

Gradient Flows on the Maximum Mean Discrepancy

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First International Conference on Prob-
abilistic Numerics (Probnum 2025)

Outline

MMD and MMD flow

- Introduction to MMD as an integral probability metric
- Connection with neural net training
- Wasserstein-2 Gradient Flow on the MMD
- Convergence: adaptive kernel
 - Neural Net implementation
 - Interpolation to χ^2

Arbel, Korba, Salim, G., Maximum Mean Discrepancy Gradient Flow (NeurIPS 2019)
Galashov, De Bortoli, G., Deep MMD Gradient Flow without adversarial training
(ICLR 2025)

Chen, Mustafi, Glaser, Korba. G, Sriperumbudur (De)-regularized Maximum
Mean Discrepancy Gradient Flow (submitted JMLR)

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Main motivation: gradient flow when the target distribution represented by samples

- A different kind of particle flow to diffusion models
- Neural network training dynamics

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The MMD, and MMD flow

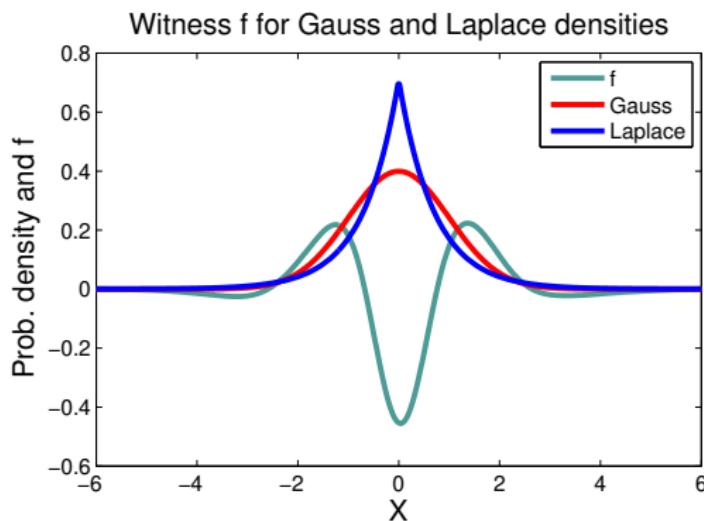
The MMD: an integral probability metric

Maximum mean discrepancy: smooth function for P vs Q

$$MMD(P, Q; F) := \sup_{\|f\| \leq 1} [\mathbb{E}_P f(X) - \mathbb{E}_Q f(Y)]$$

$$f(x) = \langle f, \varphi(x) \rangle_{\mathcal{H}}$$

$$\langle \varphi(x), \varphi(x') \rangle_{\mathcal{H}} = k(x, x')$$



The MMD: an integral probability metric

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For characteristic RKHS \mathcal{H} , $MMD(P, Q) = 0$ iff $P = Q$

Other choices for witness function class:

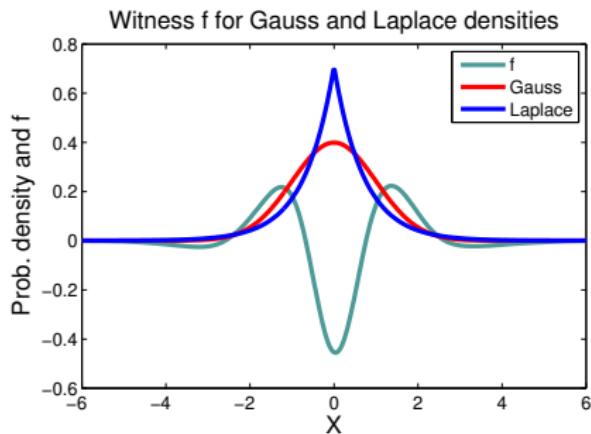
- Bounded continuous [Dudley, 2002]
- Bounded variation 1 (Kolmogorov metric) [Müller, 1997]
- Bounded Lipschitz (Wasserstein distances) [Dudley, 2002]

The MMD and witness in closed form

The MMD:

$$MMD(P, Q)$$

$$= \sup_{\|f\|_{\mathcal{H}} \leq 1} [E_P f(X) - E_Q f(Y)]$$



The MMD and witness in closed form

The MMD:

$$MMD(P, Q)$$

$$= \sup_{\|f\|_{\mathcal{H}} \leq 1} [\mathbb{E}_P f(X) - \mathbb{E}_Q f(Y)]$$

$$= \sup_{\|f\|_{\mathcal{H}} \leq 1} \langle f, \mu_P - \mu_Q \rangle_{\mathcal{H}}$$

use

$$\begin{aligned}\mathbb{E}_P f(X) &= \mathbb{E}_P \langle \varphi(X), f \rangle_{\mathcal{H}} \\ &= \langle \mathbb{E}_P [\varphi(X)], f \rangle_{\mathcal{H}} \\ &= \langle \mu_P, f \rangle_{\mathcal{H}}\end{aligned}$$

The MMD and witness in closed form

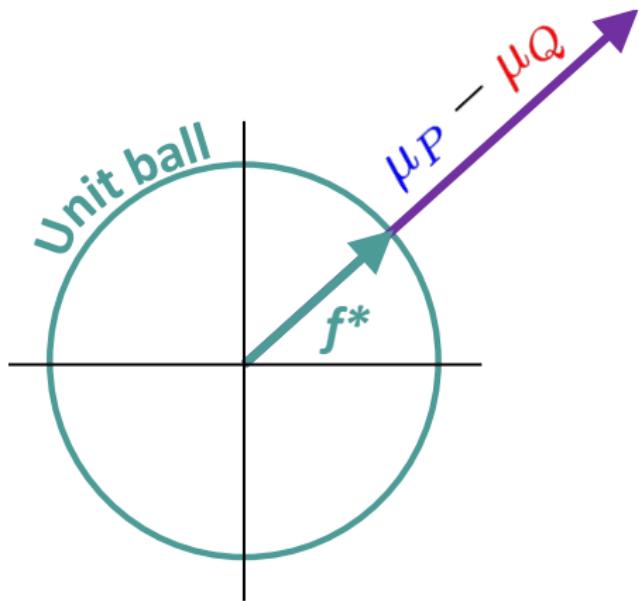
The MMD:

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$$= \|\mu_P - \mu_Q\|_{\mathcal{H}}$$



$$f^* = \frac{\mu_P - \mu_Q}{\|\mu_P - \mu_Q\|}$$

The MMD and witness in closed form

The MMD:

$$\begin{aligned}MMD(\textcolor{blue}{P}, \textcolor{red}{Q}) &= \sup_{\|\textcolor{teal}{f}\|_{\mathcal{H}} \leq 1} [\mathbb{E}_{\textcolor{blue}{P}} f(\textcolor{blue}{X}) - \mathbb{E}_{\textcolor{red}{Q}} f(\textcolor{red}{Y})] \\&= \sup_{\|\textcolor{teal}{f}\|_{\mathcal{H}} \leq 1} \langle \textcolor{teal}{f}, \mu_P - \mu_Q \rangle_{\mathcal{H}} \\&= \|\mu_P - \mu_Q\|_{\mathcal{H}}\end{aligned}$$

$$\begin{aligned}\textcolor{teal}{f}^*(x) &\propto \langle \mu_P - \mu_Q, \varphi(x) \rangle_H \\&= \mathbb{E}_{\textcolor{blue}{P}} k(\textcolor{blue}{X}, x) - \mathbb{E}_{\textcolor{red}{Q}} k(\textcolor{red}{Y}, x)\end{aligned}$$

The MMD and witness in closed form

The MMD:

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In terms of kernels:

$$\begin{aligned}MMD^2(P, Q) &= \|\mu_P - \mu_Q\|_{\mathcal{H}}^2 \\&= \underbrace{\mathbb{E}_P k(\mathbf{x}, \mathbf{x}')}_{(a)} + \underbrace{\mathbb{E}_Q k(\mathbf{y}, \mathbf{y}')}_{(a)} - 2 \underbrace{\mathbb{E}_{P, Q} k(\mathbf{x}, \mathbf{y})}_{(b)}\end{aligned}$$

(a)= within distrib. similarity, (b)= cross-distrib. similarity.

MMD Flow (NeurIPS 19)

arXiv > stat > arXiv:1906.04370

Statistics > Machine Learning

[Submitted on 11 Jun 2019 ([v1](#)), last revised 3 Dec 2019 (this version, v2)]

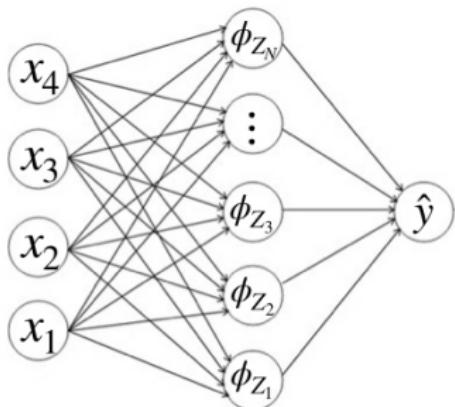
Maximum Mean Discrepancy Gradient Flow

[Michael Arbel](#), [Anna Korba](#), [Adil Salim](#), Arthur Gretton



Motivation: Neural Net training

$(x, y) \sim data$



$$\min_{Z_1, \dots, Z_N} \mathbb{E}_{data} [\|y - \frac{1}{N} \sum_{i=1}^N \phi_{Z_i}(x)\|^2]$$

$$\min_{Z_1, \dots, Z_N \in \mathcal{Z}} \mathcal{L} \left(\frac{1}{n} \sum_{i=1}^n \delta_{Z_i} \right)$$

Optimization using gradient descent:

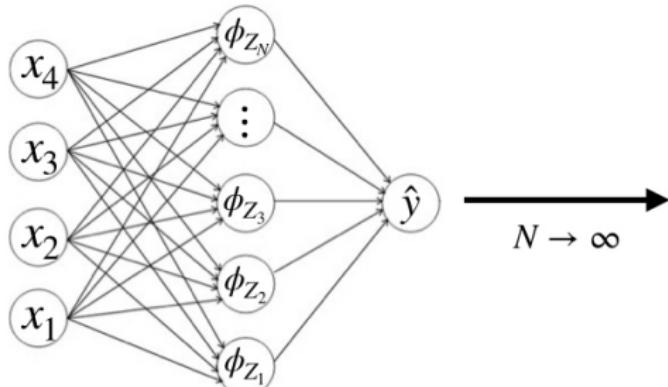
$$Z_i^{t+1} = Z_i^t - \gamma \nabla_{Z_i} \mathcal{L} \left(\frac{1}{n} \sum_{i=1}^n \delta_{Z_i^t} \right)$$

Chizat, Bach. "On the global convergence of gradient descent for over-parameterized models using optimal transport", NeurIPS (2018)

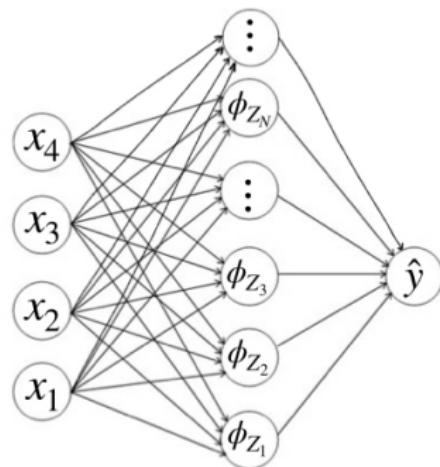
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$$\min_{Z_1, \dots, Z_n \in \mathcal{Z}} \mathcal{L} \left(\frac{1}{n} \sum_{i=1}^n \delta_{Z_i} \right) \xrightarrow{n \rightarrow \infty} \min_{\nu \in \mathcal{P}} \mathcal{L}(\nu)$$

$(x, y) \sim data$



$$N \rightarrow \infty$$



$$\min_{Z_1, \dots, Z_N} \mathbb{E}_{data} [\|y - \frac{1}{N} \sum_{i=1}^N \phi_{Z_i}(x)\|^2] \xrightarrow{N \rightarrow \infty} \min_{\nu \in \mathcal{P}} \mathbb{E}_{data} [\|y - \mathbb{E}_{Z \sim \nu} [\phi_Z(x)]\|^2]$$

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Motivation: Neural Net training

From previous slide:

$$\min_{\nu \in \mathcal{P}} \mathcal{L}(\nu) := \mathbb{E}_{(x,y)}[\|y - \mathbb{E}_{Z \sim \nu}[\phi_Z(x)]\|^2]$$

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Connection to the MMD:

- Assume well-specified setting, $y(x) = \mathbb{E}_{U \sim \nu^*} [\phi_U(x)]$
- Random feature formulation,

$$\mathcal{L}(\nu) = \mathbb{E}_x \left[\|\mathbb{E}_{U \sim \nu^*} [\phi_U(x)] - \mathbb{E}_{Z \sim \nu} [\phi_Z(x)]\|^2 \right] = MMD^2(\nu, \nu^*)$$

- The kernel is: $k(U, Z) = \mathbb{E}_x [\phi_U(x)^\top \phi_Z(x)].$

Chizat, Bach. "On the global convergence of gradient descent for over-parameterized models using optimal transport", NeurIPS (2018)

Intuition: MMD as “force field” on ν

Assume henceforth

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

MMD as free energy: target ν^* , current distribution ν

$$\mathcal{F}(\nu) := \frac{1}{2} MMD^2(\nu^*, \nu) = \underbrace{\frac{1}{2} \mathbb{E}_{\nu} k(\mathbf{x}, \mathbf{x}')}_{\text{interaction}} + \underbrace{\frac{1}{2} \mathbb{E}_{\nu^*} k(\mathbf{y}, \mathbf{y}')}_{\text{constant}} - \underbrace{\mathbb{E}_{\nu, \nu^*} k(\mathbf{x}, \mathbf{y})}_{\text{confinement}}$$

[A] Ambrosio, Gigli, and Savaré. Gradient flows: in metric spaces and in the space of probability measures. (2008)

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Consider $\{\mathbf{y}_i\}_{i=1}^n \stackrel{\text{i.i.d.}}{\sim} \nu^*$ and $\{\mathbf{x}_i\}_{i=1}^n \stackrel{\text{i.i.d.}}{\sim} \nu$.

Force on a particle \mathbf{z} :

$$-\sum_j \nabla_{\mathbf{z}} k(\mathbf{z}, \mathbf{x}_j) + \sum_j \nabla_{\mathbf{z}} k(\mathbf{z}, \mathbf{y}_j) = -\nabla_{\mathbf{z}} \hat{f}_{\nu^*, \nu_t}(z)$$

Can we formalize this?

[A] Ambrosio, Gigli, and Savaré. Gradient flows: in metric spaces and in the space of probability measures. (2008)

Wasserstein gradient flows

Tangent space of $(\mathcal{P}_2(\mathbb{R}^d), W_2)$ at μ is $h \in L^2(\mu)$ where $h : \mathbb{R}^d \rightarrow \mathbb{R}^d$.

Define $\nabla_{W_2}\mathcal{F}(\mu)$ of \mathcal{F} at μ using Taylor expansion

$$\mathcal{F}((\text{Id} + \epsilon h)_{\# \mu}) = \mathcal{F}(\mu) + \epsilon \langle \nabla_{W_2}\mathcal{F}(\mu), h \rangle_{L^2(\mu)} + o(\epsilon) \quad (1)$$

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The gradient flow is then:

$$\partial_t \nu_t = \text{div}(\nu_t \nabla_{W_2}\mathcal{F}(\nu_t))$$

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Under reasonable assumptions [A. Theorem 10.4.13]

$$\nabla_{W_2}\mathcal{F}(\mu) = \nabla \mathcal{F}'(\mu).$$

where **first variation** in direction ξ :

$$\mathcal{F}(\mu + \epsilon \xi) = \mathcal{F}(\mu) + \epsilon \int \mathcal{F}'(\mu)(x) d\xi(x) + o(\epsilon) \quad \mu + \epsilon \xi \in \mathcal{P}_2(\mathbb{R}^d) \quad (2)$$

[A] Ambrosio, Gigli, and Savaré. Gradient flows: in metric spaces and in the space of probability measures. (2008)

Wasserstein gradient flow on MMD

First variation of $\frac{1}{2} MMD^2(\nu^\star, \nu) =: \mathcal{F}(\nu)$

$$\mathcal{F}'(\nu)(z) := f_{\nu^\star, \nu}(z) = 2(\mathbb{E}_{U \sim \nu^\star}[k(U, z)] - \mathbb{E}_{U \sim \nu}[k(U, z)])$$

The W_2 gradient flow of the MMD:

$$\partial_t \nu_t = \operatorname{div}(\nu_t \nabla_{W_2} \mathcal{F}(\nu_t)) = \operatorname{div}(\nu_t \nabla f_{\nu^\star, \nu_t})$$

Ambrosio, Gigli, and Savaré. Gradient flows: in metric spaces and in the space of probability measures. (2008, Ch. 10)

Mroueh, Sercu, and Raj. Sobolev Descent. (AISTATS, 2019)

Arbel, Korba, Salim, G. (NeurIPS 2019)

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McKean-Vlasov dynamics for particles (existence and uniqueness under **Assumption A**):

$$dZ_t = -\nabla_{Z_t} f_{\nu^\star, \nu_t}(Z_t) dt, \quad Z_0 \sim \nu_0$$

Assumption A: $k(x, x) \leq K$, for all $x \in \mathbb{R}^d$, $\sum_{i=1}^d \|\partial_i k(x, \cdot)\|^2 \leq K_{1d}$ and $\sum_{i,j=1}^d \|\partial_i \partial_j k(x, \cdot)\|^2 \leq K_{2d}$, d indicates scaling with dimension.

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Wasserstein gradient flow on the MMD

Forward Euler scheme [A, Section 2.2]:

$$\begin{aligned}\nu_{n+1} &= (I - \gamma \nabla f_{\nu^*, \nu_t})_{\#} \nu_n \\ Z_{n+1} &= Z_n - \gamma \nabla_{Z_n} f_{\nu^*, \nu_n}(Z_n), \quad Z_0 \sim \nu_0, \quad Z_n \sim \nu_n\end{aligned}$$

Under **Assumption A**, ν_n approaches ν_t as $\gamma \rightarrow 0$

Wasserstein gradient flow on the MMD

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Consistency? Does ν_t converge to ν^* as $t \rightarrow \infty$?

[A] Arbel, Korba, Salim, G. (NeurIPS 2019)

Consistency

Can we use geodesic (displacement) convexity?

- A geodesic ρ_t between ν_1 and ν_2 is given by the transport map $T_{\nu_1}^{\nu_2} : \mathbb{R}^d \rightarrow \mathbb{R}^d$:

$$\rho_t = ((1-t)\text{Id} + tT_{\nu_1}^{\nu_2})_{\#\nu_1}$$

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$$\mathcal{F}(\rho_t) \leq (1-t)\mathcal{F}(\nu_1) + t\mathcal{F}(\nu_2)$$

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MMD is not displacement convex in general
(it is always mixture convex¹).

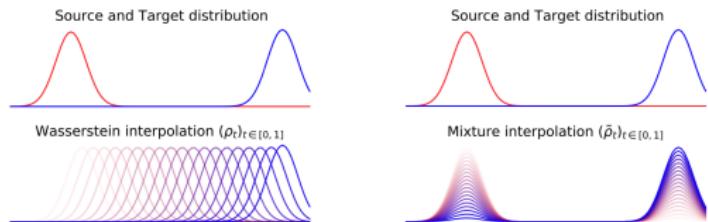
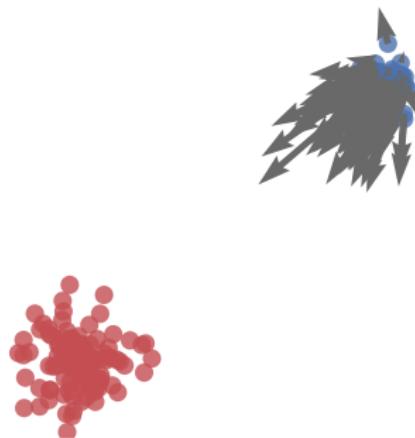


Figure from Korba, Salim, ICML 2022 Tutorial, "Sampling as First-Order Optimization over a space of probability measures"

1. $\mathcal{F}(t\nu_1 + (1-t)\nu_2) \leq t\mathcal{F}(\nu_1) + (1-t)\mathcal{F}(\nu_2) \quad \forall t \in [0, 1]).$

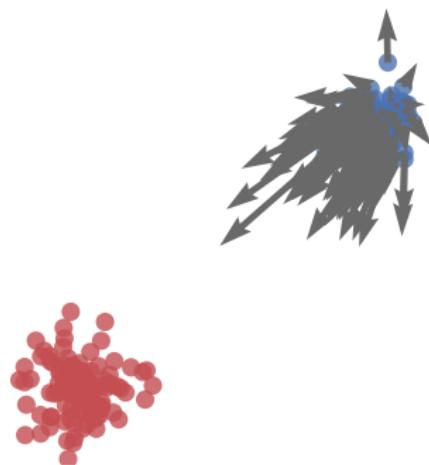
MMD flow in practice

- Data
- Particles



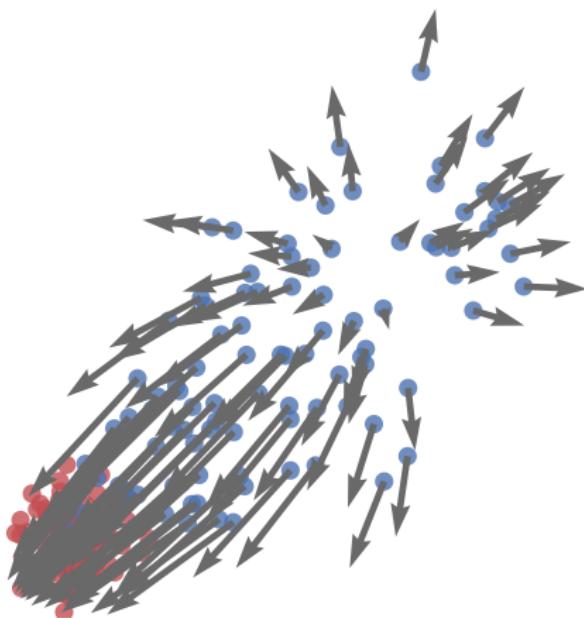
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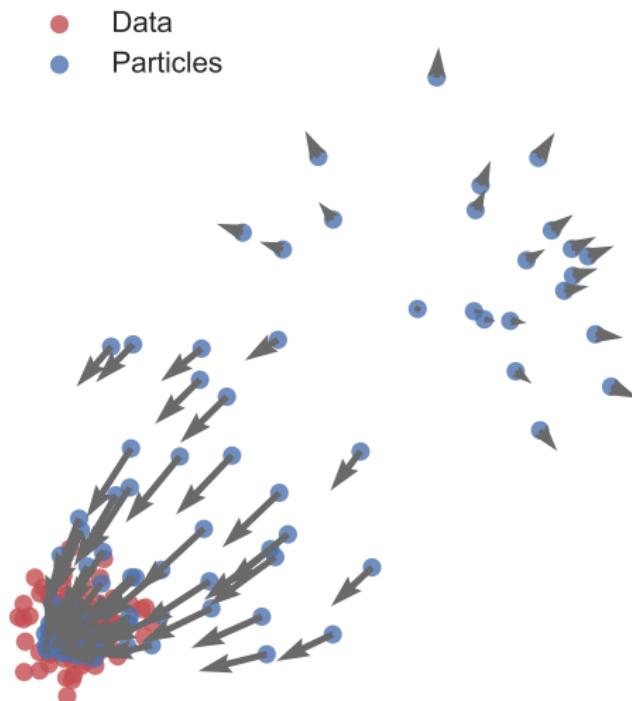


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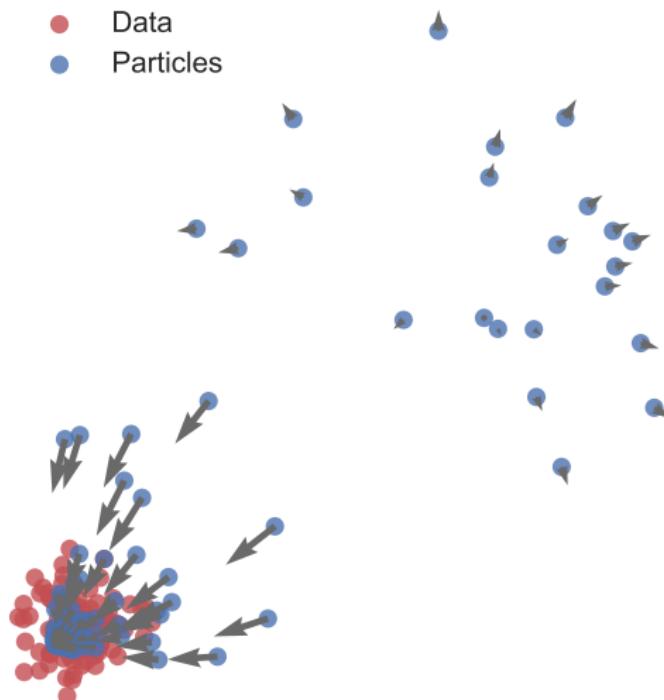
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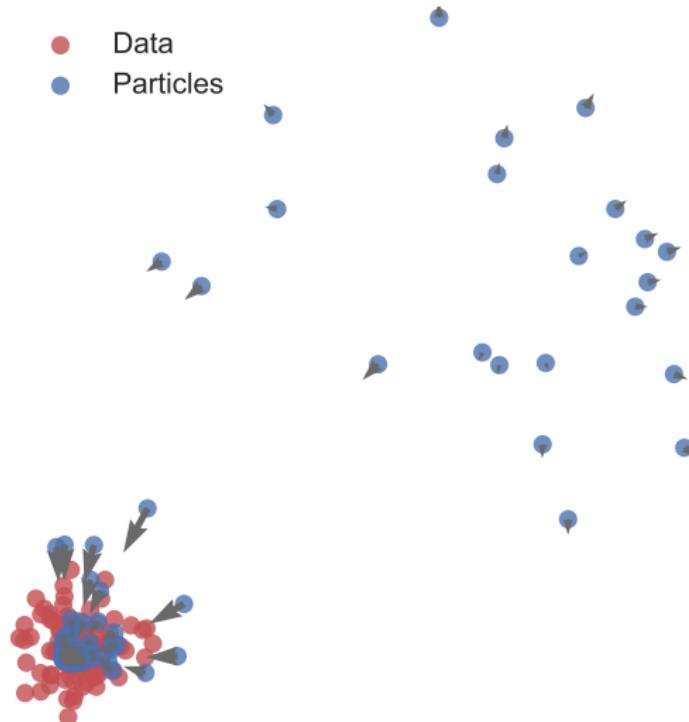
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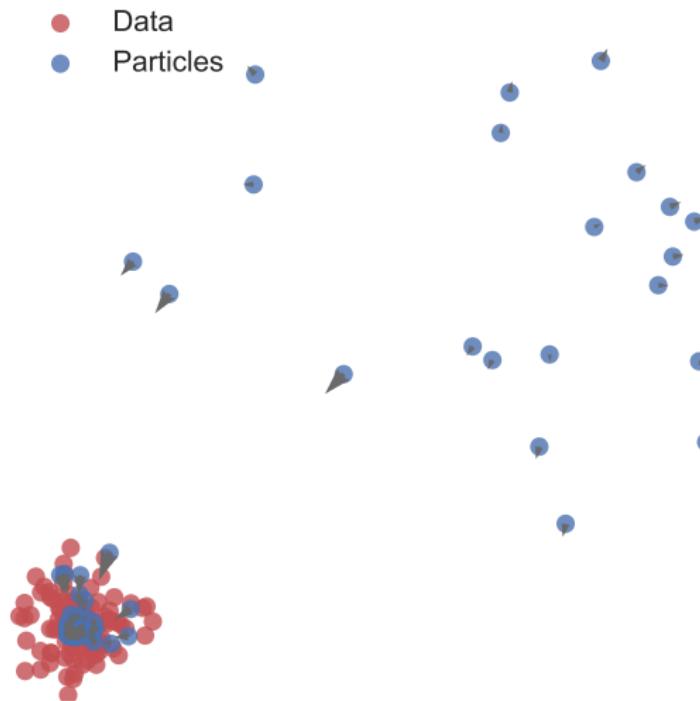
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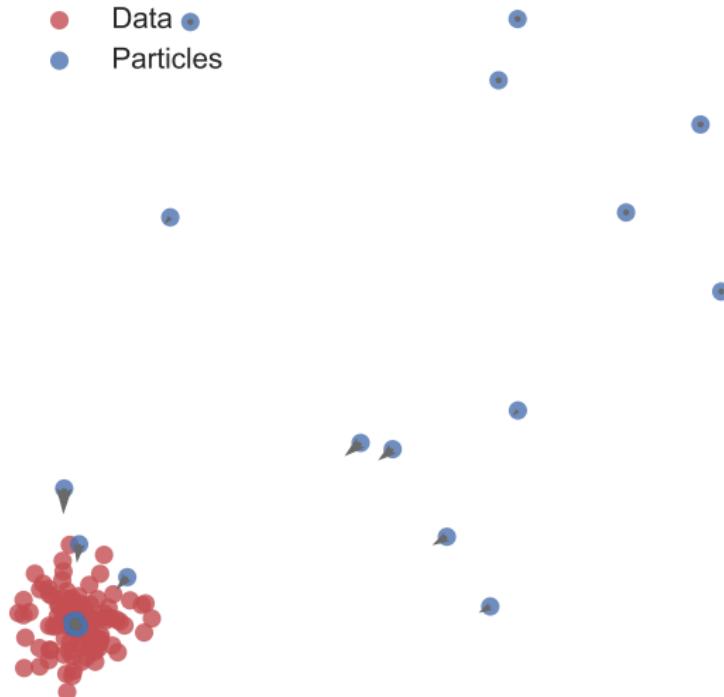
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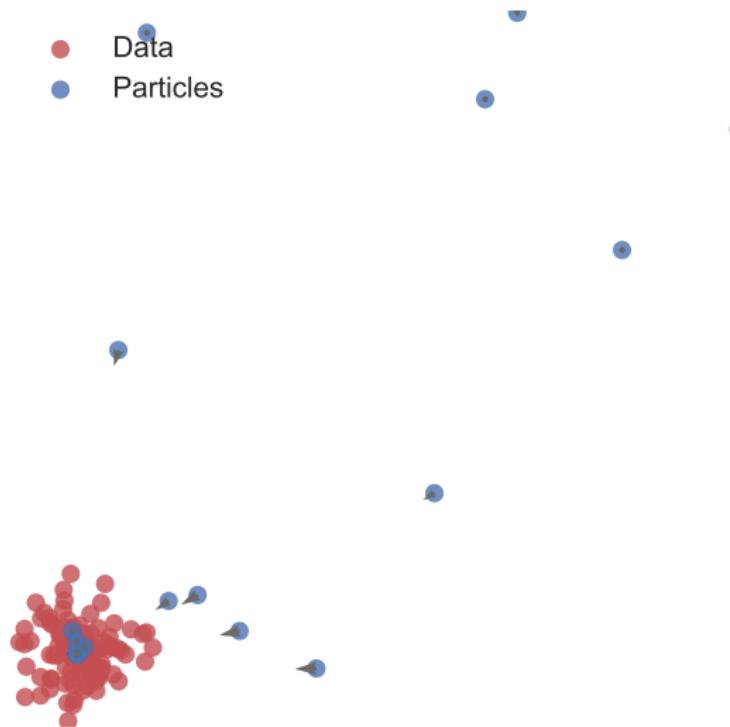
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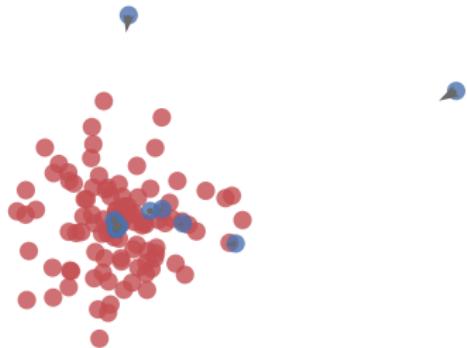


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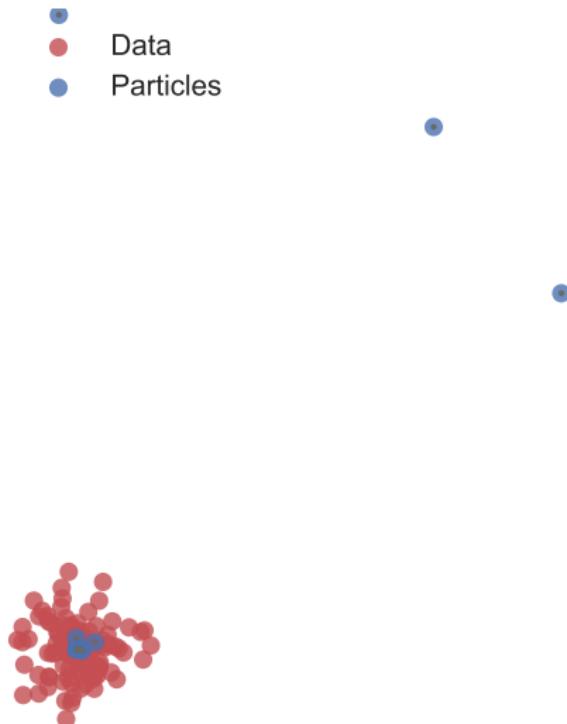


MMD flow in practice

- Data
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MMD flow in practice



Empirical observations

Some observations:

- Almost all particles tend to collapse at the center of mass m of the target ν^* , i.e.: ($\nu_t \simeq \delta_m$)
 - However, the loss stops decreasing: $\nabla f_{\nu^*, \nu_t}(z) \simeq 0$ for z on the support of ν_t (and is small when far from ν^*)...
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Idea: Adapt the kernel according to distance of ν_t to ν^* .

- “Broad” kernel when distributions far apart,
- “narrow” kernel when they are close.

Noise injection in NeurIPS 2019 was a first attempt.

Noise injection for convergence

Noise injection: Evaluate $\nabla f_{\nu^*, \nu_t}$ outside of the support of ν_t to get a better signal!

- Sample $u_t \sim \mathcal{N}(0, 1)$ and β_t is the noise level:

$$Z_{t+1} = Z_t - \gamma \nabla f_{\nu^*, \nu_t}(Z_t + \beta_t u_t); \quad Z_t \sim \nu_t$$

- Similar to continuation methods,¹ but extended to interacting particles.
- Different from entropic regularization:

$$Z_{t+1} = Z_t - \gamma \nabla f_{\nu^*, \nu_t}(Z_t) + \beta_t u_t$$

- Blur RKHS kernel with t -dependent Gaussian noise

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Noise injection for convergence

Noise injection: Evaluate $\nabla f_{\nu^*, \nu_t}$ outside of the support of ν_t to get a better signal!

- Sample $u_t \sim \mathcal{N}(0, 1)$ and β_t is the noise level:

$$Z_{t+1} = Z_t - \gamma \nabla f_{\nu^*, \nu_t}(Z_t + \beta_t u_t); \quad Z_t \sim \nu_t$$

- Similar to continuation methods,¹ but extended to interacting particles.
- Different from entropic regularization:

$$Z_{t+1} = Z_t - \gamma \nabla f_{\nu^*, \nu_t}(Z_t) + \beta_t u_t$$

- Blur RKHS kernel with t -dependent Gaussian noise

Noise injection: consistency

Recall: $Z_{t+1} = Z_t - \gamma \nabla f_{\nu^*, \nu_t}(Z_t + \beta_t u_t); \quad Z_t \sim \nu_t$

Tradeoff for β_t

- Large β_t : $\nu_{t+1} - \nu_t$ not a descent direction any more:
 $\mathcal{F}(\nu_{t+1}) > \mathcal{F}(\nu_t)$
- Small β_t : does not converge

Noise injection: consistency

Recall: $Z_{t+1} = Z_t - \gamma \nabla f_{\nu^*, \nu_t}(Z_t + \beta_t u_t); \quad Z_t \sim \nu_t$

Tradeoff for β_t

- Large β_t : $\nu_{t+1} - \nu_t$ not a descent direction any more:
 $\mathcal{F}(\nu_{t+1}) > \mathcal{F}(\nu_t)$
- Small β_t : does not converge

Need β_t such that:

$$\mathcal{F}(\nu_{t+1}) - \mathcal{F}(\nu_t) \leq -C\gamma \mathbb{E}_{\substack{X_t \sim \nu_t \\ u_t \sim \mathcal{N}(0,1)}} [\|\nabla f_{\nu^*, \nu_t}(X_t + \beta_t u_t)\|^2]$$

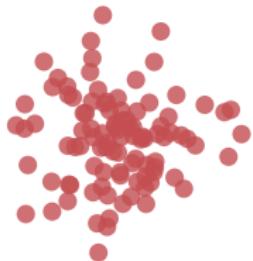
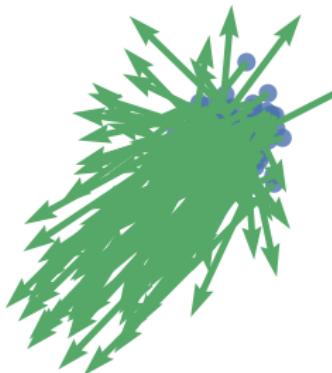
$$\sum_i^t \beta_i^2 \xrightarrow[t \rightarrow \infty]{} \infty$$

Then [A, Proposition 8]

$$\mathcal{F}(\nu_t) \leq \mathcal{F}(\nu_0) e^{-C\gamma \sum_i^t \beta_i^2}.$$

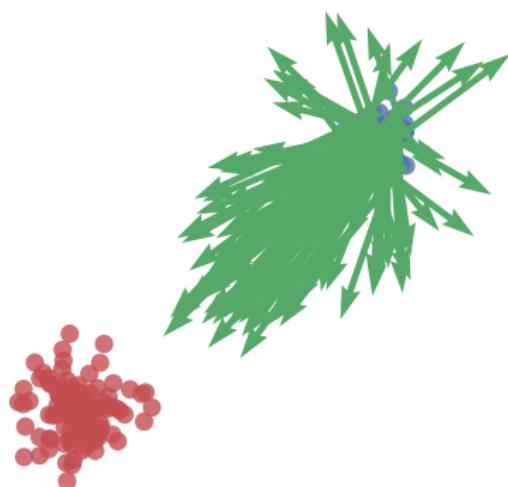
Noise injected MMD flow in practice

- Data
- Particles



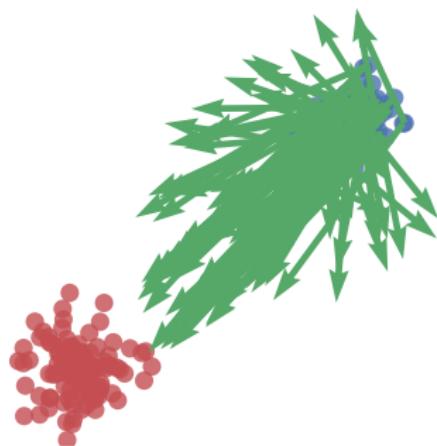
Noise injected MMD flow in practice

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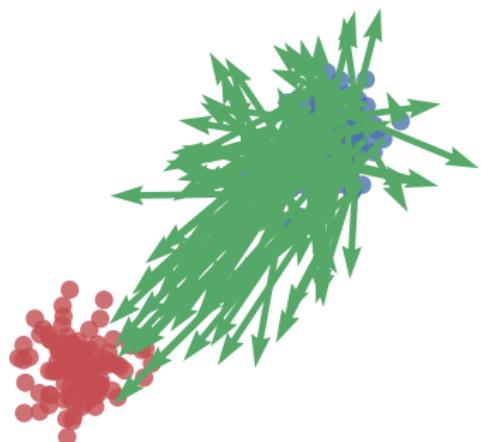
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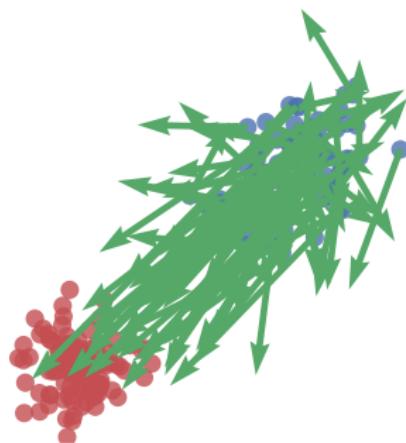
Noise injected MMD flow in practice

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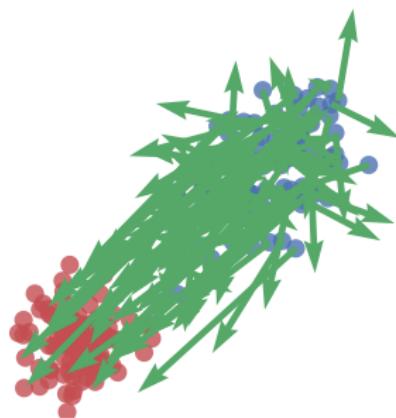
Noise injected MMD flow in practice

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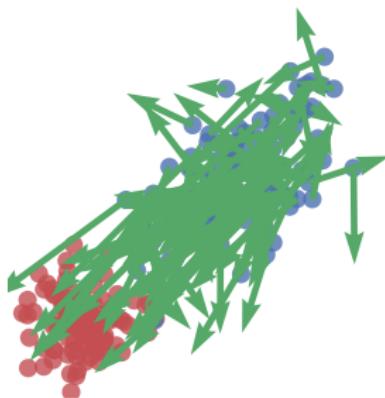
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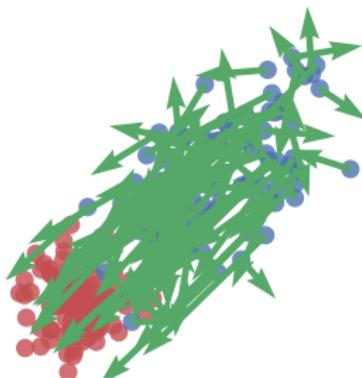
Noise injected MMD flow in practice

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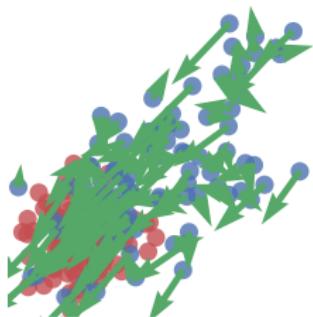
Noise injected MMD flow in practice

- Data
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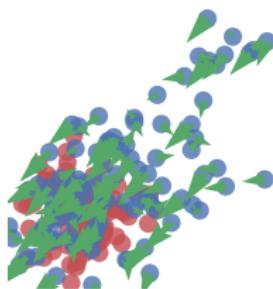
Noise injected MMD flow in practice

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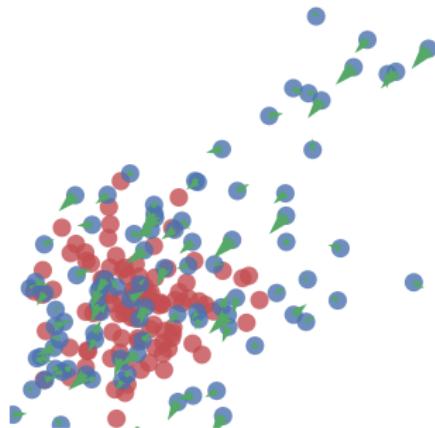
Noise injected MMD flow in practice

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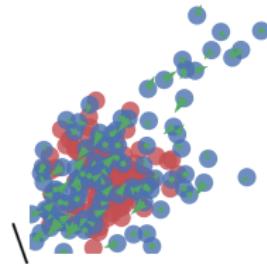
Noise injected MMD flow in practice

- Data
- Particles



Noise injected MMD flow in practice

- Data
- Particles



Adaptive MMD Flow (ICLR 25)

arXiv > cs > arXiv:2405.06780

Computer Science > Machine Learning

[Submitted on 10 May 2024]

Deep MMD Gradient Flow without adversarial training

Alexandre Galashov, Valentin de Bortoli, Arthur Gretton



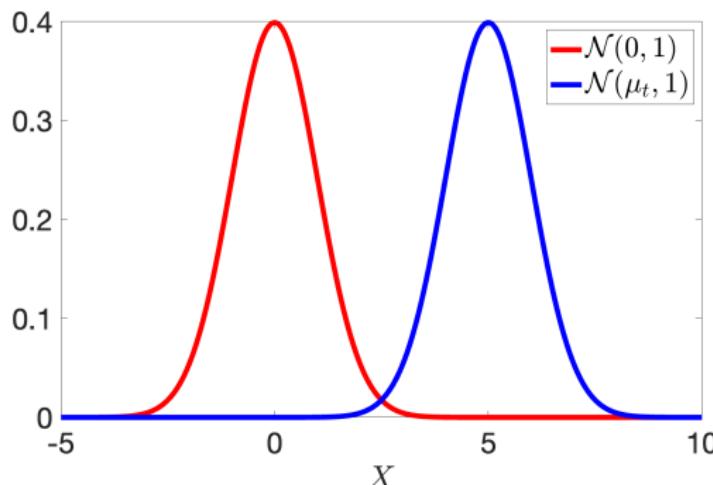
Will an adaptive kernel help?

Define the two measures:

$$\nu^* := \mathcal{N}(0, \sigma^2 \text{Id}) \quad \nu_t := \mathcal{N}(\mu_t, \sigma^2 \text{Id}).$$

Consider the family of MMDs:

$$\text{MMD}_\alpha^2(\nu^*, \nu_t) \quad \text{with} \quad k_\alpha(x, y) = \alpha^{-d} \exp[-\|x - y\|^2/(2\alpha^2)]$$



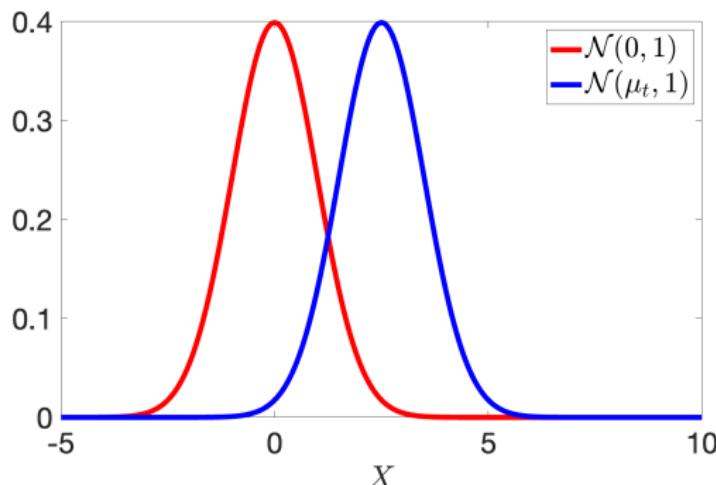
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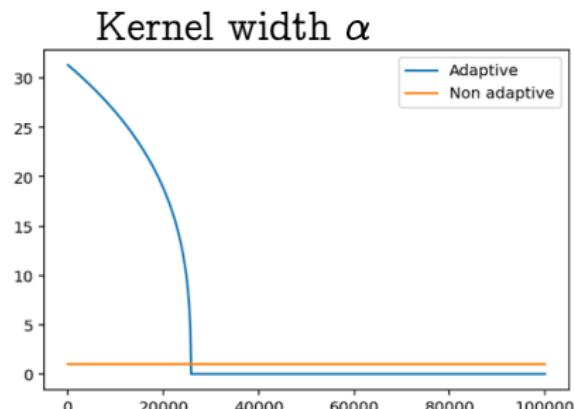
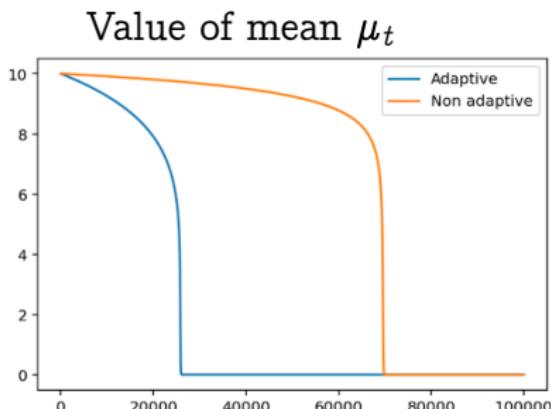
Will an adaptive kernel help?

Choose kernel such that:

$$\alpha^* = \operatorname{argmax}_{\alpha \geq 0} \|\nabla_{\mu_t} \text{MMD}_\alpha^2(\nu^*, \nu_t)\|.$$

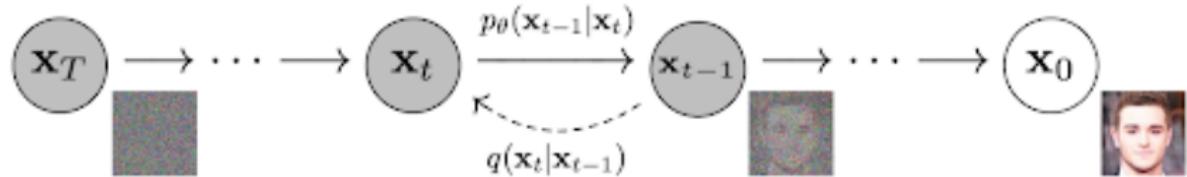
Then

$$\alpha^* = \text{ReLU}(\|\mu_t\|^2/(d+2) - 2\sigma^2)^{1/2}.$$



How to train an adaptive MMD (1)

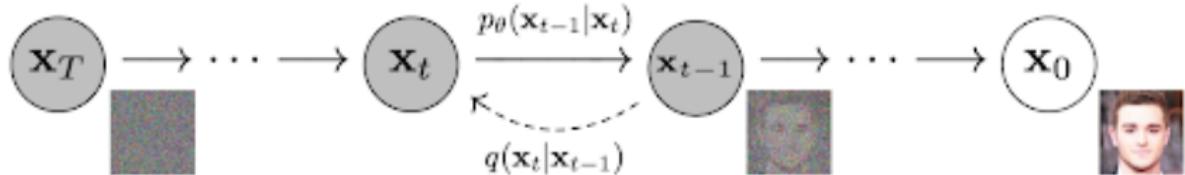
Diffusion:



Generate forward path $\tilde{\nu}_t$, $t \in [0, 1]$, such that $\tilde{\nu}_0 = \nu^*$, and $\tilde{\nu}_1 = N(0, \text{Id})$ is a Gaussian noise.

How to train an adaptive MMD (1)

Diffusion:



Generate forward path $\tilde{\nu}_t$, $t \in [0, 1]$, such that $\tilde{\nu}_0 = \nu^*$, and $\tilde{\nu}_1 = N(0, \text{Id})$ is a Gaussian noise.

Given samples $\tilde{\mathbf{x}}_0 \sim \tilde{\nu}_0$, the samples $\tilde{\mathbf{x}}_t | \tilde{\mathbf{x}}_0$ are given by

$$\tilde{\mathbf{x}}_t = \alpha_t \tilde{\mathbf{x}}_0 + \beta_t \epsilon, \quad \epsilon \sim N(0, \text{Id}),$$

with $\alpha_0 = \beta_1 = 1$ and $\alpha_1 = \beta_0 = 0$.

- low t : $\tilde{\mathbf{x}}_t$ close to the original data $\tilde{\mathbf{x}}_0$,
- high t : $\tilde{\mathbf{x}}_t$ close to a unit Gaussian

Schedule (α_t, β_t) is the variance-preserving one of Song, Sohl-Dickstein, Kingma, Kumar, Ermon, Poole. Score-based generative modeling through stochastic differential equations
(ICLR 2021) 23/30

How to train an adaptive MMD (2)

Time-dependent MMD **training loss**:

$$\mathcal{F}(\theta, t) := \frac{1}{2} \mathbb{E}_{\tilde{\nu}_t} k_{\theta, t}(\tilde{x}_t, \tilde{x}_t^l) + \mathbb{E}_{\tilde{\nu}_t, \nu^*} k_{\theta, t}(\tilde{x}_t, y)$$

with kernel

$$k_{\theta, t}(x, y) = \phi(x; t, \theta)^\top \phi(y; t, \theta)$$

and witness $f_{\nu^*, \tilde{\nu}_t}^{(\theta, t)}$.

How to train an adaptive MMD (2)

Time-dependent MMD **training loss**:

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with kernel

$$k_{\theta, t}(x, y) = \phi(x; t, \theta)^\top \phi(y; t, \theta)$$

and witness $f_{\nu^*, \tilde{\nu}_t}^{(\theta, t)}$.

Train θ by minimizing noise-conditional loss on **forward path**:

$$\mathcal{F}_{\text{tot}}(\theta, t) = \mathcal{F}(\theta, t) + \lambda_{\ell_2} \mathcal{F}_{\ell_2}(\theta, t) + \lambda_{\nabla} \mathcal{F}_{\nabla}(\theta, t),$$

$$\mathcal{F}_{\text{tot}}(\theta) = \mathbb{E}_{t \sim U[0,1]} [\mathcal{F}_{\text{tot}}(\theta, t)]$$

where

- $\mathcal{F}_{\ell_2}(\theta, t)$ is a “variance”-style penalty
- $\mathcal{F}_{\nabla}(\theta, t) = \frac{1}{N} \sum_{i=1}^N (\|\nabla f_{\nu^*, \tilde{\nu}_t}^{(\theta, t)}(\tilde{x}_{t,i})\|_2 - 1)^2$, is a gradient penalty

Gulrajani, Ahmed, Arjovsky, Dumoulin, Courville, Improved Training of Wasserstein GANs (NeurIPS 2017)

Binkowski, Sutherland, Arbel, G. (NeurIPS 2018)

Sample generation

Algorithm Noise-adaptive MMD gradient flow

Sample initial particles $Z \sim N(0, \text{Id})$

Set $\Delta t = (t_{\max} - t_{\min}) / T$

for $i = T$ to 0 do

 Set the noise level $t = i\Delta t$

 Set $Z_t^0 = Z$

 for $n = 0$ to $N_s - 1$ do

$Z_t^{n+1} = Z_t^n - \eta \nabla \textcolor{teal}{f}_{\nu^\star, \nu_t}^{(\theta^\star, t)}(Z_t^n)$

 end for

 Set $Z = Z_t^N$

end for

Output Z

Results

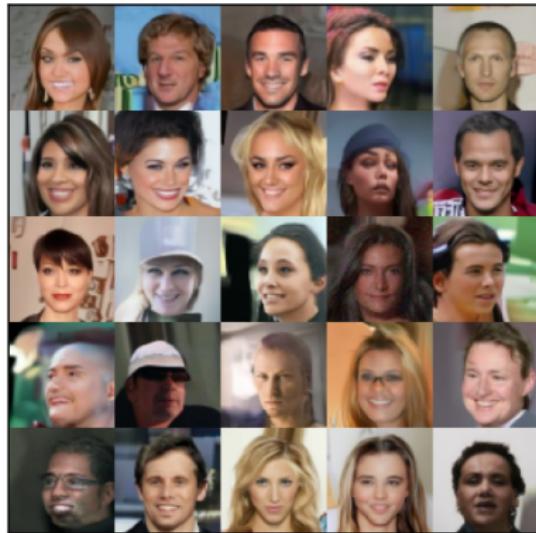
Table: Unconditional generation, CIFAR-10. MMD GAN (orig.), used mixed-RQ kernel. "Orig." – original paper, "impl." – our implementation.

Method	FID	IS	NFE
MMD GAN (orig.)	39.90	6.51	-
MMD GAN (impl.)	13.62	8.93	-
DDPM (orig.)	3.17	9.46	1000
DDPM (impl.)	5.19	8.90	100
Discriminator flows			
DGGF-KL	28.80	-	110
JKO-Flow	23.10	7.48	~ 150
GS-MMD-RK	55.00	-	86
DMMD (ours)	8.31	9.09	100
DMMD (ours)	7.74	9.12	250

DDPM from (Ho et al., 2020). Discriminator flows include two KL gradient flows trained adversarially: JKO-Flow (Fan et al., 2022) and Deep Generative Wasserstein Gradient Flows (DGGF-KL) (Heng et al., 2023). GS-MMD-RK is Generative Sliced MMD Flows with Riesz Kernels (Hertrich et al., 2024)

Images

CELEB-A (64x64)



LSUN Church (64x64)



Summary

- Gradient flows based on kernel dependence measures
- NeurIPS 2019, NeurIPS 2021, ICLR 2025, JMLR (submitted)

NeurIPS 2019:

 > stat > arXiv:1906.04370

Statistics > Machine Learning

[Submitted on 11 Jun 2019 (v1), last revised 3 Dec 2019 (this version, v2)]

Maximum Mean Discrepancy Gradient Flow

Michael Arbel, Anna Korba, Adil Salim, Arthur Gretton

NeurIPS 2021:

 > stat > arXiv:2106.08929

Statistics > Machine Learning

[Submitted on 16 Jun 2021 (v1), last revised 29 Oct 2021 (this version, v2)]

KALE Flow: A Relaxed KL Gradient Flow for Probabilities with Disjoint Support

Pierre Glaser, Michael Arbel, Arthur Gretton

Adaptive MMD (ICLR 25):

 > cs > arXiv:2405.06780

Computer Science > Machine Learning

[Submitted on 10 May 2024]

Deep MMD Gradient Flow without adversarial training

Alexandre Galashov, Valentin de Bortoli, Arthur Gretton

(De)regularized MMD
(JMLR, submitted):

 > stat > arXiv:2409.14980

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[Submitted on 23 Sep 2024]

(De)-regularized Maximum Mean Discrepancy Gradient Flow

Zonghao Chen, Aratrika Mustafi, Pierre Glaser, Anna Korba, Arthur Gretton, Bharath K. Sriperumbudur

Research support

Work supported by:

The Gatsby Charitable Foundation



Google Deepmind



Questions?

