Sampling through Optimization of Divergences

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Outline

Why sampling?

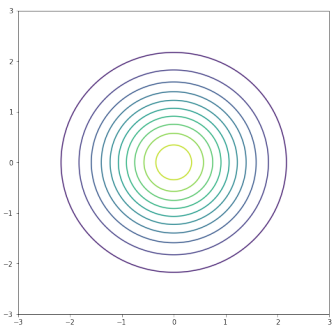
Suppose you are interested in some target probability distribution on $\mathbb{R}^d$, denoted μ^*, and you have access only to partial information, e.g.:

1. its unnormalized density (as in Bayesian inference)
2. a discrete approximation $\frac{1}{m}\sum_{k=1}^{m}\delta_{x_i} \approx \mu^*$ (e.g. i.i.d. samples, iterates of MCMC algorithms...)

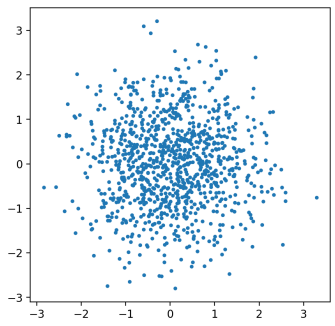
Problem: approximate $\mu^* \in \mathcal{P}(\mathbb{R}^d)$ by a finite set of n points $x_1, \dots, x_n$, e.g. to compute functionals $\int_{\mathbb{R}^d} f(x)d\mu^*(x)$.

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

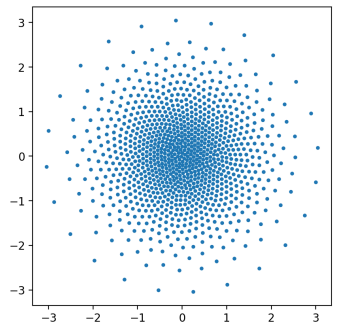
$$\left| \frac{1}{n}\sum_{i=1}^{n} f(x_i) - \int_{\mathbb{R}^d} f(x)d\mu^*(x) \right|.$$



a Gaussian density



I.i.d. samples.



Some discrete approximation

Example 1: Bayesian inference

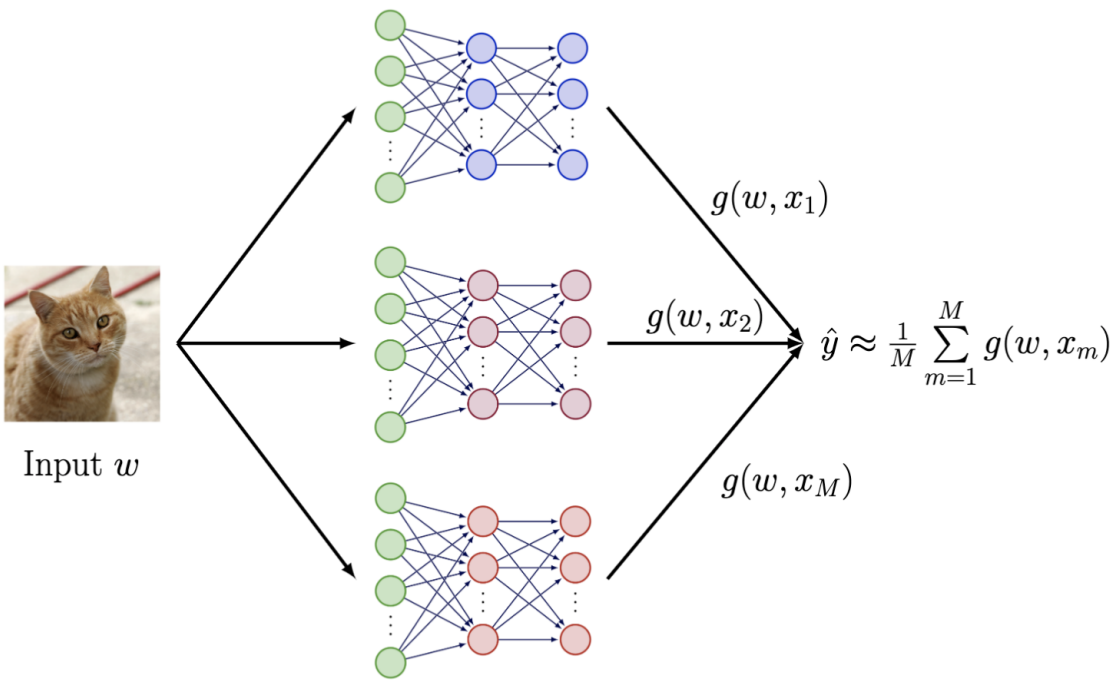
We want to sample from

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

Ensemble prediction for a new input w:

$$\hat{y} = \underbrace{\int_{\mathbb{R}^d} g(w, x) d\mu^*(x)}_{\text{"Bayesian model averaging"}}$$

Predictions of models parametrized by $x \in \mathbb{R}^d$ are reweighted by $\mu^*(x)$.

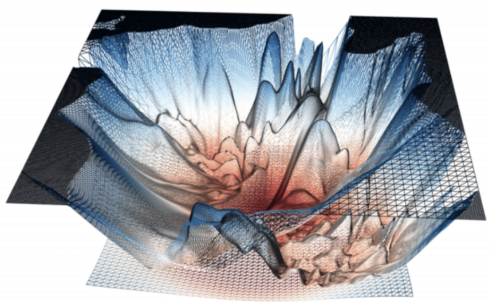


Difficult cases (in practice and in theory)

Recall that

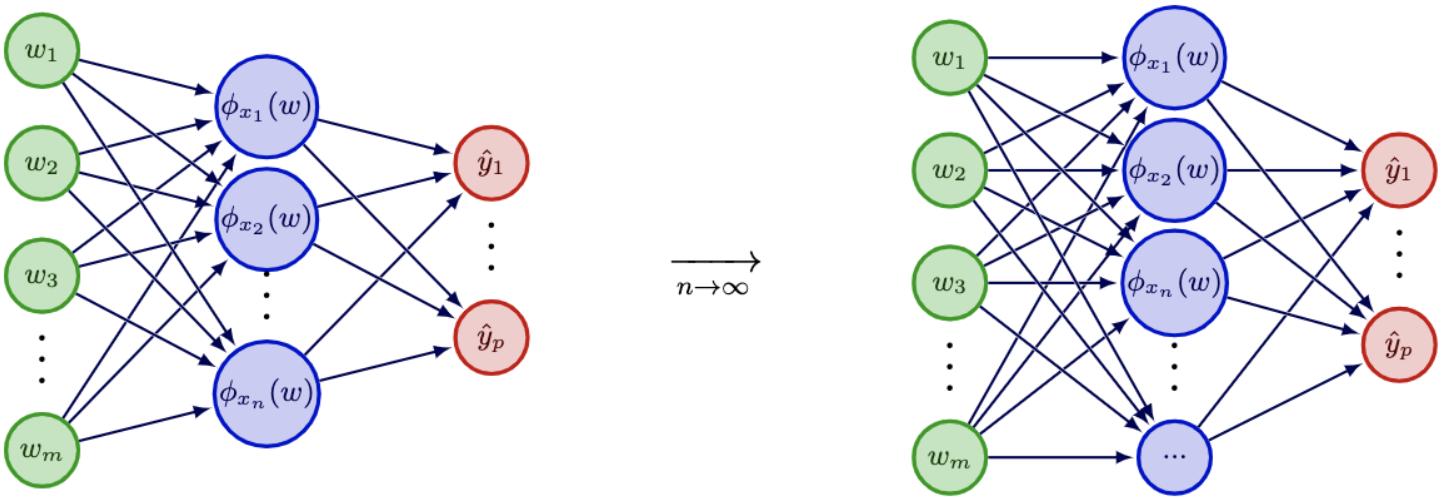
$$\mu^*(x) \propto \exp\left(-V(x)\right), \quad V(\theta) = \underbrace{\sum_{i=1}^{m} \|y_i - g(w_i, x)\|^2}_{\text{loss}} + \frac{\|x\|^2}{2}.$$

- if V is convex (e.g. $g(w, x) = \langle w, x \rangle$) many sampling methods (e.g. Langevin Monte Carlo) are known to work quite well [Durmus and Moulines, 2016, Vempala and Wibisono, 2019]
- but if its not (e.g. $g(w, x)$ 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.

Example 2 : Regression with infinite width NN



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

Define the target distribution $\mu^* \in \arg\min \mathcal{F}(\mu)$. Optimising the neural network $\iff$ approximating μ^* [Chizat and Bach, 2018, Mei et al., 2018].

If $y(w) = \frac{1}{m} \sum_{i=1}^{m} \phi_{x_i}(w)$ is generated by a neural network (as in the student-teacher network setting), then $\mathcal{F}$ can be identified to an MMD [Arbel et al., 2019].

Outline

Sampling as optimization over probability distributions

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

The sampling task can be recast as an optimization problem:

$$\mu^* = \underset{\mu \in \mathcal{P}_2(\mathbb{R}^d)}{\arg\min}\ D(\mu|\mu^*) := \mathcal{F}(\mu),$$

where D is a **dissimilarity functional**, for instance:

- a f-divergence: $\int f\left(\frac{\mu}{\mu^*}\right) d\mu^*, \quad f$ convex, $f(1) = 0$
- an integral probability metric: $\sup_{f \in \mathcal{G}} \left|\int f d\mu - \int f d\mu^*\right|$
- an optimal transport distance...

Starting from an initial distribution $\mu_0 \in \mathcal{P}_2(\mathbb{R}^d)$, one can then consider the **Wasserstein-2* gradient flow** of $\mathcal{F}$ over $\mathcal{P}_2(\mathbb{R}^d)$ to transport μ_0 to μ^*.

* $W_2^2(\nu, \mu) = \inf_{s \in \Gamma(\nu,\mu)} \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x - y\|^2 \, ds(x, y)$, where $\Gamma(\nu, \mu)$= couplings between ν, μ.

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 $\mu, \nu \in \mathcal{P}(\mathbb{R}^d)$, $\nu - \mu \in \mathcal{P}(\mathbb{R}^d)$:

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

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

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

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

It can be implemented by the deterministic process:

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

Particle system/Gradient descent approximating the WGF

Space/time discretization : Introduce a particle system $x_0^1, \dots, x_0^n \sim \mu_0$, a step-size γ, and at each step:

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

In particular, the algorithm above simply corresponds to gradient descent.

We consider several questions:

- what can we say as time goes to infinity ? (optimization error)
  $\Longrightarrow$ heavily linked with the geometry (convexity, smoothness in the Wasserstein sense) of the loss
- (for minimizers) what can we say as the number of particles grow ? ("quantization" error)

Outline

Loss function for the unnormalized densities - the KL

Many possibilities for the choice of $\mathrm{D}(\cdot|\mu^*)$ among Wasserstein distances, f-divergences, Integral Probability Metrics...

For instance, D could be the Kullback-Leibler divergence:

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

The KL as an objective is convenient when the unnormalized density of μ^* is known since it **does not depend on the normalization constant!**

Indeed writing $\mu^*(x) = e^{-V(x)}/Z$ we have:

$$\mathrm{KL}(\mu|\mu^*) = \int_{\mathbb{R}^d} \log\left(\frac{\mu}{e^{-V}}(x)\right) d\mu(x) + \log(Z).$$

But, it is not convenient when we have a discrete approximation of μ^*. Also, we cannot evaluate it for discrete μ.

KL Gradient flow in practice

- The gradient flow of the KL can be implemented via the Probability Flow (ODE):

$$d\tilde{x}_t = -\nabla \log\left(\frac{\mu_t}{\mu^*}\right)(\tilde{x}_t)dt \tag{1}$$

or the Langevin diffusion (SDE):

$$dx_t = \nabla \log \mu^*(x_t)dt + \sqrt{2}dB_t \tag{2}$$

(they share the same marginal $(\mu_t)_{t\geq 0}$)

- (2) can be discretized in time as Langevin Monte Carlo (LMC) [Roberts and Tweedie, 1996]

$$x_{m+1} = x_m + \gamma \nabla \log \mu^*(x_m) + \sqrt{2\gamma}\epsilon_m, \quad \epsilon_m \sim \mathcal{N}(0, \mathrm{Id}_{\mathbb{R}^d}).$$

- (1) can be approximated by a particle system (e.g. SVGD [Liu, 2017, He et al., 2022])
- however MCMC methods suffer an integral approximation error of order $\mathcal{O}(n^{-1/2})$ if we use $\mu_n = \frac{1}{n}\sum_{i=1}^n \delta_{x_i}$ (x_i iterates of MCMC) [Łatuszyński et al., 2013]

Another f-divergence?

- The chi-square divergence:

$$\chi^2(\mu \parallel \mu^*) := \begin{cases} \int \left(\frac{\mathrm{d}\mu}{\mathrm{d}\mu^*} - 1\right)^2 \mathrm{d}\mu^* & \mu \ll \mu^* \\ +\infty & \text{otherwise.} \end{cases}$$

  not convenient neither when μ^*'s unnormalized density is known, or if we have a discrete approximation.
- χ^2-gradient requires the normalizing constant of μ^*: $\nabla \frac{\mu}{\mu^*}$
- However, the GF of chi-square has interesting properties [Chewi et al., 2020, Craig et al., 2022] (e.g. linear convergence under Poincaré inequality on μ^*, whereas the KL flow requires log-Sobolev)

Losses for the discrete case

D could be the MMD (Maximum Mean Discrepancy):

$$\mathrm{MMD}^2(\mu, \mu^*) = \sup_{f \in \mathcal{H}_k, \|f\|_{\mathcal{H}_k} \leq 1} \left| \int f d\mu - \int f d\mu^* \right|$$

$$\iint_{\mathbb{R}^d} k(x,y) d\mu(x) d\mu(y)$$

$$+ \iint_{\mathbb{R}^d} k(x,y) d\mu^*(x) d\mu^*(y) - 2 \iint_{\mathbb{R}^d} k(x,y) d\mu(x) d\mu^*(y).$$

where $k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is a p.s.d. kernel (e.g. $k(x,y) = e^{-\|x-y\|^2}$).

It is convenient when we have a discrete approximation of μ^* (to approximate integrals).

Why we care about the loss

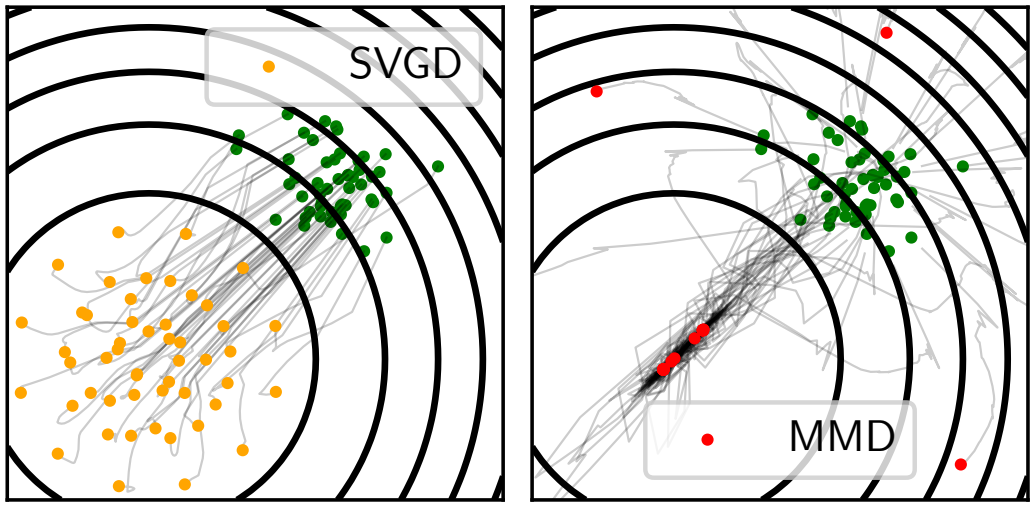


Figure: Toy example with 2D standard Gaussian. The green points represent the initial positions of the particles. The light grey curves correspond to their trajectories under the different v_{μ_t}.

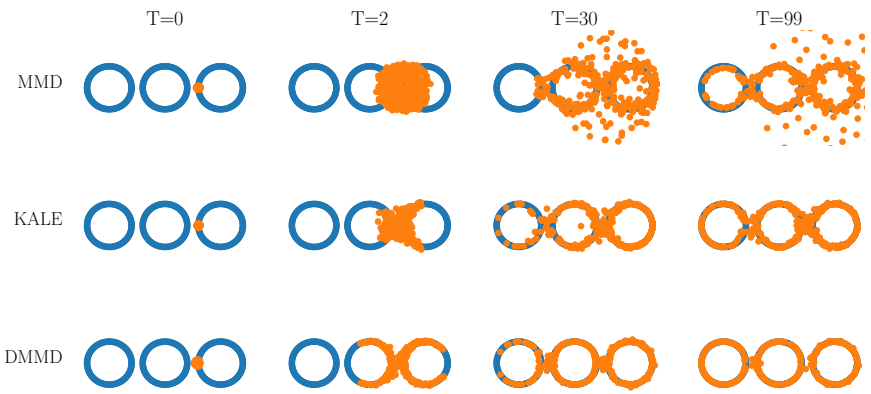
Gradient flow of the KL to a Gaussian $\mu^*(x) \propto e^{-\frac{\|x\|^2}{2}}$ is well-behaved, but not the MMD.

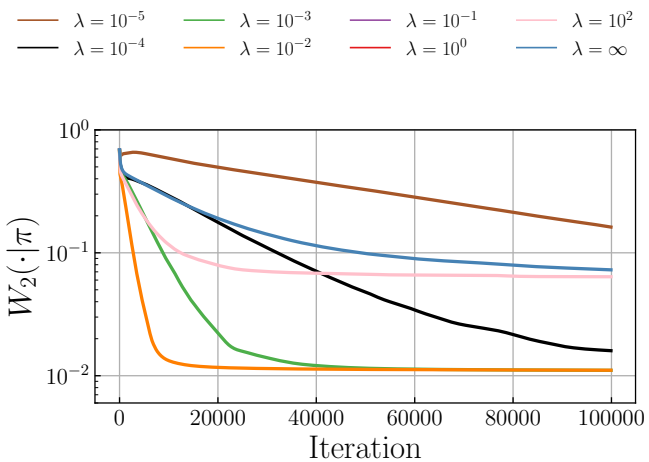
A proposal†: Interpolate between MMD and χ^2

"De-Regularized MMD" leverages the variational formulation of χ^2:

$$\mathrm{DMMD}(\mu||\mu^*) = (1+\lambda)\Big\{ \max_{h\in\mathcal{H}} \int h d\mu - \int h d\mu^* - \frac{1}{4}\int h^2 d\mu^* - \frac{1}{4}\lambda\|h\|^2_{\mathcal{H}} \Big\}$$

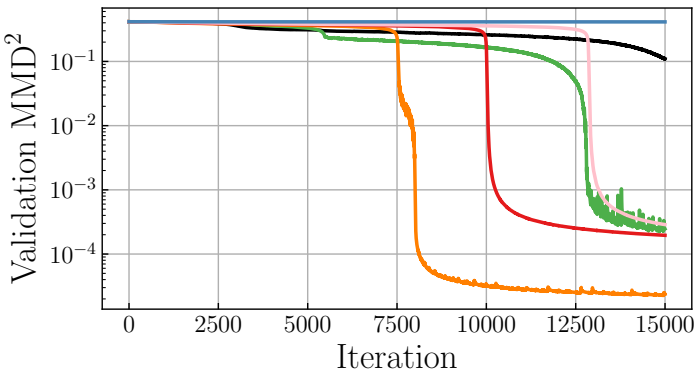
Can be written in closed-form if μ, μ^* are discrete (depends on λ and kernel matrices over samples of μ, μ^*. **It is a divergence for any λ.**
A similar idea was proposed for the KL, yielding Kale divergence [Glaser et al., 2021] but was not closed-form.

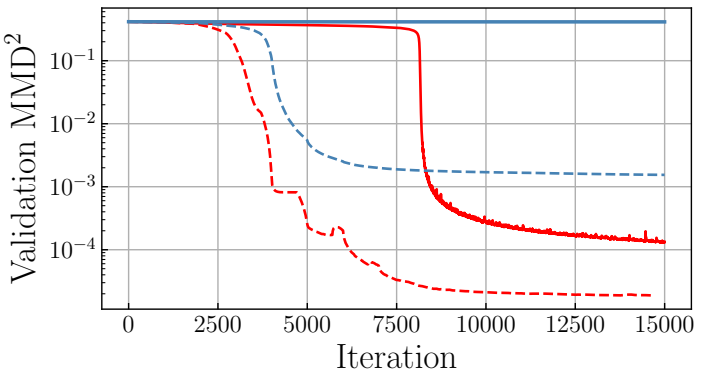




†with H. Chen, A. Gretton, P. Glaser (UCL), A. Mustafi, B. Sriperumbudur (CMU)

Student-teacher networks experiment‡





- the teacher network $w \mapsto \Psi_{\mu^*}(w)$ is given by M particles $(\xi_1, ..., \xi_M)$ which are fixed during training $\Longrightarrow \mu = \frac{1}{M}\sum_{j=1}^{M} \delta_{\xi_j}$
- the student network $w \mapsto \Psi_{\mu}(w)$ has n particles $(x_1, ..., x_n)$ that are initialized randomly $\Longrightarrow \mu = \frac{1}{n}\sum_{i=1}^{n} \delta_{x_j}$

$$\min_{\mu} \mathbb{E}_{w\sim P_{data}}\left[(\Psi_{\mu^*}(w) - \Psi_{\mu}(w)^2\right]$$

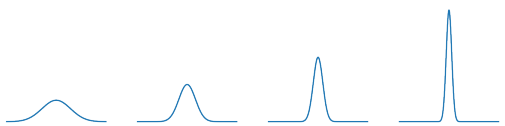
$$\Longleftrightarrow \min_{\mu} \mathrm{MMD}(\mu, \mu^*) \text{ with } k(x, x') = \mathbb{E}_{w\sim P_{data}}[\phi_{x'}(w)\phi_x(w)].$$

‡Same setting as [Arbel et al., 2019].

Another idea - "Mollified" discrepancies

Examples of mollifiers/kernels (Gaussian, Laplace, Riesz-s):

$$k_\epsilon^g(x) := \frac{\exp\left(-\frac{\|x\|_2^2}{2\epsilon^2}\right)}{Z^g(\epsilon)}, \quad k_\epsilon^g(x) := \frac{\exp\left(-\frac{\|x\|_2}{\epsilon}\right)}{Z^l(\epsilon)}, \quad k_\epsilon^s(x) := \frac{1}{(\|x\|_2^2 + \epsilon^2)^{s/2} Z^r(s,\epsilon)}$$



- Mollified chi-square [Li et al., 2022, Craig et al., 2022]:

$$\mathcal{E}_\epsilon(\mu) \quad = \quad \int \left(k_\epsilon * \frac{\mu}{\sqrt{\mu^*}}\right)(x) \frac{\mu}{\sqrt{\mu^*}}(x)\,\mathrm{d}x \quad \xrightarrow[\varepsilon \to 0]{} \quad \chi^2(\mu|\mu^*) \; + \; 1$$

- Mollified KL[§] [Craig and Bertozzi, 2016]:

$$\mathrm{KL}(k_\epsilon \star \mu|\mu^*) \xrightarrow[\varepsilon \to 0]{} \mathrm{KL}(\mu|\mu^*)$$

[§] Also ongoing work with Tom Huix (CMAP).

Outline

(Geodesically)-convex and smooth losses

$\mathcal{F}$ is said to be λ-displacement convex if along W_2 geodesics $(\rho_t)_{t\in[0,1]}$:

$$\mathcal{F}(\rho_t) \leq (1-t)\mathcal{F}(\rho_0) + t\mathcal{F}(\rho_1) - \frac{\lambda}{2}t(1-t)W_2^2(\rho_0,\rho_1) \qquad \forall\, t \in [0,1]. \quad (3)$$

The **Wasserstein Hessian** of a functional $\mathcal{F} : \mathcal{P}_2(\mathbb{R}^d) \to \mathbb{R}$ at μ is defined for any $\psi \in \mathcal{C}_c^\infty(\mathbb{R}^d)$ as:

$$\mathrm{Hess}_\mu\, \mathcal{F}(\psi,\psi) := \frac{\mathrm{d}^2}{\mathrm{d}t^2}\bigg|_{t=0} \mathcal{F}(\mu_t)$$

where $(\mu_t, v_t)_{t\in[0,1]}$ is a Wasserstein geodesic with $\mu_0 = 0, v_0 = \nabla\psi$.

$$\mathcal{F} \text{ is } \lambda\text{-displacement convex} \iff \mathrm{Hess}_\mu\, \mathcal{F}(\psi,\psi) \geq \lambda \|\nabla\psi\|^2_{L^2(\mu)}$$

(See [Villani, 2009, Proposition 16.2]). In an analog manner we can define smooth functionals as functionals with upper bounded Hessians.

Guarantees for Wasserstein gradient descent

Consider Wasserstein gradient descent (Euler discretization of Wasserstein gradient flow)

$$\mu_{l+1} = (\mathrm{Id} - \gamma \nabla \mathcal{F}'(\mu_l))_{\#}\mu_l$$

Assume $\mathcal{F}$ is M-smooth. Then, we have a descent lemma:

$$\mathcal{F}(\mu_{l+1}) - \mathcal{F}(\mu_l) \leq -\gamma \left(1 - \frac{\gamma}{2} M\right) \|\nabla \mathcal{F}'(\mu_l)\|^2_{L^2(\mu_l)}.$$

Moreover, if $\mathcal{F}$ is λ-convex, we have the global rate

$$\mathcal{F}(\mu_L) \leq \frac{W_2^2(\mu_0, \mu^*)}{2\gamma L} - \frac{\lambda}{L} \sum_{l=0}^{L} W_2^2(\mu_l, \mu^*).$$

(so the barrier term degrades with λ).

Some examples

- Let $\mu^* \propto e^{-V}$, we have [Wibisono, 2018]

$$\mathrm{Hess}_\mu \mathrm{KL}(\psi, \psi) = \int \left[\langle \mathrm{H}V(x) \nabla\psi(x), \nabla\psi(x) \rangle + \|\mathrm{H}\psi(x)\|_{HS}^2 \right] q(x)\, \mathrm{d}x.$$

  If V is m-strongly convex, then the KL is m-geo. convex; however it is not smooth (Hessian is unbounded). Similar story for χ^2-square [Ohta and Takatsu, 2011].

- For a M-smooth kernel k [Arbel et al., 2019]

$$\mathrm{Hess}_\mu \mathrm{MMD}^2(\psi, \psi) = \left\| \int \nabla\phi(x)^\top \nabla_1 k(x, \cdot) d\mu(x) \right\|_{\mathcal{H}}^2 +$$

$$2 \int \nabla\phi(x)^\top \left(\int \mathrm{H}_1 k\,(x, z)\, d\rho(z) - \int \mathrm{H}_1 k\,(x, z)\, d\mu^*(z) \right) \nabla\phi(x) d\mu(x)$$

  It is M-smooth but not geodesically convex (Hessian lower bounded by a big negative constant)

- Partial results for other discrepancies (De-Regularized MMD, mollified chi-square [Li et al., 2022] and KL)

Outline

What is known

What can we say on $\inf_{x_1,\dots,x_n} D(\mu_n|\mu^*)$ where $\mu_n = \sum_{i=1}^n \delta_{x_i}$?

- Quantization rates for the Wasserstein distance [Kloeckner, 2012, Mérigot et al., 2021]

$$W_2(\mu_n, \mu^*) \sim O(n^{-\frac{1}{d}})$$

- Forward KL [Li and Barron, 1999]: for every $g_P = \int k_\epsilon(\cdot - w)dP(w)$,

$$\arg\min_{\mu_n} \mathrm{KL}(\mu^*|k_\epsilon \star \mu_n) \leq \mathrm{KL}(\mu^*|g_P) + \frac{C^2_{\mu^*,P}\gamma}{n}$$

where $C^2_{\mu^*,P} = \int \frac{\int k_\epsilon(x-m)^2 dP(m)}{(\int k_\epsilon(x-w)dP(w))^2} d\mu^*(x)$, and $\gamma = 4\log\left(3\sqrt{e}+a\right)$ is a constant depending on ϵ with $a = \sup_{z,z'\in\mathbb{R}^d} \log\left(k_\epsilon(x-z)/k_\epsilon(x-z')\right)$.

Recent results

- For smooth and bounded kernels in [Xu et al., 2022] and μ^* with exponential tails, we get using Koksma-Hlawka inequality

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

  This bounds the integral error for $f \in \mathcal{H}_k$ by Cauchy-Schwartz:

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

- For the reverse KL (joint work with Tom Huix) we get (in the well-specified case) adapting the proof of [Li and Barron, 1999]:

$$\min_{\mu_n} \mathrm{KL}(k_\epsilon \star \mu | \mu^*) \leq C_{\mu^*}^2 \frac{\log(n) + 1}{n}.$$

A numerical example from [Li et al., 2022]

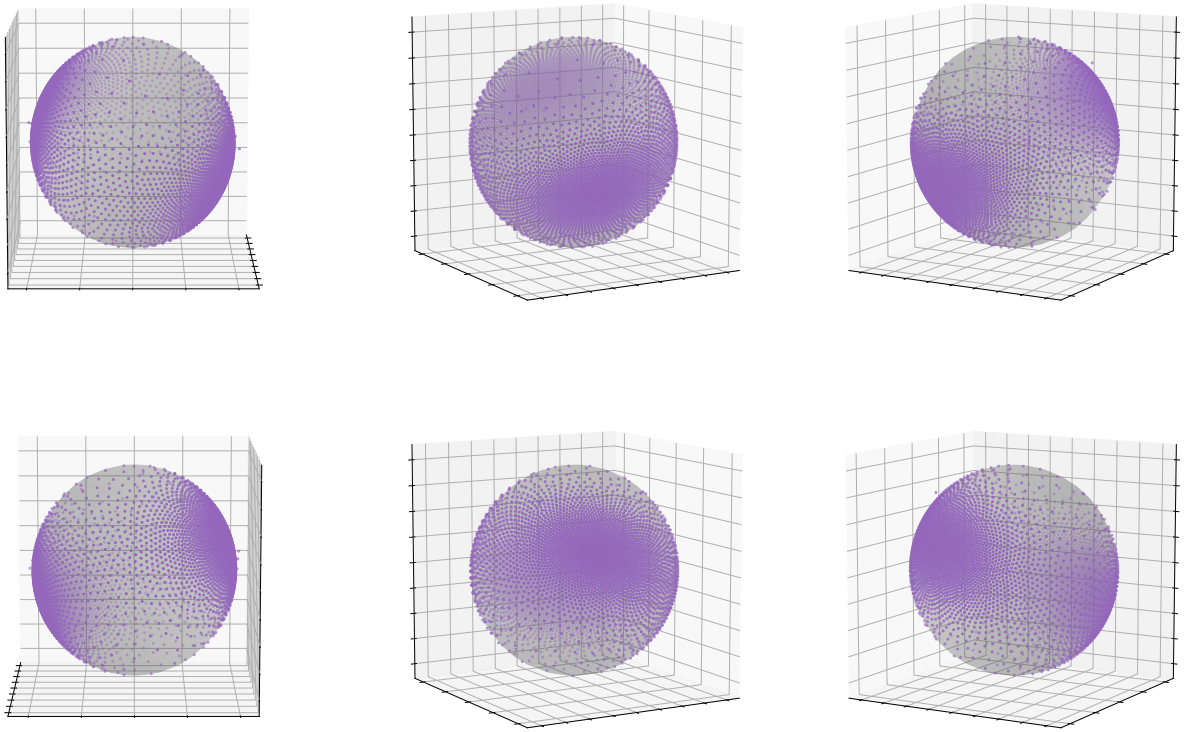


Figure: Sampling from the von Mises-Fisher distribution obtained by constraining a 3-dimensional Gaussian to the unit sphere. The unit-sphere constraint is enforced using the dynamic barrier method and the shown results are obtained using MIED with Riesz kernel and $s = 3$. The six plots are views from six evenly spaced angles.

Another numerical example from [Li et al., 2022]

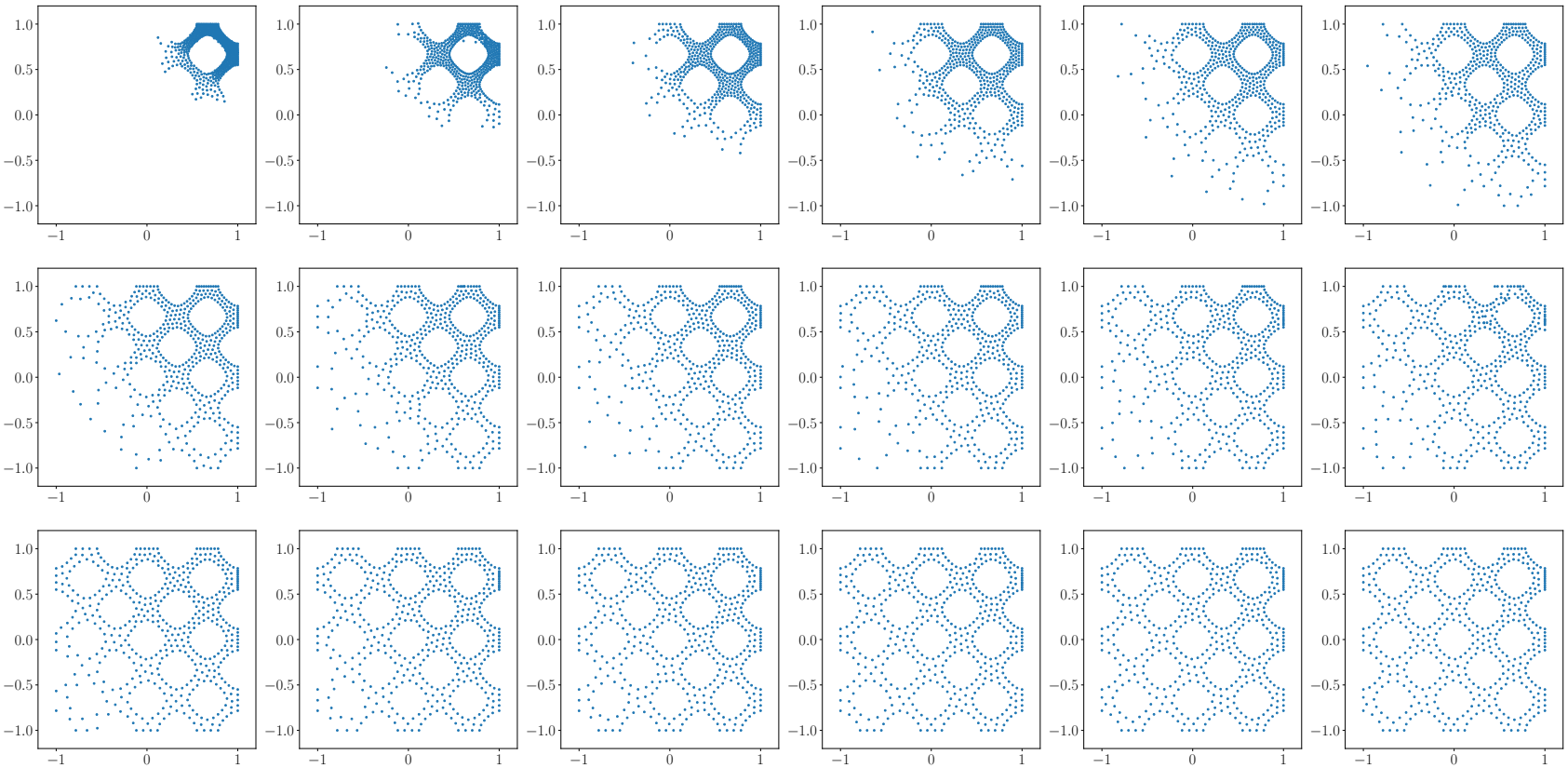


Figure: Uniform sampling of the region $\{(x, y) \in [-1, 1]^2 : (\cos(3\mu^* x) + \cos(3\mu^* y))^2 < 0.3\}$ using MIED with a Riesz mollifier ($s = 3$) where the constraint is enforced using the dynamic barrier method. The plot in row i column j shows the samples at iteration $100 + 200(6i + j)$. The initial samples are drawn uniformly from the top-right square $[0.5, 1.0]^2$.

Open questions

- Finite-particle/quantization guarantees are still missing for many losses or in the non-well specified case

$$\mathrm{D}(\mu_n||\mu^*) \leq f(n, \mu^*)?$$

- How to improve the performance of the algorithms for highly non-log concave targets? e.g. through sequence of targets $(\mu^*)_{t\in[0,1]}$ interpolating between μ_0 and μ^*?

References (with code):

- Maximum Mean Discrepancy Gradient Flow. Arbel, M., Korba, A., Salim, A., and Gretton, A. (Neurips 2019).
- Accurate quantization of measures via interacting particle-based optimization. Xu, L., Korba, A., and Slep$^{\vee}$cev, D. (ICML 2022).
- Sampling with mollified interaction energy descent. Li, L., Liu, Q., Korba, A., Yurochkin, M., and Solomon, J. (ICLR 2023).

References I

Ambrosio, L., Gigli, N., and Savaré, G. (2008).

Gradient flows: in metric spaces and in the space of probability measures.
Springer Science & Business Media.

Arbel, M., Korba, A., Salim, A., and Gretton, A. (2019).

Maximum mean discrepancy gradient flow.
In *Advances in Neural Information Processing Systems*, pages 6481–6491.

Chewi, S., Le Gouic, T., Lu, C., Maunu, T., and Rigollet, P. (2020).

Svgd as a kernelized wasserstein gradient flow of the chi-squared divergence.
Advances in Neural Information Processing Systems, 33:2098–2109.

Chizat, L. and Bach, F. (2018).

On the global convergence of gradient descent for over-parameterized models using optimal transport.
Advances in neural information processing systems, 31.

Chopin, N., Crucinio, F. R., and Korba, A. (2023).

A connection between tempering and entropic mirror descent.
arXiv preprint arXiv:2310.11914.

Craig, K. and Bertozzi, A. (2016).

A blob method for the aggregation equation.
Mathematics of computation, 85(300):1681–1717.

Craig, K., Elamvazhuthi, K., Haberland, M., and Turanova, O. (2022).

A blob method method for inhomogeneous diffusion with applications to multi-agent control and sampling.
arXiv preprint arXiv:2202.12927.

Durmus, A. and Moulines, E. (2016).

Sampling from strongly log-concave distributions with the unadjusted langevin algorithm.
arXiv preprint arXiv:1605.01559, 5.

References II

Glaser, P., Arbel, M., and Gretton, A. (2021).

Kale flow: A relaxed kl gradient flow for probabilities with disjoint support.
Advances in Neural Information Processing Systems, 34:8018–8031.

He, Y., Balasubramanian, K., Sriperumbudur, B. K., and Lu, J. (2022).

Regularized stein variational gradient flow.
arXiv preprint arXiv:2211.07861.

Kloeckner, B. (2012).

Approximation by finitely supported measures.
ESAIM: Control, Optimisation and Calculus of Variations, 18(2):343–359.

Łatuszyński, K., Miasojedow, B., and Niemiro, W. (2013).

Nonasymptotic bounds on the estimation error of mcmc algorithms.
Bernoulli, 19(5A):2033–2066.

Li, J. and Barron, A. (1999).

Mixture density estimation.
Advances in neural information processing systems, 12.

Li, L., Liu, Q., Korba, A., Yurochkin, M., and Solomon, J. (2022).

Sampling with mollified interaction energy descent.
arXiv preprint arXiv:2210.13400.

Liu, Q. (2017).

Stein variational gradient descent as gradient flow.
In *Advances in neural information processing systems*, pages 3115–3123.

References III

Mei, S., Montanari, A., and Nguyen, P.-M. (2018).

A mean field view of the landscape of two-layer neural networks.
Proceedings of the National Academy of Sciences, 115(33):E7665–E7671.

Mérigot, Q., Santambrogio, F., and Sarrazin, C. (2021).

Non-asymptotic convergence bounds for wasserstein approximation using point clouds.
Advances in Neural Information Processing Systems, 34:12810–12821.

Ohta, S.-i. and Takatsu, A. (2011).

Displacement convexity of generalized relative entropies.
Advances in Mathematics, 228(3):1742–1787.

Roberts, G. O. and Tweedie, R. L. (1996).

Exponential convergence of langevin distributions and their discrete approximations.
Bernoulli, pages 341–363.

Vempala, S. and Wibisono, A. (2019).

Rapid convergence of the unadjusted langevin algorithm: Isoperimetry suffices.
Advances in neural information processing systems, 32.

Villani, C. (2009).

Optimal transport: old and new, volume 338.
Springer.

Wibisono, A. (2018).

Sampling as optimization in the space of measures: The langevin dynamics as a composite optimization problem.
In *Conference on Learning Theory*, pages 2093–3027. PMLR.

References IV

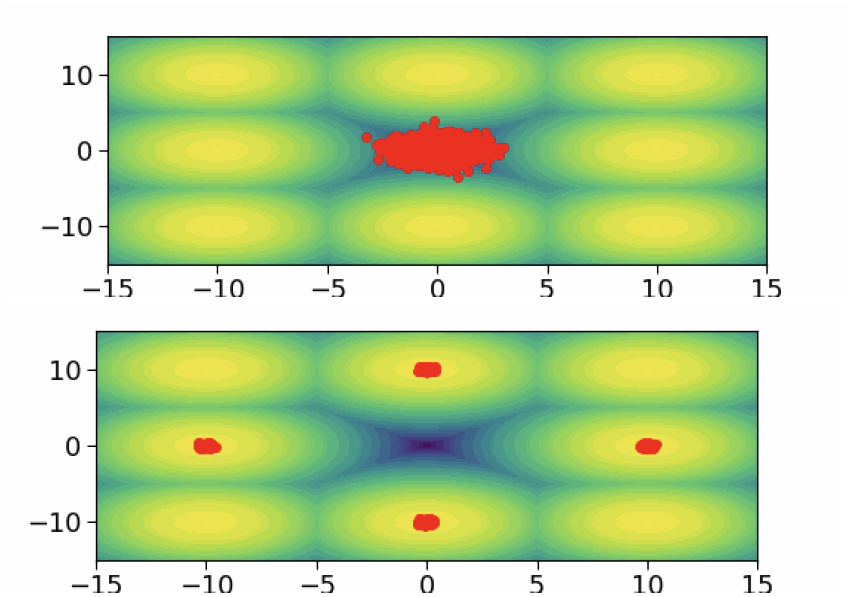
Xu, L., Korba, A., and Slepčev, D. (2022).

Accurate quantization of measures via interacting particle-based optimization.

International Conference on Machine Learning.

Mixture of Gaussians

Langevin Monte Carlo on a mixture of Gaussians does not manage to target all modes in reasonable time, even in low dimensions.

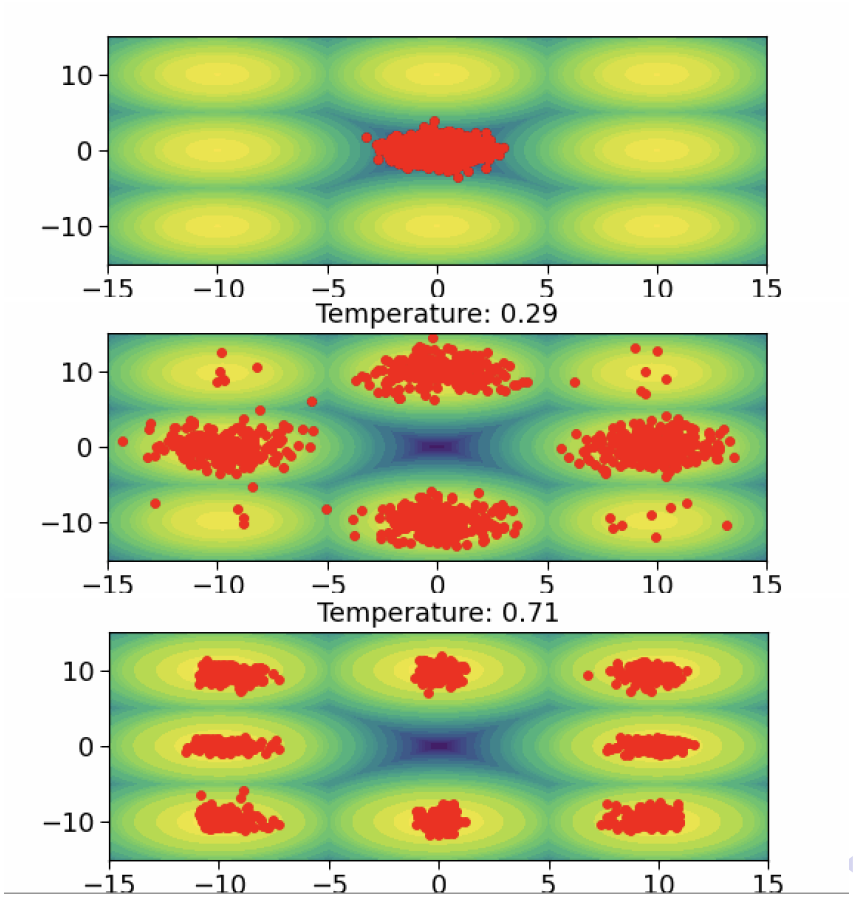


Annealing

One possible fix : sequence of tempered targets as:

$$\mu_\beta^* \propto \mu_0^\beta (\mu^*)^{1-\beta}, \quad \beta \in [0,1]$$

Can be seen as **discretized Fisher-Rao gradient flow** [Chopin et al., 2023].



Other tempered path

"Convolutional path" ($\beta \in [0, +\infty[$) frequently used in Diffusion Models

$$\mu_\beta^* = \frac{1}{\sqrt{1-\beta}}\mu_0\left(\frac{\cdot}{\sqrt{1-\beta}}\right) * \frac{1}{\sqrt{\beta}}\mu^*\left(\frac{\cdot}{\sqrt{\beta}}\right)$$

(vs "geometric path" $\mu_\beta^* \propto \mu_0^\beta (\mu^*)^{1-\beta}$)