## Gradient Flows on the Maximum Mean Discrepancy

#### Arthur Gretton



Gatsby Computational Neuroscience Unit, Google Deepmind

2nd RSS/Turing Workshop on Gradient Flows for Sampling, Inference, and Learning (2025)

### Outline

#### $\ensuremath{\mathsf{MMD}}\xspace$ and $\ensuremath{\mathsf{MMD}}\xspace$ flow

- Introduction to MMD as an integral probability metric
- Connection with neural net training
- Wasserstein-2 Gradient Flow on the MMD
- Convergence: noise injection, adaptive kernel

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

### Outline

#### $\ensuremath{\mathsf{MMD}}\xspace$ and $\ensuremath{\mathsf{MMD}}\xspace$ flow

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

- MMD (and related IPMs) are GAN critics
- Understand dynamics of GAN training
- Neural network training dynamics

Arbel, Korba, Salim, G., Maximum Mean Discrepancy Gradient Flow (NeurIPS 2019)

Galashov, De Bortoli, G., Deep MMD Gradient Flow without adversarial training (ICLR 2025) 2/50

# The MMD, and MMD flow

### The MMD: an integral probability metric

 $\begin{array}{l} \text{Maximum mean discrepancy: smooth function for $P$ vs $Q$}\\ MMD(P, Q; F) := \sup_{||f|| \leq 1} \left[ \operatorname{E}_{P} f(X) - \operatorname{E}_{Q} f(Y) \right] \\ f(x) = \langle f, \varphi(x) \rangle_{\mathcal{F}} \\ \langle \varphi(x), \varphi(x') \rangle_{\mathcal{F}} = k(x, x') \end{array}$ 



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# The MMD: an integral probability metric

 $\begin{array}{l} \text{Maximum mean discrepancy: smooth function for $P$ vs $Q$}\\ MMD(P, Q; F) \coloneqq \sup_{||f|| \leq 1} \left[ \operatorname{E}_P f(X) - \operatorname{E}_Q f(Y) \right]\\ f(x) = \langle f, \varphi(x) \rangle_{\mathcal{F}}\\ \langle \varphi(x), \varphi(x') \rangle_{\mathcal{F}} = k(x, x') \end{array}$ 

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

Other choices for witness function class:

Bounded continuous [Dudley, 2002]
 Bounded varation 1 (Kolmogorov metric) [Müller, 1997]
 Bounded Lipschitz (Wasserstein distances) in an

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The MMD:

$$egin{aligned} MMD(P, oldsymbol{Q}; F) \ &= \sup_{||f||_{\mathcal{F}} \leq 1} \left[ \mathrm{E}_{P}f(X) - \mathrm{E}_{oldsymbol{Q}}f(Y) 
ight] \end{aligned}$$



#### The MMD:

MMD(P, Q; F)

- $= \sup_{||f||_{\mathcal{F}} \leq 1} \left[ \mathbb{E}_{P} f(X) \mathbb{E}_{Q} f(Y) \right]$
- $= \sup_{||f||_{\mathcal{F}} \leq 1} \langle f, \mu_P \mu_Q 
  angle_{\mathcal{F}}$

use

$$egin{aligned} & \mathrm{E}_{P}f(X) = \mathrm{E}_{P}\left\langle arphi(X),f
ight
angle _{\mathcal{F}} \ & = \left\langle \mathrm{E}_{P}\left[arphi(X)
ight],f
ight
angle _{\mathcal{F}} \ & = \left\langle oldsymbol{\mu}_{P},f
ight
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  angle_{\mathcal{F}}$
- $= \|\boldsymbol{\mu}_P \boldsymbol{\mu}_Q\|_{\mathcal{F}}$



#### The MMD:

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ight] \ &= \sup_{||f||_{\mathcal{F}} \leq 1} \left\langle f, \mu_P - \mu_Q 
ight
angle_{\mathcal{F}} \ &= \left\| \mu_P - \mu_Q 
ight\|_{\mathcal{F}} \end{aligned}$$

$$egin{aligned} f^*(x) &\propto \left< \mu_P - \mu_Q, arphi(x) 
ight>_{\mathcal{F}} \ &= \mathrm{E}_P k(X, x) - \mathrm{E}_Q k(Y, x) \end{aligned}$$

#### The MMD:

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ight
angle_{\mathcal{F}} \end{aligned}$$

$$= \|\boldsymbol{\mu}_P - \boldsymbol{\mu}_Q\|_{\mathcal{F}}$$

In terms of kernels:

$$MMD^{2}(P, Q) = \left\| \mu_{P} - \mu_{Q} \right\|_{\mathcal{F}}^{2}$$
$$= \underbrace{\mathbb{E}_{P}k(x, x')}_{(a)} + \underbrace{\mathbb{E}_{Q}k(y, y')}_{(a)} - 2\underbrace{\mathbb{E}_{P,Q}k(x, y)}_{(b)}$$

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

# MMD Flow (NeurIPS 19)



#### 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





 $(x, y) \sim data$ 



$$\min_{Z_1,...,Z_N \in \mathcal{Z}} \mathcal{L}\left(rac{1}{n}\sum_{i=1}^n \delta_{Z_i}
ight)$$

Optimization using gradient descent:

$$Z_i^{t+1} = Z_i^t - \gamma 
abla_{Z_i} \mathcal{L}\left(rac{1}{n}\sum_{i=1}^n \delta_{Z_i^t}
ight)$$

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



Chizat, Bach. "On the global convergence of gradient descent for over-parameterized models using optimal transport", NeurIPS (2018) 8/50

From previous slide:

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

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

From previous slide:

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

#### Connection to the MMD:

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

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

• 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 $\nu$

Assume henceforth

$${oldsymbol 
u}, {oldsymbol 
u}^st \in \mathcal{P}_2(\mathbb{R}^d) := \left\{ \mu \in \mathcal{P}(\mathbb{R}^d) \ : \ \int ||x||^2 d\mu(x) < \infty 
ight\}.$$

MMD as free energy: target  $\nu^*$ , current distribution  $\nu$ 

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

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Consider  $\{\mathbf{y}_i\}_{i=1}^n \stackrel{\text{i.i.d.}}{\sim} \boldsymbol{\nu}^*$  and  $\{\mathbf{x}_i\}_{i=1}^n \stackrel{\text{i.i.d.}}{\sim} \boldsymbol{\nu}$ . Force on a particle  $\boldsymbol{z}$ :

$$-\sum_{j} \nabla_{z} k(z, \mathbf{x}_{j}) + \sum_{j} \nabla_{z} k(z, \mathbf{y}_{j}) = -\nabla_{z} \hat{f}_{\boldsymbol{\nu}^{\star}, \boldsymbol{\nu}_{t}}(z)$$

#### Can we formalize this?

#### Wasserstein gradient flows

Tangent space of  $(\mathcal{P}_2(\mathbb{R}^d), W_2)$  is  $h \in L^2(\mu)$  where  $h : \mathbb{R}^d \to \mathbb{R}^d$ . Define  $\nabla_{W_2} \mathcal{F}(\mu)$  of  $\mathcal{F}$  at  $\mu$  using Taylor expansion

$$\mathcal{F}((\mathrm{Id} + \epsilon h)_{\#\mu}) = \mathcal{F}(\mu) + \epsilon \langle \nabla_{W_2} \mathcal{F}(\mu), h \rangle_{\mu} + o(\epsilon)$$
(1)

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(1)

Under reasonable assumptions [A. Theorem 10.4.13]

$$abla_{W_2}\mathcal{F}(\mu)=
abla\mathcal{F}'(\mu).$$

where first variation in direction  $\xi$ :

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

#### Wasserstein gradient flows

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

The gradient flow is then:

$$\partial_t \boldsymbol{\nu}_t = \operatorname{div}(\boldsymbol{\nu}_t \nabla_{W_2} \mathcal{F}(\boldsymbol{\nu}_t))$$

#### Wasserstein gradient flow on MMD

First variation of 
$$\frac{1}{2}MMD^2(\nu^*,\nu) =: \mathcal{F}(\nu)$$
  
 $\mathcal{F}'(\nu)(z) := f_{\nu^*,\nu}(z) = 2\left(\mathbb{E}_{U \sim \nu^*}[k(U,z)] - \mathbb{E}_{U \sim \nu}[k(U,z)]\right)$   
The  $W_2$  gradient flow of the MMD:

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

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)

#### Wasserstein gradient flow on MMD

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

$$dZ_t = - 
abla_{Z_t} f_{oldsymbol{
u}^\star,oldsymbol{
u}_t}(Z_t) dt, \qquad Z_0 \sim oldsymbol{
u}_0$$

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.

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)

#### Wasserstein gradient flow on the MMD

Forward Euler scheme [A, Section 2.2]:

$$egin{aligned} oldsymbol{
u}_{n+1} &= (I - \gamma 
abla f_{oldsymbol{
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u}_t})_{\#}oldsymbol{
u}_n \ Z_{n+1} &= Z_n - \gamma 
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Under Assumption A,  $\nu_n$  approaches  $\nu_t$  as  $\gamma \to 0$ 

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

#### Wasserstein gradient flow on the MMD

Forward Euler scheme [A, Section 2.2]:

$$\begin{split} \boldsymbol{\nu}_{n+1} &= (I - \gamma \nabla f_{\boldsymbol{\nu}^{\star}, \boldsymbol{\nu}_{t}})_{\#} \boldsymbol{\nu}_{n} \\ Z_{n+1} &= Z_{n} - \gamma \nabla_{Z_{n}} f_{\boldsymbol{\nu}^{\star}, \boldsymbol{\nu}_{n}}(Z_{n}), \qquad Z_{0} \sim \boldsymbol{\nu}_{0}, \ Z_{n} \sim \boldsymbol{\nu}_{n} \end{split}$$

Under Assumption A,  $\nu_n$  approaches  $\nu_t$  as  $\gamma \to 0$ 

Consistency? Does  $\nu_t$  converge to  $\nu^*$  as  $t \to \infty$ ?

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

### Consistency

Can we use geodesic (displacement) convexity?

• A geodesic  $\rho_t$  between  $\nu_1$  and  $\nu_2$  is given by the transport map  $T_{\nu_1}^{\nu_2}$  :  $\mathbb{R}^d \to \mathbb{R}^d$ :

$$ho_t = \left((1-t) {
m Id} + t T^{
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• A functional  $\mathcal{F}$  is displacement convex if:

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ho_t) \leq (1-t)\mathcal{F}(
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MMD is not displacement convex in general (it is always mixture convex<sup>1</sup>).



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

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

#### Noise injection for convergence

Noise injection: Evaluate  $\nabla f_{\nu^{\star},\nu_{t}}$  outside of the support of  $\nu_{t}$  to get a better signal!

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

$$Z_{t+1} = Z_t - \gamma \nabla f_{\nu^{\star},\nu_t}(Z_t + \boldsymbol{\beta}_t u_t); \qquad Z_t \sim \boldsymbol{\nu}_t$$

Similar to continuation methods,<sup>1</sup> but extended to interacting particles.
 Different from entropic regularization:

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

<sup>&</sup>lt;sup>1</sup>Chaudhari, Oberman, Osher, Soatto, Carlier. Deep relaxation: partial differential equations for optimizing deep neural networks. Research in the Mathematical Sciences (2017) Hazan, Levy, Shalev-Shwartz. On graduated optimization for stochastic non-convex problems. ICML (2016).

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### Noise injection: consistency

 $\begin{array}{ll} \text{Recall:} & Z_{t+1} = Z_t - \gamma \nabla f_{\nu^\star,\nu_t} (Z_t + \pmb{\beta}_t u_t); & Z_t \sim \nu_t \\ \text{Tradeoff for } \pmb{\beta}_t \end{array}$ 

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

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

Need  $\beta_t$  such that:

$$egin{aligned} \mathcal{F}(oldsymbol{
u}_{t+1}) &- \mathcal{F}(oldsymbol{
u}_t) \leq -C \gamma \mathbb{E}_{\substack{X_t \sim oldsymbol{
u}_t \sim \mathcal{N}(0,1)}} [\| 
abla f_{oldsymbol{
u}^\star,oldsymbol{
u}_t}(X_t + oldsymbol{eta}_t u_t) \|^2] \ &\sum_i^t oldsymbol{eta}_i^2 \ \stackrel{ oldsymbol{
u}_t 
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abla f_{oldsymbol{
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u}_t}(X_t + oldsymbol{eta}_t u_t) \|^2] \end{aligned}$$

Then [A, Proposition 8]

$$\mathcal{F}(\boldsymbol{\nu}_t) \leq \mathcal{F}(\boldsymbol{\nu}_0) e^{-C\gamma \sum_i^t \boldsymbol{\beta}_i^2}.$$

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

DataParticles









Data

Particles











Data

Particles























Data

Particles



### Noise injection: neural net setting





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### Noise injection: neural net setting



#### Noise injection: neural net setting



KSD is Kernel Sobolev Discrepancy. Y. Mroueh, T. Sercu, and A. Raj. "Sobolev Descent." In: AISTATS. 2019.

# Adaptive MMD Flow (ICLR 25)



**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:

$$\boldsymbol{\nu}^{\star} := \mathcal{N}(0, \sigma^2 \mathrm{Id}) \qquad \boldsymbol{\nu}_t := \mathcal{N}(\boldsymbol{\mu}_t, \sigma^2 \mathrm{Id}).$$

Consider the family of MMDs:

 $\mathrm{MMD}_{\alpha}^{2}(\boldsymbol{\nu^{\star}},\boldsymbol{\nu_{t}}) \qquad \mathrm{with} \qquad k_{\alpha}(x,y) = \alpha^{-d} \exp[-||x-y||^{2}/(2\alpha^{2})]$ 



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 $\mathrm{MMD}_{\alpha}^{2}(\boldsymbol{\nu^{\star}},\boldsymbol{\nu_{t}}) \qquad \mathrm{with} \qquad k_{\alpha}(x,y) = \alpha^{-d} \exp[-||x-y||^{2}/(2\alpha^{2})]$ 



#### Will an adaptive kernel help?

Choose kernel such that:

$$lpha^{\star} = \operatorname{argmax}_{lpha \geq 0} || 
abla_{\mu_t} \operatorname{MMD}^2_{lpha}(oldsymbol{
u^{\star}},oldsymbol{
u}_t) ||.$$

Then

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



### 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  $\tilde{\nu}_1 = N(0, Id)$  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  $\tilde{\nu}_1 = N(0, Id)$  is a Gaussian noise.

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

$$ilde{x}_t = lpha_t ilde{x}_0 + eta_t \epsilon, \quad \epsilon \in \mathrm{N}(0,\mathrm{Id}),$$

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

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

Schedule  $(\alpha_t, \beta_t)$  is the variance-preserving one of Song, Sohl-Dickstein, Kingma, Kumar, Ermon, Poole. Score-based generative modeling through stochastic differential equations (ICLR 2021)

### How to train an adaptive MMD (2)

Time-dependent MMD training loss:

$$\mathcal{F}(\theta,t) := \frac{1}{2} \mathrm{E}_{\tilde{\boldsymbol{\nu}}_t} k_{\theta,t}(\tilde{\boldsymbol{x}}_t, \tilde{\boldsymbol{x}}_t') + \mathrm{E}_{\tilde{\boldsymbol{\nu}}_t, \boldsymbol{\nu}^*} k_{\theta,t}(\tilde{\boldsymbol{x}}_t, \boldsymbol{y})$$

with kernel

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

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

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

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

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Train  $\theta$  by minimizing noise-conditional loss on forward path:

$$egin{aligned} \mathcal{F}_{ ext{tot}}( heta,t) &= \mathcal{F}( heta,t) + \lambda_{\ell_2}\mathcal{F}_{\ell_2}( heta,t) + \lambda_
abla \mathcal{F}_
abla( heta,t), \ \mathcal{F}_{ ext{tot}}( heta) &= \mathbb{E}_{t\sim U[0,1]}\left[\mathcal{F}_{ ext{tot}}( heta,t)
ight] \end{aligned}$$

where

Gulrajani, Ahmed, Arjovsky, Dumoulin, Courville, Improved Training of Wasserstein GANs (NeurIPS 2017) Binkowski, Sutherland, Arbel, G. (NeurIPS 2018) 24/50

### Sample generation

#### Algorithm Noise-adaptive MMD gradient flow

```
Sample initial particles Z \sim N(0, Id)
Set \Delta t = (t_{\text{max}} - t_{\text{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_{\rm s} - 1 do
      Z_t^{n+1} = Z_t^n - \eta \nabla 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
MND CAN (orig)	20.00	6 51	
MMD GAN (orig.)	39.90 12.60	0.01	-
MMD GAN (Impl.)	13.02	0.93	-
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	$\sim 150$
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)



#### CELEB-A (64x64)



#### LSUN Church (64x64)



### Summary

Gradient flows based on kernel dependence measures:

- MMD flow is simpler, KALE flow is mode-seeking
- Noise injection can improve convergence
- NeurIPS 2019, ICLR 2025

#### NeurIPS 2019:

 $\exists \mathbf{r} \langle \mathbf{i} \mathbf{V} \rangle$  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

#### Adaptive MMD (ICLR 25):



#### Summary

Gradient flows based on kernel dependence measures:

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 $\exists \mathbf{r} \mathbf{i} \mathbf{V} > \text{stat} > \text{arXiv:1906.04370}$ 

Statistics > Machine Learning

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#### NeurIPS 2021:

arxiv > 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):



#### $\exists \mathbf{r} \mathsf{i} \mathsf{V} > \mathsf{stat} > \mathsf{ar} \mathsf{Xiv}: 2409.14980$

Statistics > Machine Learning

[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

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## Questions?

