Accurate Quantization of Measures via Interacting Particle-based Optimization

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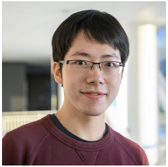
Ellis Theory workshop



Joint work with Lantian Xu, Dejan Slepčev (Carnegie Mellon University).

Outline

Quantization problem

Problem : approximate a target distribution $\pi \in \mathcal{P}(\mathbb{R}^d)$ by a finite set of n points $x_1, \dots, x_n$, e.g. to compute functionals $\int_{\mathbb{R}^d} f(x) d\pi(x)$.

The quality of the set can be measured by the integral approximation error:

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

Several approaches, among which :

- MCMC methods : generate a Markov chain whose law converges to π, $\mathrm{err}(x_1, \dots, x_n) = \mathcal{O}(n^{-1/2})$
  [Łatuszyński et al., 2013]
- **deterministic particle systems**, $\mathrm{err}(x_1, \dots, x_n)$?

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 w, e.g. :

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

Goal: learn the best distribution over parameter x to fit the data.

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1. Compute the Likelihood:

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

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$$x \sim p, \quad \text{e.g. } p(x) \propto \exp\left(-\frac{\|x\|^2}{2}\right).$$

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3. Bayes' rule yields:

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

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

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- prediction for a new input w:

$$y_{pred} = \int_{\mathbb{R}^d} g(w, x) d\pi(x)$$

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

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

Question: how can we approximate π?

Outline

Sampling as optimization over distributions

3 algorithms/particle systems at study:

- Maximum Mean Discrepancy Descent [Arbel et al., 2019]
- Kernel Stein Discrepancy Descent [Korba et al., 2021]
- Stein Variational Gradient Descent [Liu and Wang, 2016]

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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:

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

where D is a **dissimilarity functional** and $\mathcal{F}$ **"a loss"**.

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.

Euclidean gradient flow and continuity equation

Let $V : \mathbb{R}^d \to \mathbb{R}$ and consider minimizing V. The gradient flow of V can be written

$$\boxed{\frac{dx_t}{dt} = -\nabla V(x_t)}$$

and assume x_0 random with density μ_0.

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and assume x_0 random with density μ_0.

What are the dynamics of the density μ_t of x_t ? Let $\phi \in C_c\infty(\mathbb{R}^d)$.

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

and applying the chain rule and using I.P.P.,

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

Therefore,

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

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.

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

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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 (Benamou-Brenier formula):

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

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

The first variation of $\mu \mapsto \mathcal{F}(\mu)$ evaluated at $\mu \in \mathcal{P}(\mathbb{R}^d)$ is the unique function $\frac{\partial \mathcal{F}(\mu)}{\partial \mu} : \mathbb{R}^d \to \mathbb{R}$ s. t. for any $\mu, \nu \in \mathcal{P}(\mathbb{R}^d)$, $\nu - \mu \in \mathcal{P}(\mathbb{R}^d)$:

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

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The family $\mu : [0, \infty] \to \mathcal{P}_2(\mathbb{R}^d), t \mapsto \mu_t$ satisfies a Wasserstein gradient flow of $\mathcal{F}$ if:

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

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

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It can be implemented by the deterministic process:

$$\boxed{\frac{dx_t}{dt} = -\nabla_{W_2} \mathcal{F}(\mu_t)(x_t), \quad \text{where } x_t \sim \mu_t}$$

Particle system approximating the WGF

Euler time-discretization : in $\mathbb{R}^d$, move particles as:

$$x_{l+1} = Xx_l - \gamma \nabla_{W_2} \mathcal{F}(\mu_l)(x_l) \sim \mu_{l+1}, \quad x_0 \sim \mu_0.$$

But μ_l is unknown.

Space discretization/particle system : Introduce a particle system $x_0^1, \ldots, x_0^n \sim \mu_0$, and at each step:

$$x_{l+1}^i = x_l^i - \gamma \nabla_{W_2} \mathcal{F}(\hat{\mu}_l)(x_l^i) \quad \text{for } i = 1, \ldots, n,$$

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

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 $x_1, \dots, x_n \in \mathbb{R}^d)$
- examples:
  - the Gaussian kernel $k(x, y) = \exp\left(-\frac{\|x-y\|^2}{h}\right)$
  - the Laplace kernel $k(x, y) = \exp\left(-\frac{\|x-y\|}{h}\right)$
- $\mathcal{H}_k$ 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 $\|.\|_{\mathcal{H}_k}$.
- It satisfies the reproducing property:

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

Maximum Mean Discrepancy [Gretton et al., 2012]

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

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

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

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

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

The differential of $\mu \mapsto \frac{1}{2}\mathrm{MMD}^2(.,\pi)$ evaluated at $\mu \in \mathcal{P}_2(\mathbb{R}^d)$ is:

$$\int k(x,.)d\mu(x) - \int k(x,.)d\pi(x) : \mathbb{R}^d \to \mathbb{R}.$$

Hence, for k regular enough, $\nabla_{W_2}\frac{1}{2}\mathrm{MMD}^2(\mu,\pi)$ is:

$$\int \nabla_2 k(x,.)d\mu(x) - \int \nabla_2 k(x,.)d\pi(x) : \mathbb{R}^d \to \mathbb{R}.$$

Kernel Stein Discrepancy [Chwialkowski et al., 2016, Liu et al., 2016]

If one does not have access to samples of π but only to its score, it is still possible to compute the KSD:

$$\mathrm{KSD}^2(\mu|\pi) = \iint k_\pi(x,y)d\mu(x)d\mu(y),$$

where $k_\pi : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is the **Stein kernel**, defined through

- the score function $s(x) = \nabla \log \pi(x)$,
- a p.s.d. kernel $k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$, $k \in C^2(\mathbb{R}^d)$[1]

For $x, y \in \mathbb{R}^d$,

$$\begin{aligned} k_\pi(x,y) = &\ s(x)^T s(y)\, k(x,y) + s(x)^T\, \nabla_2 k(x,y) \\ &+ \nabla_1 k(x,y)^T\, s(y) + \boldsymbol{\nabla} \cdot_1 \nabla_2 k(x,y) \\ = &\sum_{i=1}^d \frac{\partial \log \pi(x)}{\partial x_i} . \frac{\partial \log \pi(y)}{\partial y_i} . k(x,y) + \frac{\partial \log \pi(x)}{\partial x_i} . \frac{\partial k(x,y)}{\partial y_i} \\ &+ \frac{\partial \log \pi(y)}{\partial y_i} . \frac{\partial k(x,y)}{\partial x_i} + \frac{\partial^2 k(x,y)}{\partial x_i \partial y_i} \in \mathbb{R}. \end{aligned}$$

[1] e.g. : $k(x,y) = \exp(-\|x-y\|^2/h)$, $\quad \pi(x) \propto e^{-\|x\|^2}$, $s(x) = -x$

KSD vs 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]

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

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

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

MMD and KSD Descent

Let $\mathcal{F}(\mu) = \mathrm{D}(\mu|\pi)$ where D is the MMD or KSD.

For discrete measures $\mu = \frac{1}{n}\sum_{i=1}^n \delta_{X^i}$, let $F(X^1, \dots, X^n) := \mathcal{F}(\mu)$. Then, for $i = 1, \dots, n$,

$$x_{l+1}^i = x_l^i - \gamma \nabla_{W_2}\mathcal{F}(\hat{\mu}_l)(x_l^i), \quad \hat{\mu}_l = \frac{1}{n}\sum_{i=1}^n \delta_{x_l^i}$$

$$\Updownarrow$$

$$\boxed{x_{l+1}^i = x_l^i - \gamma \nabla_{x^i} F(x_l^1, \dots, x_l^n).}$$

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$$\boxed{x_{l+1}^i = x_l^i - \gamma \nabla_{x^i} F(x_l^1, \ldots, x_l^n).}$$

- If D is the MMD, the gradient of F is:

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

- In contrast, if D is the KSD, it is:

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

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- The MMD/KSD/their W_2 gradient write as sums of integrals of μ and π
- Hence they can be evaluated in closed form for discrete μ and $\pi \implies$ use L-BFGS to automatically select the best step-size
- depending on the information on π, choose the KSD (unnormalized density) or MMD (samples)
- The MMD upper bounds the integral approximation error for functions in the RKHS, since by the reproducing property and Cauchy-Schwartz:

$$\left|\int_{\mathbb{R}^d} f(x)d\pi(x) - \int_{\mathbb{R}^d} f(x)d\mu(x)\right| \leq \|f\|_{\mathcal{H}_k} \mathrm{MMD}(\mu,\pi).$$

Similarly for the KSD with $\mathcal{H}_{k_\pi}$.

Stein Variational Gradient Descent [Liu and Wang, 2016]

Stein Variational Gradient Descent (SVGD) performs gradient descent in $\mathcal{P}(\mathbb{R}^d)$ of the Kullback-Leibler (KL) divergence :

$$\mathrm{KL}(\mu|\pi) = \begin{cases} \int_{\mathbb{R}^d} \log\left(\frac{\mu}{\pi}(x)\right) d\mu(x) & \text{if } \mu \ll \pi \\ +\infty & \text{otherwise.} \end{cases}$$

with respect to a "kernelized Wasserstein distance" depending on **a kernel** k [Liu, 2017, Duncan et al., 2019]:

$$W_k^2(\mu_0, \mu_1) = \inf_{(\mu_t, v_t)_{t\in[0,1]}} \left\{ \int_0^1 \|v_t\|^2_{\mathcal{H}_k^d} dt(x) : \frac{\partial \mu_t}{\partial t} = \boldsymbol{\nabla} \cdot (\mu_t v_t) \right\}.$$

Stein Variational Gradient Descent [Liu and Wang, 2016]

In continuous time, SVGD flow is defined by the continuity equation

$$\frac{\partial \mu_t}{\partial t} + \boldsymbol{\nabla} \cdot (\mu_t v_{\mu_t}) = 0,\ v_{\mu_t} = S_{\mu_t,k} \nabla \log \left(\frac{\mu_t}{\pi}\right)$$

where

- $\nabla \log \left(\frac{\mu}{\pi}\right) = \nabla_{W_2} \mathrm{KL}(\mu|\pi)$,
- $S_{\mu,k} : L^2(\mu) \to \mathcal{H}_k,\ f \mapsto \int k(x,.)f(x)d\mu(x)$,

and one can write $v_{\mu_t} = k \star (\mu_t \nabla \log \pi) - \nabla k \star \mu_t$.

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Let $\gamma > 0$ be a fixed step-size. Starting from $x_0^1, \ldots, x_0^n \sim \mu_0$, SVGD algorithm updates the n particles as follows at each iteration :

$$x_{l+1}^i = x_l^i + \frac{\gamma}{n} \sum_{j=1}^{n} \left[\nabla \log \pi(x_l^j) k(x_l^i, x_l^j) - \nabla_{x_l^j} k(x_l^i, x_l^j) \right].$$

Remarks

- for discrete measures, the KL is not defined
- SVGD does not minimize a well-defined functional for discrete measures, it is only a discrete approximation of the KL flow
- cannot be used with L-BFGS (or not straightforwardly)
- how to measure the quantization, i.e. the quality of the particles obtained?

Outline

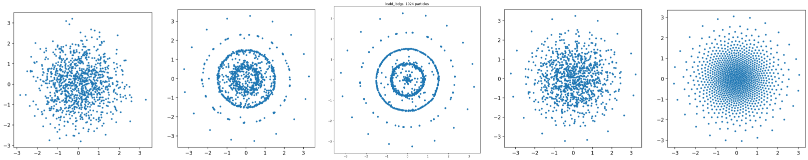
Problem and Motivation

Background on Interacting Particle Systems

MMD and KSD Quantization

Experiments

Motivation - Final states for a Gaussian target



(a) i.i.d. (b) MMD k_G (c) KSD k_G (d) SVGD k_G (e) SVGD k_L

Figure: Final states of the algorithms for 1000 particles, kernel bandwidth = 1. k_G is the Gaussian kernel and k_L is the Laplace kernel.

We run MMD/KSD descent with Gaussian kernel only, since

$$(1)\ \nabla_{x^i} \mathrm{MMD}^2(\mu_n, \pi) = \frac{1}{n} \sum_{j=1,\dots,n} \nabla_2 k(x^i, x^j) - \int \nabla_2 k(x^i, x) d\pi(x),$$

$$(2)\ \nabla_{x^i} \mathrm{KSD}^2(\mu_n, \pi) = \frac{1}{n} \sum_{j=1,\dots n} \nabla_2 k_\pi(x^i, x^j),$$

$$(3)\ \nabla_{x^i} \mathrm{SVGD} = \frac{1}{n} \sum_{j=1,\dots,n} \nabla \log \pi(x^i) k(x^i, x) + \nabla_{x^i} k(x^i, x)$$

(1) available in closed form for π and k Gaussian, (2) involves high order derivatives of the kernel, (3) can be run with any kernel including k_L

We are interested in establishing bounds on the quantization error

$$Q_n = \inf_{X_n = x_1, \ldots, x_n} \mathrm{D}(\pi, \mu_n), \quad \text{for } \mu_n = \frac{1}{n} \sum_{i=1}^{n} \delta_{x_i},$$

where D is the MMD or KSD.

Remark: For $x_1, \ldots, x_n \overset{i.i.d.}{\sim} \pi$, the rate is known to be $\mathcal{O}(n^{-1/2})$ [Gretton et al., 2006, Tolstikhin et al., 2017, Lu and Lu, 2020].

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Assumption A1: Assume that the kernel is d-times continuously differentiable. Assume also that any mixed partial derivative of the kernel of order smaller than d has a RKHS norm bounded by a constant $C_{k,d} \geq 0$.

First result for the MMD

Theorem: Suppose A1 holds. Assume that (i) π is the Lebesgue measure or (ii) a probability measure on $[0,1]^d$. Then, there exists a constant C_d, such that for all $n \geq 2$,

- if (i): there exist points $x_1, \ldots, x_n$ such that

$$\mathrm{MMD}(\pi, \mu_n) \leq C_d \frac{(\log n)^{d-1}}{n}.$$

- if (ii): there exist points $x_1, \ldots, x_n$ such that

$$\mathrm{MMD}(\pi, \mu_n) \leq C_d \frac{(\log n)^{\frac{3d+1}{2}}}{n}.$$

Proof: We use the well-known Koksma-Hlawka inequality [Aistleitner and Dick, 2015](Th1):

$$\left| \int_{[0,1]^d} f(x) d\pi(x) - \frac{1}{n} \sum_{i=1}^{n} f(x_i) \right| \leq \mathcal{D}(X_n, \pi) V(f),$$

- $\mathcal{D}(X_n, \pi) = \sup_{I=\Pi_{i=1}^{n}[a_i,b_i]} |\pi(I) - \mu_n(I)|$ is the discrepancy of the point set X_n, can be bounded by $C_{\pi,d} g(n)$ [Aistleitner and Dick, 2015]
- The variation of a function $f : [0,1]^d \to \mathbb{R}$ with continuous mixed partial derivatives is defined as

$$V(f) = \sum_{\alpha \subseteq \{1,\ldots,d\}} \int_{[0,1]^{|\alpha|}} \left| \frac{\partial^{|\alpha|} f(x_\alpha, 1)}{\partial x_\alpha} \right| dx_\alpha.$$

Then, use the reproducing property on partial derivatives with Cauchy-Schwarz inequality, and **A1**:

$$\left| \frac{\partial^{|\alpha|} f(x_\alpha, 1)}{\partial x_\alpha} \right| \leq \left\| \frac{\partial^{|\alpha|} k((x_\alpha, 1), \cdot)}{\partial^{|\alpha|} x_\alpha} \right\|_{\mathcal{H}_k} \|f\|_{\mathcal{H}_k} \leq C_{k,d}.$$

Result for non compactly supported distributions π

Proposition 1: Suppose A1 holds and that k is bounded. Assume π is a light-tailed distribution on $\mathbb{R}^d$ (i.e. which has a thinner tail than an exponential distribution). Then, for $n \geq 2$ there exist points $x_1, ..., x_n$ such that

$$\mathrm{MMD}(\pi, \mu_n) \leq C_d \frac{(\log n)^{\frac{5d+1}{2}}}{n}.$$

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Proof: Decompose $\mathrm{MMD}(\pi, \mu_n) \leq \mathrm{MMD}(\pi, \mu) + \mathrm{MMD}(\mu, \mu_n)$, choosing μ compactly supported on $A_n = [-\log n, \log n]^d$.

As π is light-tailed, $\|\mu - \pi\|_{TV} \leq C_1/n$ distance, and we first get $\mathrm{MMD}(\pi, \mu) \leq C_k \|\mu - \pi\|_{TV} \leq C/n$.

Then, we can take a discrete μ_n supported on A_n and bound $\mathrm{MMD}(\mu, \mu_n)$ using similar arguments as in the previous Theorem.

Result for the KSD

Theorem: Assume that k is Gaussian and that $\pi \propto \exp(-U)$ with $U \in C^\infty(\mathbb{R}^d)$. Assume furthermore that $U(x) > c_1\|x\|$ for large enough x, and that there exists a real-valued polynomial V of degree $m \geq 0$, such that for any multi-index β, $\left|\frac{\partial^\beta U(x)}{\partial^{\beta_1}x_1 \ldots \partial^{\beta_j}x_j}\right| \leq V(x)$ for all $1 \leq |\beta| \leq d+1$. Then there exist points $x_1, \ldots, x_n$ such that

$$\mathrm{KSD}(\mu_n|\pi) \leq C_d \frac{(\log n)^{\frac{6d+2m+1}{2}}}{n}.$$

Satisfied for gaussian mixtures π.

Result for the KSD

Theorem: Assume that k is Gaussian and that $\pi \propto \exp(-U)$ with $U \in C^\infty(\mathbb{R}^d)$. Assume furthermore that $U(x) > c_1\|x\|$ for large enough x, and that there exists a real-valued polynomial V of degree $m \geq 0$, such that for any multi-index β, $\left|\frac{\partial^\beta U(x)}{\partial^{\beta_1}x_1 \dots \partial^{\beta_j}x_j}\right| \leq V(x)$ for all $1 \leq |\beta| \leq d+1$. Then there exist points $x_1, ..., x_n$ such that

$$\mathrm{KSD}(\mu_n|\pi) \leq C_d \frac{(\log n)^{\frac{6d+2m+1}{2}}}{n}.$$

Satisfied for gaussian mixtures π.

Proof: The proof relies on bounding the first and last term of the

$$\begin{aligned}\mathrm{KSD}(\mu_n, \pi) = 2 \iint \nabla \log(\pi)(x)^T \nabla_y k(x, y) d\mu(x) d\mu(y) \\ + \underbrace{\iint \nabla \log(\pi)(x)^T \nabla \log(\pi)(y) k(x, y) d\mu(x) d\mu(y)}_{(1)} + \underbrace{\iint \boldsymbol{\nabla} \cdot_x \nabla_y k(x, y) d\mu(x) d\mu(y)}_{(2)},\end{aligned}$$

$\mu = \mu_n - \pi$, as the cross terms can be upper bounded by the former ones by CS and reproducing property.

(1) $\mathrm{MMD}(\mu_n, \pi)$, with $k_1(x, y) = s(x)^T s(y) k(x, y)$, bounded by controlling $\|\nabla \log \pi\|_{H^d}$

(2) $\mathrm{MMD}(\mu_n, \pi)$, with $k_2(x, y) = \boldsymbol{\nabla} \cdot_x \nabla_y k(x, y)$, bounded by Prop 1 for bounded kernels.

Outline

Algorithms

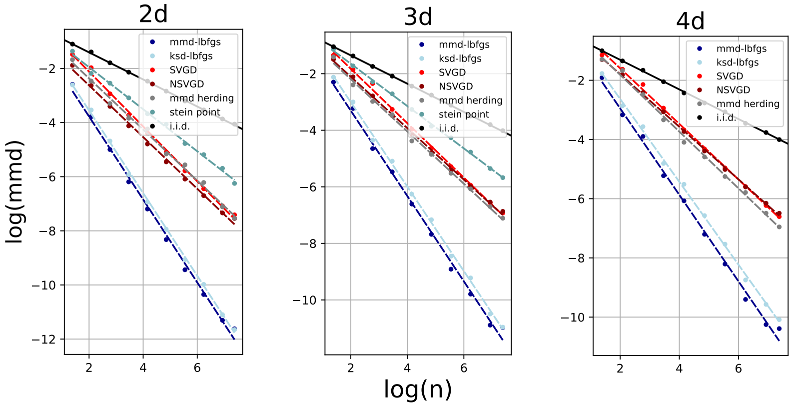
we investigate numerically the quantization properties of :

- SVGD
- MMD descent
- KSD Descent
- Kernel Herding (KH) : greedy minimization of the MMD
- Stein points (SP) : greedy minimization of the KSD

Hyperparameters:

- kernel: Gaussian, Laplace...
- bandwith of the kernel
- step-size

Quantization rates of the algorithms, $\pi = \mathcal{N}(0, 1/d\, I_d)$



Averaged over 3 runs of each algorithm, run for 1e4 iterations, where the initial particles are i.i.d. samples of π. MMD/KSD Descent use bandwidth 1; the same bandwith is used for evaluation.

d	Eval.	SVGD	MMD-lbfgs	KSD-lbfgs	KH	SP
2	**KSD**	-0.98	-1.48	-1.46	-0.84	-0.77
	MMD	-1.04	-1.60	-1.54	-0.93	-0.77
3	**KSD**	-0.91	-1.38	-1.44	-0.84	-0.78
	MMD	-0.96	-1.51	-1.49	-0.92	-0.75
4	**KSD**	-0.91	-1.35	-1.39	-0.89	–
	MMD	-0.94	-1.46	-1.40	-0.95	–
8	**KSD**	-0.84	-1.14	-1.16	–	–
	MMD	-0.77	-1.25	-1.13	–	–

Some remarks:

- The slopes remain much steeper than the Monte Carlo rate (-0.5), even when the dimension increases
- The slopes are better than our theoretical upper bounds

Robustness to evaluation discrepancy

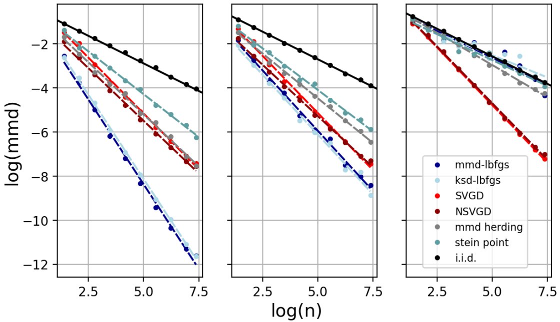


Figure: Importance of the choice of the bandwidth in the MMD evaluation metric when evaluating the final states, in 2D. From Left to Right: (evaluation) MMD bandwidth = 1, 0.7, 0.3.

- if we measure the discrepancy using a kernel with smaller bandwidth, MMD and KSD results deteriorate significantly and SVGD/NSVGD perform the best.
- likely reason : Samples of MMD and KSD with Gaussian kernel have internal structures which can affect the discrepancy at lower bandwidths.

For $\nu, \mu \in \mathcal{P}_p(\mathbb{R}^d)$, the Sliced p-Wasserstein (SW) distance is defined as:

$$d_{sw,p}(\nu, \mu) = \int_{\mathbb{S}^{d-1}} W_p(P_{\theta\#}\nu, P_{\theta\#}\mu) d\theta, \quad P_\theta : x \mapsto x \cdot \theta.$$

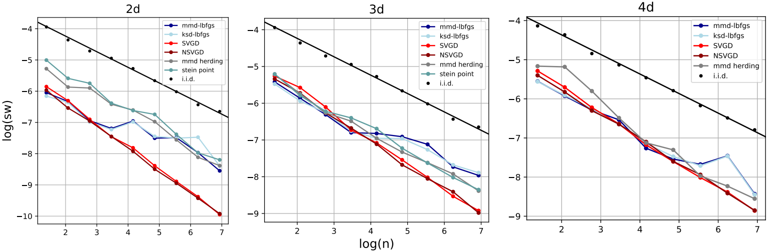


Figure: Quantization rates measured in SW distance of the algorithms $\pi = \mathcal{N}(0, {}^1\!/_d I_d)$. We use $p = 1$ and 50 random directions drawn uniformly on $\mathbb{S}^{d-1}$ to discretize the integration.

The rates for SVGD are approximately $n^{-0.72}, n^{-0.65}, n^{-0.63}$ for $d = 2, 3$, and 4. We note that these are quite close to the rate we theoretically predict for the distance between the measure on a grid in $[0, 1]^d$, and the Lebesgue measure: $d_{sw,1} \sim n^{-\frac{1}{2} - \frac{1}{2d}}$, which is $n^{-0.75}, n^{-0.67}, n^{-0.625}$ for $d = 2, 3$, and 4.

Conclusion

- MMD/ KSD descent, SVGD can create "super samples" that approximate π at fast rates

Open questions/future work:

- improve our quantization bounds for MMD/KSD (dependence in dimension, Laplace kernel?)
- obtain quantization bounds for SVGD

Thank you !

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Alternative assumption for the MMD bound:

A2. Let $k(x, y) = \eta(x - y)$ a translation invariant kernel on $\mathbb{R}^d$. Assume that $\eta \in C(\mathbb{R}^d) \cap L^1(\mathbb{R}^d)$, and that its Fourier transform verifies : $\exists C_{k,d} \geq 0$ such that $(1 + |\xi|^2)^d \leq C_{k,d} |\hat{\eta}(\xi)|^{-1}$ for any $\xi \in \mathbb{R}^d$.

A2 includes kernels which are not smooth, such as Matern kernels that can be defined through their Fourier transform $\hat{\eta}(\xi) \propto \frac{1}{(1+\|\xi\|^2)^j}$, $j \geq d$ whose RKHS correspond to Sobolev spaces of order j, and which are not smooth at $z = 0$.

Laplace kernel $k(x, y) = \exp(-\|x - y\|)$ corresponds to $j =: fracd + 12$ and does not satisfy **A2.**

A1 is satisfied by the Gaussian kernel with $C_{k,d} = (2d)!$.

Proof. By the reproducing property, we have

$$\left\| \frac{\partial^{|\alpha|} k((x_\alpha, 1), \cdot)}{\partial^{|\alpha|} x_\alpha} \right\|_{\mathcal{H}_k} = \left(\frac{\partial^{|\alpha|,|\alpha|} k((x_\alpha, 1), (x_\alpha, 1))}{\partial^{|\alpha|} x_\alpha \partial^{|\alpha|} y_\alpha} \right)^{\frac{1}{2}}.$$

Consider the Gaussian kernel, i.e. for $x, y \in \mathbb{R}^d$, $k(x, y) = e^{-\|x-y\|^2/h}$. Hence, for any $x, y \in \mathbb{R}^d$, the $|\alpha|$-th partial derivative of the kernel in both variables is equal to

$$\frac{\partial^{|\alpha|,|\alpha|} k(x, y)}{\partial^{|\alpha|} x_\alpha \partial^{|\alpha|} y_\alpha} = (-1)^{|\alpha|} \frac{\partial^{2|\alpha|} e^{-t^2}}{\partial^{2|\alpha|} t} = (-1)^{|\alpha|} e^{-t^2} h_{2|\alpha|}(t)$$

where h_u, $u \geq 0$ denotes the u-th Hermite polynomial. In particular for $x = y$, i.e. $t = 0$, evaluations of Hermite polynomials at zero correspond to the well-known Hermite numbers $(-1)^{|\alpha|} 2^{|\alpha|} (2|\alpha| - 1)!!$ with $(2|\alpha| - 1)!! = 1 \times 3 \times \cdots \times (2|\alpha| - 1)$. We conclude using $|\alpha| \leq d$.

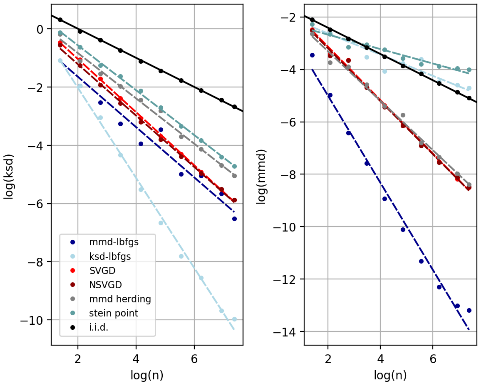

Figure: Quantization rates of the algorithms at study when the target distribution is a 2D-Gaussian mixture distribution with variance 0.3, centred at [1,0] and [-1,0]. We evaluate them using MMD and KSD with bandwidth 1. We run algorithms under the same setting as the 2-4D experiments on Figure 30.

L-BFGS

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

$$x_{l+1} = x_l - \gamma_l B_l^{-1} \nabla F(x_l) := x_l + \gamma_l d_l \tag{1}$$

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

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

$$B_{l+1}^{-1} = \left(I - \frac{\Delta x_l y_l^T}{y_l^T \Delta x_l} \right) B_l^{-1} \left(I - \frac{y_l \Delta x_l^T}{y_l^T \Delta x_l} \right) + \frac{\Delta x_l \Delta x_l^T}{y_l^T \Delta x_l}$$

$$\text{where} \quad \begin{aligned} \Delta x_l &= x_{l+1} - x_l \\ y_l &= \nabla F(x_{l+1}) - \nabla F(x_l) \end{aligned}$$

Step2. (requires F and ∇F) A line-search is performed to find the best step-size in (1) :

$$\begin{aligned} F(x_l + \gamma_l d_l) &\leq F(x_l) + c_1 \gamma_l \nabla F(x_l)^T d_l \\ \nabla F(x_l + \gamma_l d_l)^T d_l &\geq c_2 \nabla F(x_l)^T d_l \end{aligned}$$

Kernel Herding (KH) and Stein Points (SP)

They attempt to solve MMD or KSD quantization in a greedy manner, i.e. by sequentially constructing μ_n, adding one new particle at each iteration to minimize MMD/KSD.

Kernel Herding (KH) for the MMD [Chen et al., 2012]:

$$x^{n+1} = \underset{x \in \mathbb{R}^d}{\operatorname{argmax}} \langle w_n, k(x,.) \rangle_{\mathcal{H}_k}$$

$$w_{n+1} = w_n + m_\pi - k(x_{n+1},.)$$

[Bach et al., 2012] obtain a linear rate of convergence $\mathcal{O}(e^{-bn})$

- if the mean embedding $m_\pi = \mathbb{E}_{x\sim\pi}[k(x,.)]$ lies in the relative interior of the marginal polytope *convexhull*$(\{k(x,.), x \in \mathbb{R}^d\})$ with distance b away from the boundary
- however for infinite-dimensional kernels $b = 0$ and the rate does not hold.

Stein Points for the KSD [Chen et al., 2018] greedily minimizes the KSD similarly. The authors establish a $\mathcal{O}((\log(n)/n)^{\frac{1}{2}})$ rate, which seem slower than their empirical observations.

Forward method for the KL

Problem: $\nabla_{W_2} \mathrm{KL}(\mu_n|\pi) = \nabla \log\left(\frac{\mu_n}{\pi}\right)$ 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. with[2] :

1. **Kernel Density Estimation (KDE)**:

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

Then,

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

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

[2] assume 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

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

Then,

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

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

$$\implies \nabla_{W_2} \mathrm{KL}(\mu_n | \pi)(.) \approx -(\nabla V(.) + \sum_{i=1}^{N} \frac{\nabla k(. - X_n^i)}{\sum_{m=1}^{N} k(X_n^i - X_n^m)} + \frac{\sum_{i=1}^{N} \nabla k(. - X_n^i)}{\sum_{i=1}^{N} k(. - X_n^i)})$$