Gradient Flows on Kernel Divergence Measures

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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, consistency
- Noise injection for improved convergence

KALE and KALE flow

- Introduction to KALE as a variational lower bound on the KL divergence
- Wasserstein-2 gradient flow on KALE
- Properties in relation to MMD

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

Glaser, Arbel, G., KALE Flow: A Relaxed KL Gradient Flow for Probabilities with Disjoint Support (NeurIPS 2021)

Motivation

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

Gradient flow on MMD

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

Gradient flow on KALE

- The KALE (and other lower bounds on ϕ-divergences) are GAN critics
- Understand dynamics of GAN training

Source and target might have disjoint support: KL undefined!

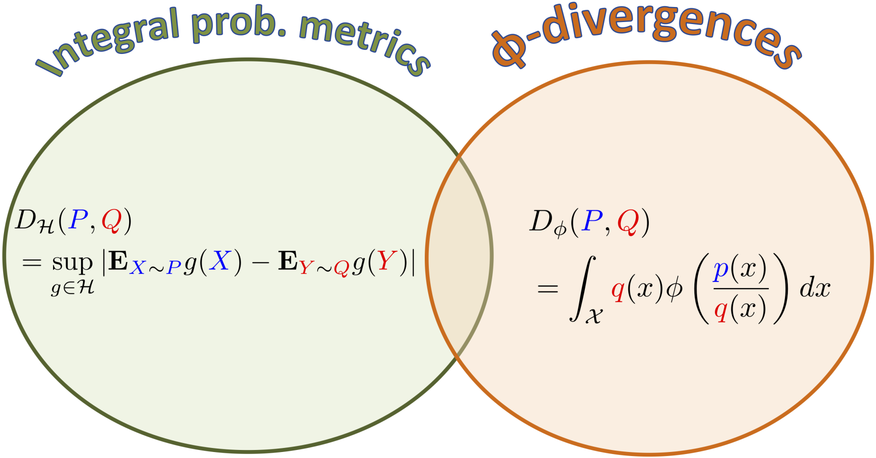
Binkowski, Sutherland, Arbel, G., Demystifying MMD GANs (ICLR 2018)

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

Arbel, Zhou, G. Generalized Energy-Based Models, (ICLR 2021)

Nowozin, Cseke, Tomioka, NeurIPS (2016)

Divergences



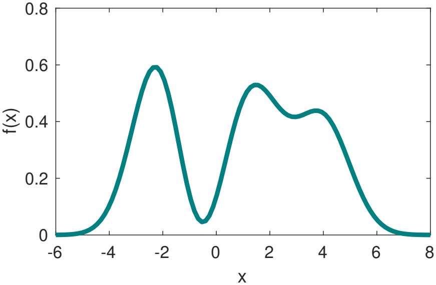
The MMD, and MMD flow

All of kernel methods

"The kernel trick"

$$f(x) = \sum_{\ell=1}^{\infty} f_\ell \varphi_\ell(x)$$

$$= \sum_{i=1}^{m} \alpha_i \underbrace{k(x_i, x)}_{\langle \varphi(x_i), \varphi(x) \rangle_{\mathcal{F}}}$$



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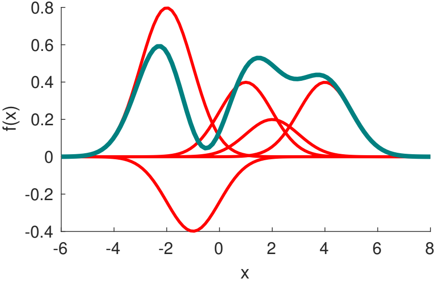


$$f_\ell := \sum_{i=1}^{m} \alpha_i \varphi_\ell(x_i)$$

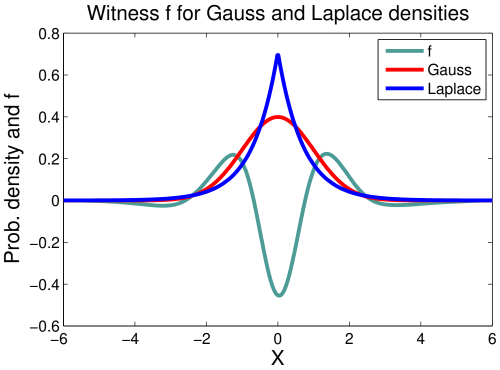
Function of infinitely many features expressed using m coefficients.

MMD as an integral probability metric

Maximum mean discrepancy: smooth function for P vs Q

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

$$(F = \text{unit ball in RKHS } \mathcal{F})$$



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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) [Dudley, 2002]

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A result for the proof on the next slide:

$$\mathrm{E}_P(f(X)) = \mathrm{E}_P \left\langle f, \varphi(X) \right\rangle_{\mathcal{F}} = \left\langle f, \mathrm{E}_P \varphi(X) \right\rangle_{\mathcal{F}} = \left\langle f, \mu_P \right\rangle_{\mathcal{F}}$$

(always true if kernel is bounded)

Integral prob. metric vs feature difference

The MMD:

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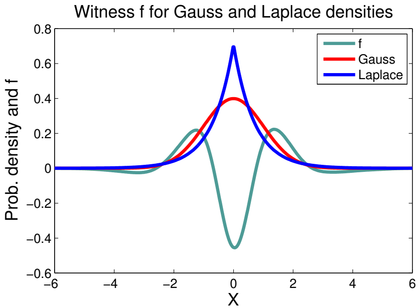

Integral prob. metric vs feature difference

The MMD:

$$
\begin{aligned}
& MMD(P, Q; F) \\
&= \sup_{\|f\|_{\mathcal{F}} \leq 1} \left[\mathrm{E}_P f(X) - \mathrm{E}_Q f(Y) \right] \\
&= \sup_{\|f\|_{\mathcal{F}} \leq 1} \langle f, \mu_P - \mu_Q \rangle_{\mathcal{F}}
\end{aligned}
$$

use

$$\mathrm{E}_P f(X) = \langle \mu_P, f \rangle_{\mathcal{F}}$$

Integral prob. metric vs feature difference

The MMD:

$$MMD(P, Q; F)$$
$$= \sup_{\|f\|_{\mathcal{F}} \leq 1} \left[\mathrm{E}_P f(X) - \mathrm{E}_Q f(Y) \right]$$
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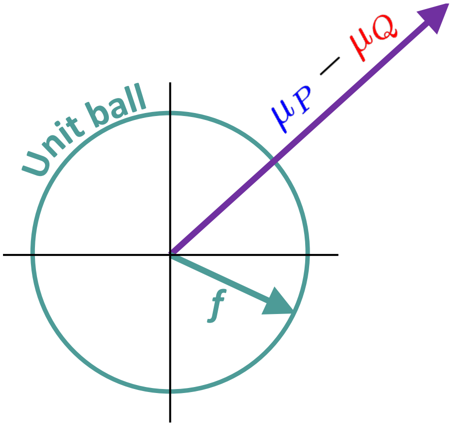

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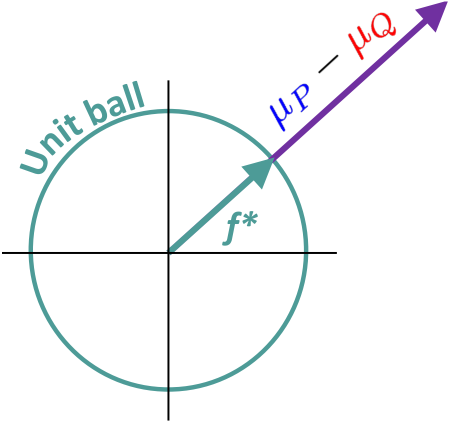

$$f^* = \frac{\mu_P - \mu_Q}{\|\mu_P - \mu_Q\|}$$

Integral prob. metric vs feature difference

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&= \sup_{\|f\|_{\mathcal{F}} \le 1} \langle f, \mu_P - \mu_Q \rangle_{\mathcal{F}} \\
&= \|\mu_P - \mu_Q\|
\end{aligned}
$$

$$f^*(x) \propto \mu_P(x) - \mu_Q(x) = \mathrm{E}_P k(X, x) - \mathrm{E}_Q k(Y, x)$$

Function view and feature view equivalent

Computing the MMD

The maximum mean discrepancy is the distance between feature means:

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

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

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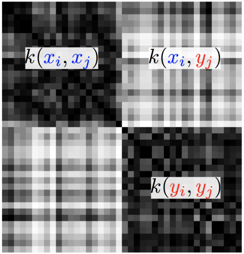
\end{aligned}
$$

Empirical estimate:

$$
\begin{aligned}
\widehat{MMD}^2 = &\frac{1}{n(n-1)} \sum_{i \neq j} k(x_i, x_j) \\
&+ \frac{1}{n(n-1)} \sum_{i \neq j} k(y_i, y_j) \\
&- \frac{2}{n^2} \sum_{i,j} k(x_i, y_j)
\end{aligned}
$$



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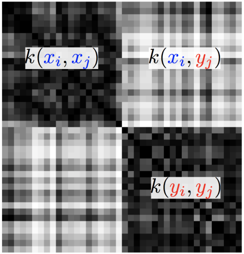
Empirical witness:

$$\hat{f}_{\nu^\star,\nu_t}(z) \propto \sum_j k(z, x_j) - \sum_j k(z, y_j)$$

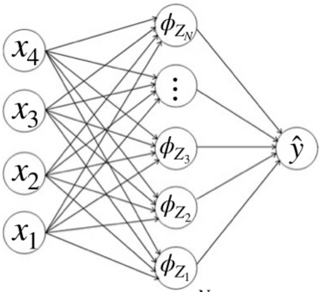


MMD Flow



Motivation: Neural Net training

$(x, y) \sim data$



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

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

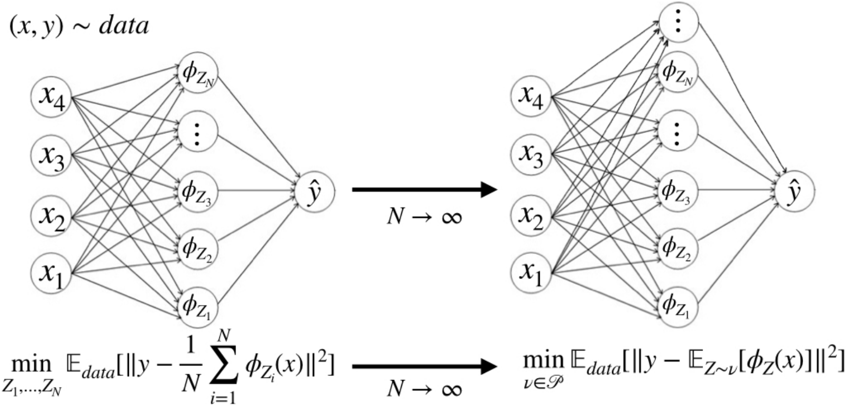
Optimization using gradient descent:

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

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

Motivation: Neural Net training

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



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Motivation: Neural Net training

From previous slide:

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

Want to prove global convergence of GD when $n \to \infty$ and

$$\phi_Z(x) = w\, g_\theta(x), \qquad Z = (w, \theta)$$

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$$\phi_Z(x) = w\, g_\theta(x), \qquad Z = (w, \theta)$$

Connection to the MMD:

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

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

- 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)

Preliminaries: Wasserstein gradient flow on MMD

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

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

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

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Consider $\{\mathrm{y}_i\}_{i=1}^n \overset{\text{i.i.d.}}{\sim} \nu^*$ and $\{x_i\}_{i=1}^n \overset{\text{i.i.d.}}{\sim} \nu$.
Force on a particle z:

$$-\sum_j \nabla_z k(z, x_j) + \sum_j \nabla_z k(z, \mathrm{y}_j) = -\nabla_z \hat{f}_{\nu^\star, \nu_t}(z)$$

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Wasserstein gradient flows

Tangent space of $\left(\mathcal{P}_2(\mathbb{R}^d), W_2\right)$ 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 μ using Taylor expansion

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

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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:

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

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The gradient flow is then:

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

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Wasserstein gradient flow on MMD

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

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

The W_2 gradient flow of the MMD:

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

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)

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

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

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]:

$$\nu_{n+1} = (I - \gamma \nabla f_{\nu^\star, \nu_t})_{\#} \nu_n$$
$$Z_{n+1} = Z_n - \gamma \nabla_{Z_n} f_{\nu^\star, \nu_n}(Z_n), \qquad Z_0 \sim \nu_0,\ Z_n \sim \nu_n$$

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

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Consistency? Does ν_t converge to $\nu^\star$ as $t \to \infty$?

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

Consistency (1)

Can we use geodesic (displacement) convexity?

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

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

- A functional $\mathcal{F}$ is displacement convex if:

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

MMD is not displacement convex in general (it is always mixture[1] convex).

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

Consistency (2)

Dissipation inequalities:

- Rate by which $\mathcal{F}$ decreases along the gradient flow [A, Proposition 2]

$$\frac{d\mathcal{F}(\nu_t)}{dt} = -\mathbb{E}_{\nu_t}[\|\nabla f_{\nu^\star,\nu_t}\|^2]$$

- Assume the dissipation rate is controlled (path-dependent Lojasiewicz inequality)

$$\mathcal{F}(\nu_t) \leq C\mathbb{E}_{\nu_t}[\|\nabla f_{\nu^\star,\nu_t}\|^2]$$

- From above, [A, Proposition 7]:

$$\mathcal{F}(\nu_t) \leq \frac{1}{\mathcal{F}(\nu_0)^{-1} + 2C^{-1}t}$$

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Consistency (2)

Check: Lojasiewicz inequality for MMD?

- Does there exist $C > 0$ such that

$$\mathcal{F}(\nu_t) \leq C\mathbb{E}_{\nu_t}[||\nabla f_{\nu^\star,\nu_t}||^2]$$

- By Cauchy-Schwarz in the RKHS,[A, eq. 16]

$$\mathcal{F}(\nu_t) =: \frac{1}{2}MMD^2(\nu_t, \nu^\star) \leq S(\nu^\star|\nu_t)\mathbb{E}_{\nu_t}[||\nabla f_{\nu^\star,\nu_t}||^2]$$

where $S(\nu^\star|\nu_t)$ is the Negative Sobolev Distance[2]

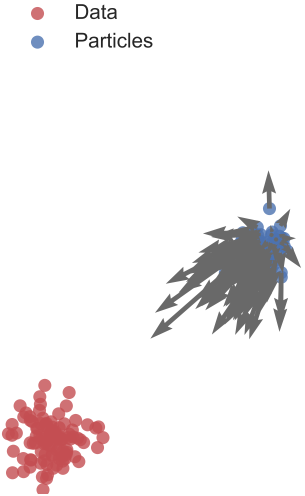
- Require $S(\nu^\star|\nu_t) < C$ for entire sequence ν_t: hard to check in theory, fails in practice.

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

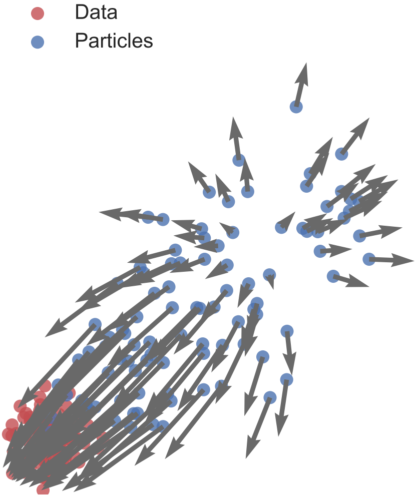
[2] $S(\nu^\star|\nu_t) = \sup_{g,\mathbb{E}_{Z\sim\nu_t}[||\nabla g(Z)||^2]\leq 1} |\mathbb{E}_{Z\sim\nu_t}[g(Z)] - \mathbb{E}_{U\sim\nu^\star}[g(U)]|$

MMD flow in practice

MMD flow in practice



MMD flow in practice



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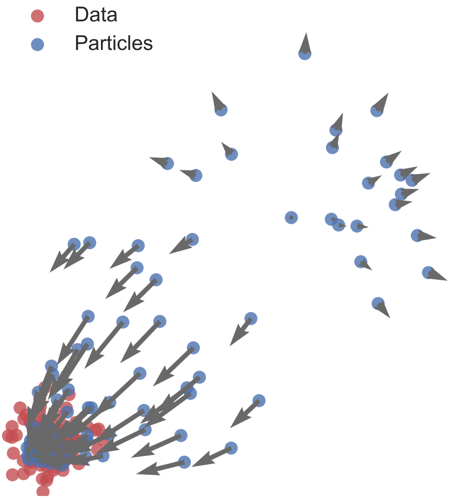

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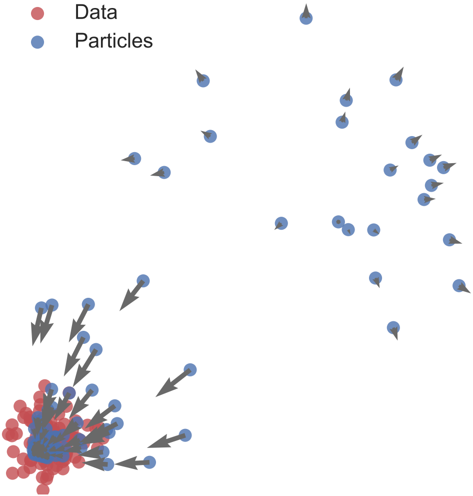

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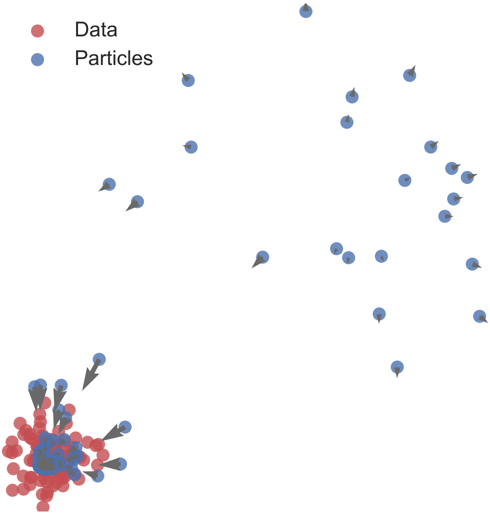

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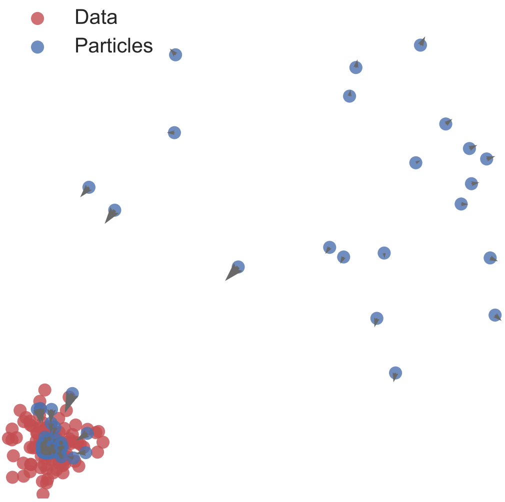

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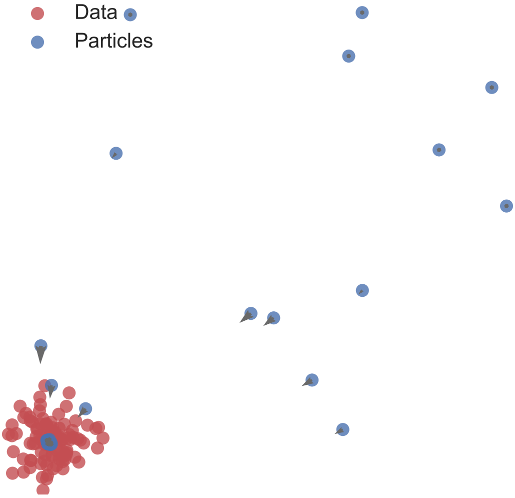

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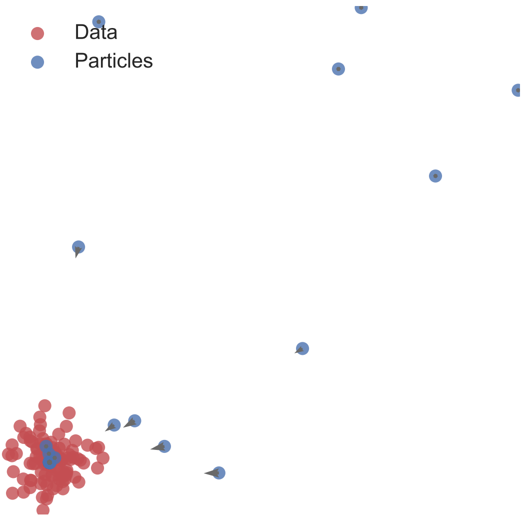

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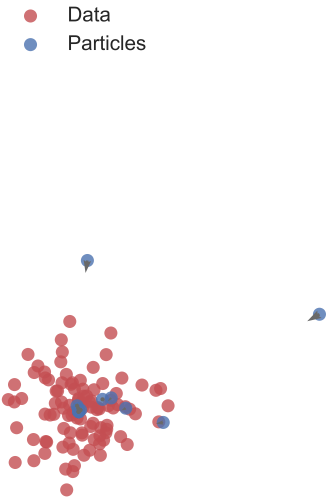

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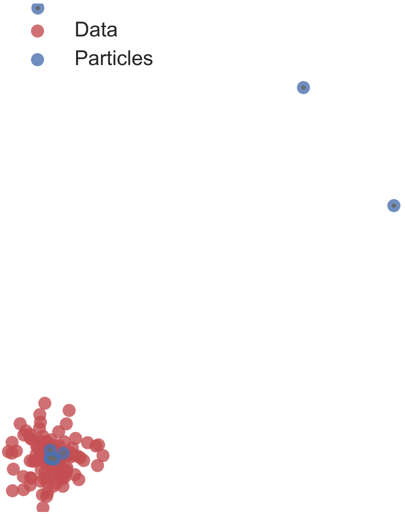

Empirical observations

Some observations:

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

Can these observations be used to improve convergence?

Noise injection to improve convergence

Noise injection: Evaluate $\nabla f_{\nu^\star,\nu_t}$ 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:

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

- Similar to continuation methods,[3] but extended to interacting particles.
- Different from entropic regularization:

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

[3] 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).

Noise injection: consistency

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

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: Back to the failure mode: $\nabla f_{\nu^\star,\nu_t}(Z_t + \beta_t u_t) \simeq 0$

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

Noise injection: consistency

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Need β_t such that:

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

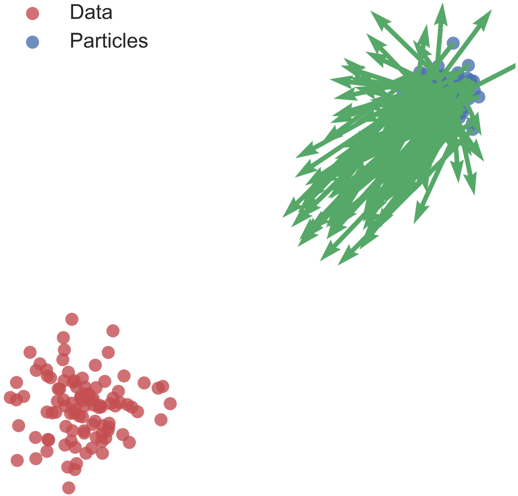
$$\sum_i^t \beta_i^2 \underset{t \to \infty}{\rightarrow} \infty$$

Then [A, Proposition 8]

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

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

Noise injected MMD flow in practice



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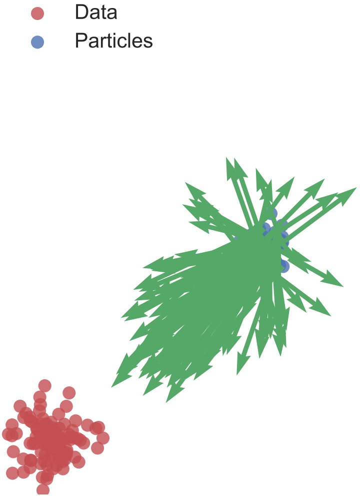

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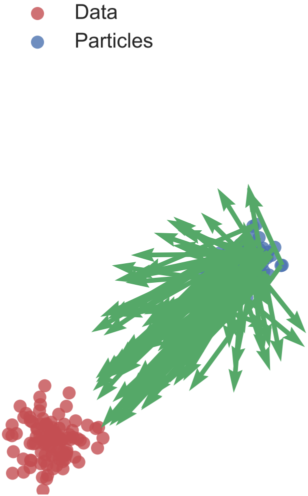

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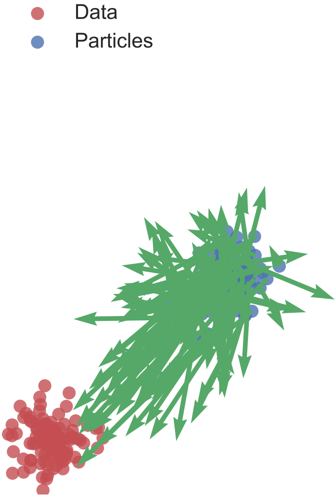

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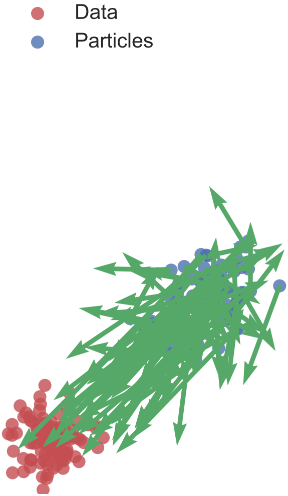

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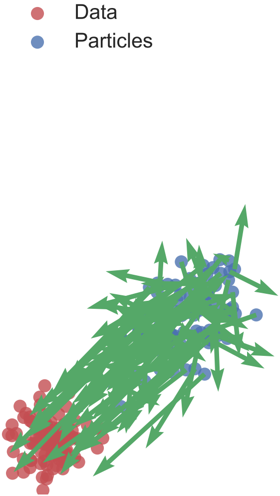

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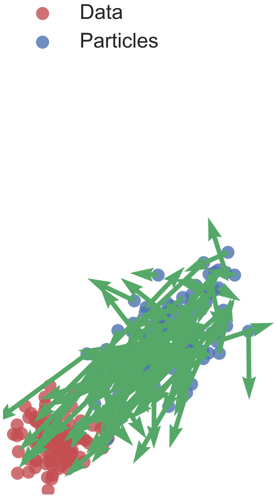

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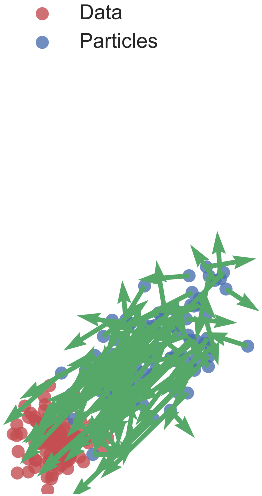

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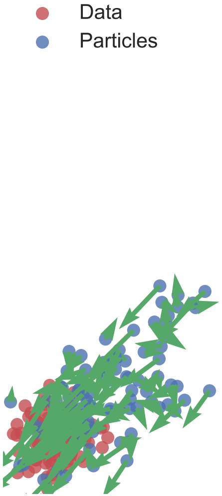

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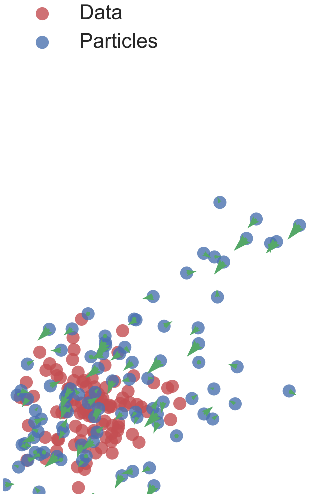
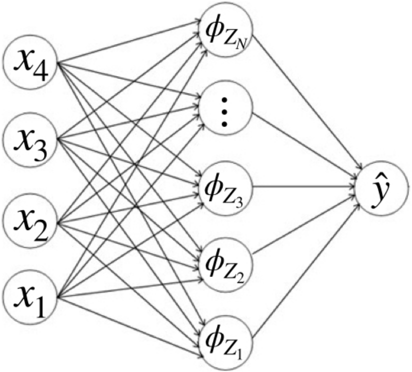


Noise injected MMD flow in practice

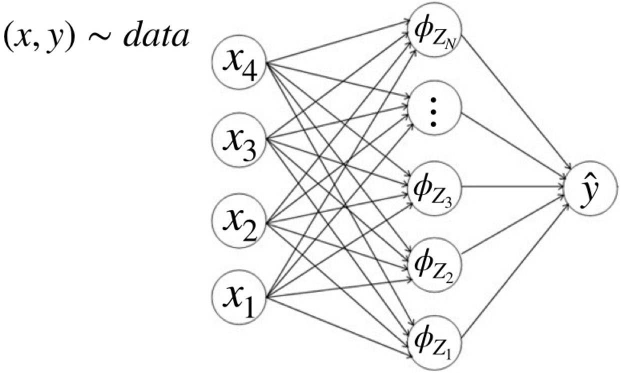
Noise injection: neural net setting

$(x, y) \sim data$



$$\min_{Z_1,\ldots,Z_N} \mathbb{E}_{data}[\| \frac{1}{M} \sum_{m}^{M} \phi_{U^m}(x) - \frac{1}{N} \sum_{n=1}^{N} \phi_{Z^n}(x) \|^2]$$

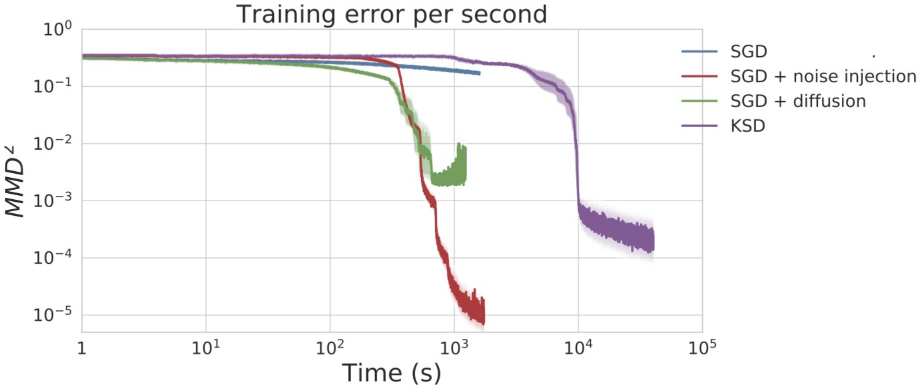
Noise injection: neural net setting



$$\min_{Z_1,\ldots,Z_N} MMD^2(\nu^*, \frac{1}{N}\sum_{n=1}^{N} \delta_{Z^n})$$

$$k(Z, Z') = \mathbb{E}_{data}[\phi_Z(x)\phi_{Z'}(x)]$$

Noise injection: neural net setting



The KALE, and KALE flow

The ϕ-divergences

Define the ϕ-divergence(f-divergence):

$$D_\phi(P, Q) = \int \phi\left(\frac{p(z)}{q(z)}\right) q(z)dz$$

where ϕ is convex, lower-semicontinuous, $\phi(1) = 0$.

- Example: $\phi(u) = u\log(u)$ gives KL divergence,

$$\begin{aligned} D_{KL}(P, Q) &= \int \log\left(\frac{p(z)}{q(z)}\right) p(z)dz \\ &= \int \left(\frac{p(z)}{q(z)}\right) \log\left(\frac{p(z)}{q(z)}\right) q(z)dz \end{aligned}$$

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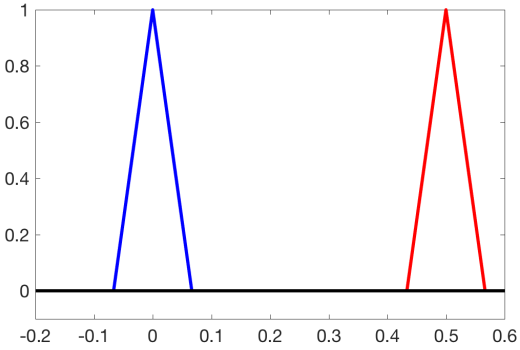
The challenge of disjoint support

Simple example: disjoint support.

Goodfellow et al. (NeurIPS 2014), Arjovsky and Bottou [ICLR 2017]

$$D_{KL}(P, Q) = \infty \qquad D_{JS}(P, Q) = \log 2$$



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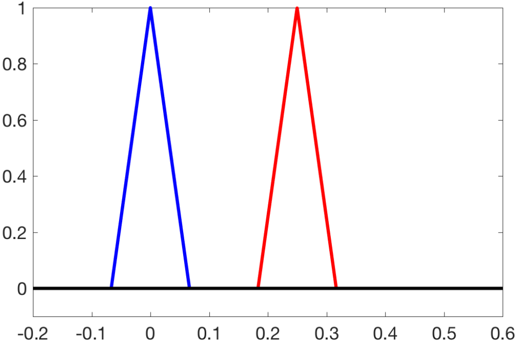
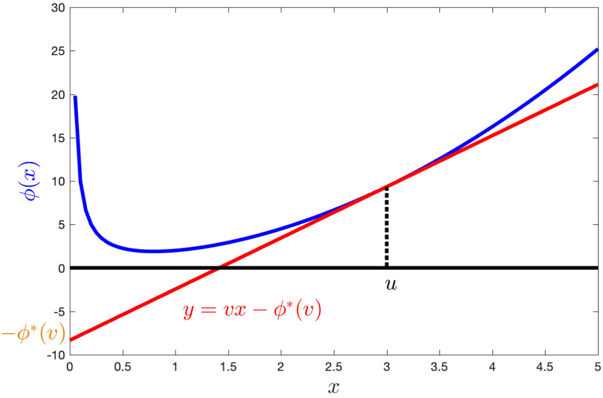


ϕ-divergences in practice

Notation: the conjugate (Fenchel) dual

$$\phi^*(v) = \sup_{u \in \mathbb{R}} \{uv - \phi(u)\}.$$



- $\phi^*(v)$ is negative intercept of tangent to ϕ with slope v

ϕ-divergences in practice

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- For a convex l.s.c. ϕ we have

$$\phi^{**}(x) = \phi(x) = \sup_{v \in \mathbb{R}} \{xv - \phi^*(v)\}$$

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- KL divergence:

$$\phi(x) = x \log(x) \qquad \phi^*(v) = \exp(v - 1)$$

A variational lower bound

A lower-bound ϕ-divergence approximation:

$$D_\phi(P, Q) = \int q(z)\phi\left(\frac{p(z)}{q(z)}\right) dz$$

Nguyen, Wainwright, Jordan, IEEE Transactions on Information Theory (2010);
Nowozin, Cseke, Tomioka, NeurIPS (2016)

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$$= \int q(z) \underbrace{\sup_{f_z}\left(\frac{p(z)}{q(z)} f_z - \phi^*(f_z)\right)}_{\phi\left(\frac{p(z)}{q(z)}\right)}$$

$\phi^*(v)$ is dual of $\phi(x)$.

A variational lower bound

A lower-bound ϕ-divergence approximation:

$$
\begin{aligned}
D_\phi(P, Q) &= \int q(z)\phi\left(\frac{p(z)}{q(z)}\right) dz \\
&= \int q(z) \sup_{f_z} \left(\frac{p(z)}{q(z)} f_z - \phi^*(f_z)\right) \\
&\geq \sup_{f \in \mathcal{H}} \mathrm{E}_P f(X) - \mathrm{E}_Q \phi^*(f(Y))
\end{aligned}
$$

(restrict the function class)

Nguyen, Wainwright, Jordan, IEEE Transactions on Information Theory (2010); Nowozin, Cseke, Tomioka, NeurIPS (2016)

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(restrict the function class)

Bound tight when:

$$f^\diamond(z) = \partial\phi\left(\frac{p(z)}{q(z)}\right)$$

if ratio defined.

Nguyen, Wainwright, Jordan, IEEE Transactions on Information Theory (2010); Nowozin, Cseke, Tomioka, NeurIPS (2016)

Case of the KL

$$D_{KL}(P, Q) = \int \log\left(\frac{p(z)}{q(z)}\right) p(z)\,dz$$

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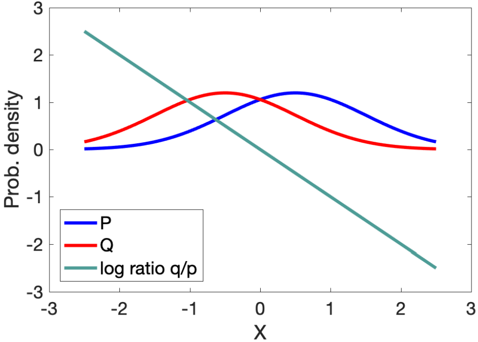

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$$\approx \sup_{f \in \mathcal{H}} \left[\frac{1}{n}\sum_{j=1}^{n} f(x_i) - \frac{1}{n}\sum_{i=1}^{n} \exp(f(y_i))\right] + 1$$

$$x_i \overset{\text{i.i.d.}}{\sim} P$$

$$y_i \overset{\text{i.i.d.}}{\sim} Q$$

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This is a

KL

Approximate

Lower-bound

Estimator.

Nguyen, Wainwright, Jordan, IEEE Transactions on Information Theory (2010);
Nowozin, Cseke, Tomioka, NeurIPS (2016)

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This is a

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Nguyen, Wainwright, Jordan, IEEE Transactions on Information Theory (2010); Nowozin, Cseke, Tomioka, NeurIPS (2016)

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The KALE divergence

Nguyen, Wainwright, Jordan, IEEE Transactions on Information Theory (2010);
Nowozin, Cseke, Tomioka, NeurIPS (2016)

Empirical properties of KALE

$$KALE(P, Q; \mathcal{H}) = \sup_{f \in \mathcal{H}} E_P f(X) - E_Q \exp\left(f(Y)\right) + 1$$

$$f = \langle w, \phi(x) \rangle_{\mathcal{H}} \qquad \mathcal{H} \text{ an RKHS}$$

$$\|w\|^2_{\mathcal{H}} \quad \text{penalized}$$

Glaser, Arbel, G. "KALE Flow: A Relaxed KL Gradient Flow for Probabilities with Disjoint Support," (NeurIPS 2021, Section 2)

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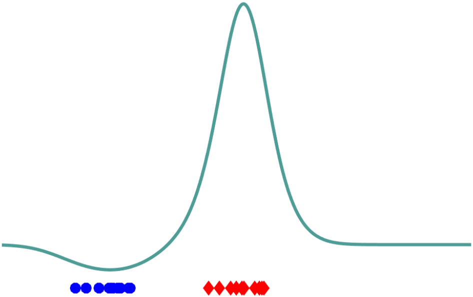
$\|w\|_{\mathcal{H}}^2$ penalized

$KALE(Q, P; \mathcal{H})$=0.18



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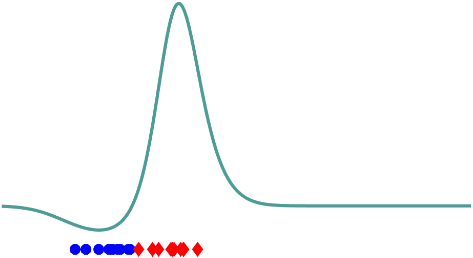
$\|w\|^2_{\mathcal{H}}$ penalized

$$KALE(Q, P; \mathcal{H}) = 0.12$$



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Topological properties of KALE (1)

Key requirements on $\mathcal{H}$ and $\mathcal{X}$:

- Compact domain $\mathcal{X}$,
- $\mathcal{H}$ dense in the space $C(\mathcal{X})$ of continuous functions on $\mathcal{X}$ wrt $\|\cdot\|_\infty$.
- If $f \in \mathcal{H}$ then $-f \in \mathcal{H}$ and $cf \in \mathcal{H}$ for $0 \leq c \leq C_{\max}$.

Theorem: $KALE(P, Q; \mathcal{H}) \geq 0$ and $KALE(P, Q; \mathcal{H}) = 0$ iff $P = Q$.

Zhang, Liu, Zhou, Xu, and He. "On the Discrimination-Generalization Tradeoff in GANs" (ICLR 2018, Corollary 2.4; Theorem B.1)
Arbel, Liang, G. (ICLR 2021, Proposition 1)

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$\mathcal{H}$ dense in $C(\mathcal{X})$ for $\mathcal{X} \subset \mathbb{R}^d$ when:

$$\mathcal{H} = \operatorname{span}\{\sigma(w\top x + b) : [w, b] \in \Theta\}$$

$\sigma(u) = \max\{u, 0\}^\alpha$, $\alpha \in \mathbb{N}$, and $\{\lambda\theta : \lambda \geq 0, \theta \in \Theta\} = \mathbb{R}^{d+1}$.

Zhang, Liu, Zhou, Xu, and He. “On the Discrimination-Generalization Tradeoff in GANs”

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Arbel, Liang, G. (ICLR 2021, Proposition 1)

Topological properties of KALE (2)

Additional requirement: all functions in $\mathcal{H}$ Lipschitz in their inputs with constant L

Theorem: $\text{KALE}(P, Q^n; \mathcal{H}) \to 0$ iff $Q^n \to P$ under the weak topology.

Liu, Bousquet, Chaudhuri. "Approximation and Convergence Properties of Generative Adversarial Learning" (NeurIPS 2017); Arbel, Liang, G. (ICLR 2021, Proposition 1)

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Partial proof idea:

$$\begin{aligned}
\mathrm{KALE}(P, Q; \mathcal{H}) &= \int f \, dP - \int \exp(f) \, dQ + 1 \\
&= -\int f(x) \, dQ(x) + f(x') \, dP(x') \\
&\quad - \int \underbrace{(\exp(f) - f - 1)}_{\geq 0} \, dQ \\
&\leq \int f(x') \, dP(x') - \int f(x) \, dQ(x) \leq L W_1(P, Q)
\end{aligned}$$

Liu, Bousquet, Chaudhuri. "Approximation and Convergence Properties of Generative Adversarial Learning" (NeurIPS 2017); Arbel, Liang, G. (ICLR 2021, Proposition 1)

KALE vs KL vs MMD

A scaled KALE (non-degenerate for $\lambda = 0$ or $\lambda \to \infty$):

$$\mathrm{KALE}_\lambda(P, Q; \mathcal{H}) = (1+\lambda) \sup_{f \in \mathcal{H}} \left[E_P f(X) - E_Q \exp(f(Y)) + 1 - \frac{\lambda}{2} \|f\|_{\mathcal{H}}^2 \right]$$

MMD limit:

$$\lim_{\lambda \to +\infty} \mathrm{KALE}_\lambda(P, Q; \mathcal{H}) = \frac{1}{2} \mathrm{MMD}^2(P, Q).$$

KL limit (assuming $\log \frac{\mathrm{d}P}{\mathrm{d}Q} \in \mathcal{H}$):

$$\lim_{\lambda \to 0} \mathrm{KALE}_\lambda(P, Q; \mathcal{H}) = \mathrm{KL}(P, Q).$$

Glaser, Arbel, G. (NeurIPS 2021, Proposition 1)

Wasserstein gradient flow on KALE

First variation of the $KALE_\lambda(\nu, \nu^\star)$

$$\frac{\partial \mathrm{KALE}_\lambda}{\partial \nu}(\nu)(z) := (1+\lambda)\, f_{\nu,\nu^\star}(z)$$

where $f_{\nu,\nu^\star}$ is the solution of

$$f_{\nu,\nu^\star} = \arg\max_{f \in \mathcal{H}} \{\mathcal{K}(f, \nu)\},$$

where

$$\mathcal{K}(f, \nu) := E_\nu f(X) - E_{\nu^*} \exp(f(Y)) + 1 - \frac{\lambda}{2}\|f\|^2_{\mathcal{H}}$$

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Proof (idea):

$$\frac{\partial \mathrm{KALE}_\lambda}{\partial \nu} = \frac{\partial \mathcal{K}(f_{\nu,\nu^\star}, \nu)}{\partial \nu} + \underbrace{\frac{\partial \mathcal{K}(f,\nu)}{\partial f}\bigg|_{f=f_{\nu,\nu^\star}}}_{=0} \frac{\partial f_{\nu,\nu^\star}}{\partial \nu}$$

as long as $\frac{\partial f_{\nu,\nu^\star}}{\partial \nu}$ exists (via implicit function theorem)

Wasserstein gradient flow on KALE

The W_2 gradient flow of the KALE:

$$\partial_t \nu_t = -(1+\lambda)\mathrm{div}(\nu_t \nabla f_{\nu_t,\nu^\star}), \qquad \nu_0 = P_0$$

where

$$f_{\nu,\nu^\star} = \arg\max_f \mathcal{K}(f,\nu)$$

Glaser, Arbel, G. (NeurIPS 2021, Lemma 3)

Consistency (2)

Again, under the (strong!) assumption

$$S(\nu^\star|\nu_t) := \sup_{g, \mathbb{E}_{Z\sim\nu_t}[||\nabla g(Z)||^2]\leq 1} |\mathbb{E}_{Z\sim\nu_t}[g(Z)] - \mathbb{E}_{U\sim\nu^\star}[g(U)]|$$
$$\leq C$$

we have

$$\text{KALE}(\nu_t) \leq \frac{1}{\text{KALE}(\nu_0)^{-1} + C^{-1}t}$$

Once again, noise injection can be used (similar result to MMD flow).

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Once again, noise injection can be used (similar result to MMD flow).

Compare with linear rate for Wasserstein-2 flow on KL when $\nu^\star$ satisfies log-Sobolev inequality with constant ρ:

$$\frac{d}{dt}KL(\nu_t, \nu^\star) \leq -2\rho KL(\nu_t, \nu^\star)$$

Glaser, Arbel, G. (NeurIPS 2021, Proposition 3)

KALE flow vs MMD flow in practice

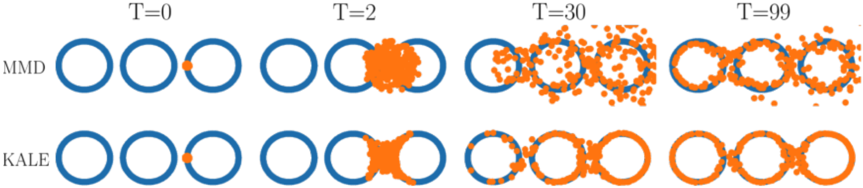

Figure 1: MMD and KALE flow trajectories for “three rings” target

Glaser, Arbel, G. (NeurIPS 2021)

Summary

- Gradient flows based on kernel dependence measures:
  - MMD flow is simpler, KALE flow is mode-seeking
  - Noise injection can improve convergence
- NeurIPS 2019, NeurIPS 2021

NeurIPS 2019:

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

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arXiv > stat > arXiv:2106.08929

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

Pierre Glaser, Michael Arbel, Arthur Gretton

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KALE as GAN critic:

ICLR 2021:

arXiv.org > stat > arXiv:2003.05033

Statistics > Machine Learning

[Submitted on 10 Mar 2020 (v1), last revised 24 Jun 2020 (this version, v3)]

Generalized Energy Based Models

Michael Arbel, Liang Zhou, Arthur Gretton

NeurIPS 2020:

arXiv.org > cs > arXiv:2003.06060

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Your GAN is Secretly an Energy-based Model and You Should use Discriminator Driven Latent Sampling

Tong Che, Ruixiang Zhang, Jascha Sohl-Dickstein, Hugo Larochelle, Liam Paull, Yuan Cao, Yoshua Bengio

Questions?


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