} \sum_{j=1}^N \delta_{Z^j}$, $N \ll M$ tries to learn the mapping $x \mapsto \int \phi_Z(x) d\pi(Z)$.

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Gradient descent on $(Z_j)_{j=1}^N \iff$ implementing a discretized Wasserstein gradient flow of the MMD [Arbel et al., 2019].

Stein Fisher information

Stationary condition : $\text{KSD}^2(\mu_t|\pi) = \left\| S_{\mu_t} \nabla \log \left(\frac{\mu_t}{\pi} \right) \right\|_{\mathcal{H}}^2 = 0$.

Implies weak convergence of μ_t to π if [Gorham and Mackey, 2017]:

- ▶ π is y dissipative (e.g. gaussian mixtures):

$$\liminf_{r \rightarrow \infty} \kappa(r) > 0,$$

$$\kappa(r) = \inf \left\{ -2 \frac{\langle \nabla \log \pi(x) - \nabla \log \pi(y), x - y \rangle}{\|x - y\|_2^2}; \|x - y\|_2^2 = r \right\}$$

- ▶ k is translation invariant with a non-vanishing Fourier transform and the sequence is uniformly tight;
or k is the IMQ kernel defined by $k(x, y) = (c^2 + \|x - y\|_2^2)^{\beta}$ for $c > 0$ and $\beta \in [-1, 0]$ (slow decay rate).

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Proposition: [Korba et al., 2020] if k is bounded, $\pi \propto \exp(-V)$ with H_V bounded above and if $\exists C > 0$, $\int \|x\|^2 d\mu_t(x) < C$ for all $t > 0$, then $\text{KSD}^2(\mu_t|\pi) \rightarrow 0$.

SVGD- Propagation of chaos

Recall that the practical SVGD implementation is :

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

where $\hat{\mu}_n$ denotes the empirical distribution of the interacting particles.

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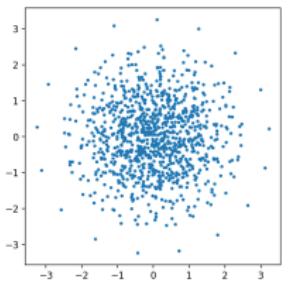
Propagation of chaos result

Let $n \geq 0$ and $T > 0$. Under boundedness and Lipschitzness assumptions for all $k, \nabla k, V$; for any $0 \leq n \leq \frac{T}{\gamma}$ we have :

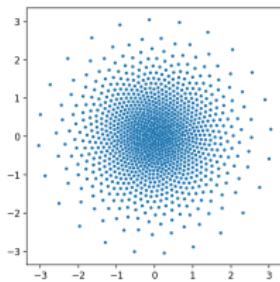
$$\mathbb{E}[W_2^2(\bar{\mu}_n, \hat{\mu}_n)] \leq \frac{1}{2} \left(\frac{1}{\sqrt{N}} \sqrt{\text{var}(\mu_0)} e^{LT} \right) (e^{2LT} - 1)$$

where L is a constant depending on k and π and $\bar{\mu}_n = \frac{1}{N} \sum_{j=1}^N \delta_{\bar{X}_n^j}$ with $\bar{X}_n^j \sim \mu_n$ i.i.d.

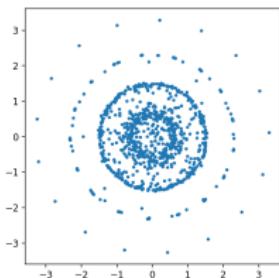
Ongoing work - quantization of these methods - gaussian target



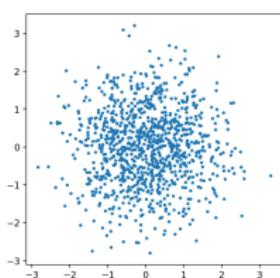
(d) SVGD Gaussian



(e) NSVGD Laplace



(f) MMD-lbfgs



(g) i.i.d.

Figure: (a)-(c) Final states of the algorithms for 1000 particles, after 1e4 iterations. The kernel bandwidth for all algorithms is set to 1.

Ongoing work - quantization of these methods - gaussian target

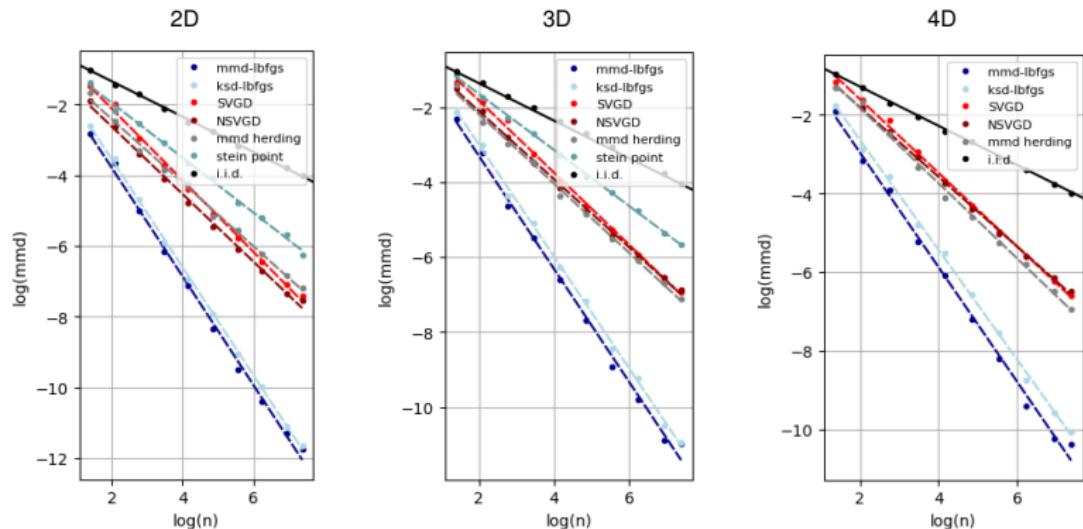


Figure: target distribution: $\pi = \mathcal{N}(0, 1/d I_d)$.

Ongoing work - quantization of these methods - gaussian target

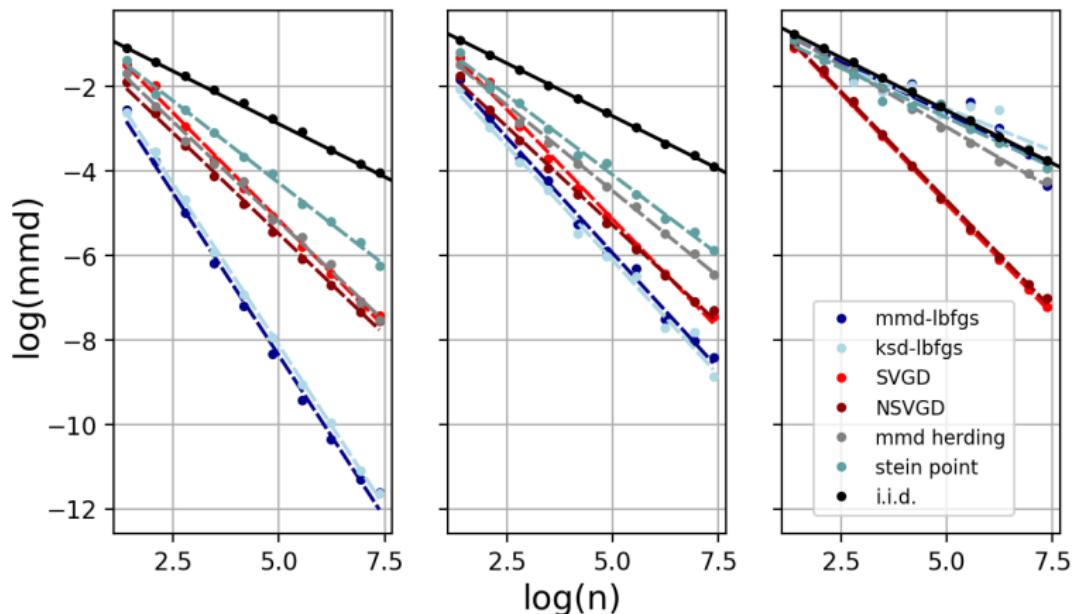


Figure: (same target π) Importance of the choice of the bandwidth in the MMD evaluation metric when evaluating the final states, in 2D.
From Left to Right: (evaluation) MMD bandwidth = 1, 0.7, 0.3.

MMD

Assume $m_\mu : \mu \mapsto \int k(x, \cdot) d\mu(x)$ injective.

The Maximum Mean Discrepancy defines a distance on $\mathcal{P}_2(\mathbb{R}^d)$:

$$\begin{aligned}\text{MMD}^2(\mu, \pi) &= \sup_{f \in \mathcal{H}_k, \|f\|_{\mathcal{H}_k} \leq 1} \left| \int f d\mu - \int f d\pi \right|^2 \\ &= \|m_\mu - m_\pi\|_{\mathcal{H}_k}^2 \\ &= \iint_{\mathbb{R}^d} k(x, y) d\mu(x) d\mu(y) + \iint_{\mathbb{R}^d} k(x, y) d\pi(x) d\pi(y) \\ &\quad - 2 \iint_{\mathbb{R}^d} k(x, y) d\mu(x) d\pi(y),\end{aligned}$$

by the reproducing property $\langle f, k(x, \cdot) \rangle_{\mathcal{H}_k} = f(x)$ for $f \in \mathcal{H}_k$.

MMD and KSD Descent

For discrete measures $\mu_N = 1/N \sum_{i=1}^N \delta_{X^i}$, we can define $F(X^1, \dots, X^N) := \mathcal{F}(\mu_N)$ when it is well defined (e.g., for the MMD or KSD).

In that case, Forward method for WGF = Gradient descent for F on the position of the particles.

- ▶ If D is the MMD, the gradient of F is readily obtained as

$$\nabla_{x^i} F(X^1, \dots, X^N) = \frac{1}{N} \sum_{j=1}^N \nabla_2 k(X^i, X^j) - \int \nabla_2 k(X^i, x) d\pi(x).$$

⇒ requires to know the density π , or at least samples from it !

- ▶ In contrast, if D is the KSD,

$$\nabla_{x^i} F(X^1, \dots, X^N) = \frac{1}{N} \sum_{j=1}^N \nabla_2 k_\pi(X^i, X^j).$$

Algorithm: at each time $n \geq 0$, for any $i = 1, \dots, N$:

$$X_{n+1}^i = X_n - \gamma \nabla_{x^i} F(X_n^1, \dots, X_n^N).$$

KSD is a particular MMD

Under mild assumptions on k and π , the Stein kernel k_π is p.s.d. and satisfies a **Stein identity** [Oates et al., 2017]

$$\int_{\mathbb{R}^d} k_\pi(x, \cdot) d\pi(x) = 0.$$

Consequently, **KSD is an MMD** with kernel k_π , since:

$$\begin{aligned}\text{MMD}^2(\mu|\pi) &= \int k_\pi(x, y) d\mu(x) d\mu(y) + \int k_\pi(x, y) d\pi(x) d\pi(y) \\ &\quad - 2 \int k_\pi(x, y) d\mu(x) d\pi(y) \\ &= \int k_\pi(x, y) d\mu(x) d\mu(y) \\ &= \text{KSD}^2(\mu|\pi)\end{aligned}$$

First strategy : functional inequality?

$$\mathcal{F}(\mu|\pi) = \iint k_\pi(x, y) d\mu(x) d\mu(y).$$

We have

$$\frac{\partial \mathcal{F}(\mu)}{\partial \mu} = \int k_\pi(x, \cdot) d\mu(x) = \mathbb{E}_{x \sim \mu}[k_\pi(x, \cdot)]$$

and under appropriate growth assumptions on k_π :

$$\nabla_{W_2} \mathcal{F}(\mu) = \mathbb{E}_{x \sim \mu}[\nabla_2 k_\pi(x, \cdot)],$$

Hence

$$\begin{aligned}\frac{d\mathcal{F}(\mu_t)}{dt} &= \langle \nabla_{W_2} \mathcal{F}(\mu_t), -\nabla_{W_2} \mathcal{F}(\mu_t) \rangle_{L^2(\mu_t)} \\ &= -\mathbb{E}_{y \sim \mu_t} \left[\|\mathbb{E}_{x \sim \mu_t}[\nabla_2 k_\pi(x, y)]\|^2 \right] \leq 0.\end{aligned}$$

⇒ **Difficult to identify a functional inequality to relate $d\mathcal{F}(\mu_t)/dt$ to $\mathcal{F}(\mu_t)$, and establish convergence in continuous time (similar to [Arbel et al., 2019]).**

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

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

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

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

⇒ **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 :

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

where

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

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

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 ($\subset L^2(\pi)$)?

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

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

Curvature near equilibrium - negative result

The previous inequality

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

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

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

- ▶ 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 $P_{\pi, k_\pi} : L^2(\pi) \rightarrow L^2(\pi)$, $f \mapsto \int k_\pi(x, \cdot) f(x) d\pi(x)$.

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

Functional inequalities

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

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

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

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

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

It can be shown that:

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

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

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)