

Maximum Mean Discrepancy Gradient Flow

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Problem and Outline

Problem:

- ▶ Transport mass from a starting probability distribution to a target distribution
- ▶ How? By finding a *continuous* path on the space of distributions, decreasing some loss
- ▶ **This work:** Minimize the Maximum Mean Discrepancy (MMD) on the space of probability distributions.

Application : Insights on the theoretical properties of some large neural networks and alteration of the dynamics to improve convergence.

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1. Background and motivation
2. Wasserstein gradient flow of the MMD
3. Convergence properties
4. A noise-injection algorithm for better convergence

Outline

Background and motivation

Wasserstein gradient flow of the MMD

Convergence properties of the MMD gradient flow

A noise-injection algorithm for better convergence

Reproducing Kernel Hilbert Spaces (RKHS)

- ▶ Let $k : \mathcal{Z} \times \mathcal{Z} \rightarrow \mathbb{R}$ a positive, semi-definite kernel
- ▶ $\mathcal{H}$ its corresponding RKHS.

Recall: $\mathcal{H}$ is a Hilbert space with inner product $\langle ., . \rangle_{\mathcal{H}}$ and norm $\|.\|_{\mathcal{H}}$. It satisfies the reproducing property:

$$\forall \quad f \in \mathcal{H}, f(z) = \langle f, k(z, .) \rangle_{\mathcal{H}}$$

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$$\forall f \in \mathcal{H}, f(z) = \langle f, k(z, \cdot) \rangle_{\mathcal{H}}$$

Let $\mathcal{P}$ the set of probability distributions on $\mathcal{Z}$ with finite second moment. Suppose k is characteristic, ie the map:

$$\begin{aligned} \mathcal{P} &\rightarrow \mathcal{H} \\ \nu &\mapsto \underbrace{\int_{\mathcal{Z}} k(z, \cdot) d\nu(z)}_{\text{"mean embedding of } \nu"} \end{aligned}$$

is injective.

Maximum Mean Discrepancy (MMD)

Maximum Mean Discrepancy ([Gretton et al., 2012a]) defines a distance on $\mathcal{P}$:

$MMD(\mu, \nu) = \|f_{\mu, \nu}\|_{\mathcal{H}}$, where

$$f_{\mu, \nu}(\cdot) = \int k(z, \cdot) d\mu(z) - \int k(z, \cdot) d\nu(z)$$

$f_{\mu, \nu}$ is called the **witness function** and is the difference between the mean embeddings of μ and ν .

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Now fix the (target) distribution μ . We consider the functional:

$$\begin{aligned}\mathcal{L}: \quad \mathcal{P} &\rightarrow \mathbb{R} \\ \nu &\mapsto \frac{1}{2} MMD^2(\mu, \nu)\end{aligned}$$

MMD functional

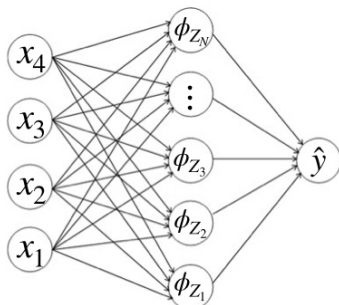
For a target distribution μ (fixed), for any $\nu \in \mathcal{P}$:

$$\begin{aligned}\mathcal{L}(\nu) &= \frac{1}{2} \text{MMD}^2(\mu, \nu) \\ &= \frac{1}{2} \|f_{\mu, \nu}\|_{\mathcal{H}}^2 \\ &= \frac{1}{2} \langle f_{\mu, \nu}, f_{\mu, \nu} \rangle_{\mathcal{H}} \\ &= \frac{1}{2} \langle f_{\mu, \nu}, \int k(z, \cdot) d\nu(z) - \int k(z, \cdot) d\mu(z) \rangle_{\mathcal{H}} \\ &= \frac{1}{2} \left(\int f_{\mu, \nu}(z) d\nu(z) - \int f_{\mu, \nu}(z) d\mu(z) \right) \\ &= \frac{1}{2} \int k(z, z') d\nu(z) d\nu(z') + \frac{1}{2} \int k(z, z') d\mu(z) d\mu(z') \\ &\quad - \int k(z, z') d\nu(z) d\mu(z')\end{aligned}$$

General problem

Consider the following regression problem:

$$(x, y) \sim \text{data}$$

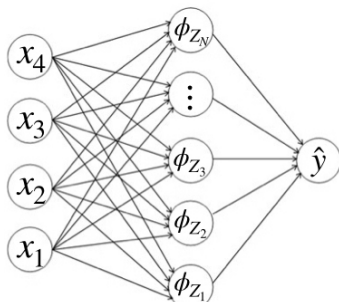


$$\min_{Z_1, \dots, Z_N} \mathbb{E}_{\text{data}} \left[\left\| y - \frac{1}{N} \sum_{i=1}^N \phi_{Z_i}(x) \right\|^2 \right]$$

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Consider the following regression problem:

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

► $\phi_{Z_i}(x) = w_i g(x, \theta_i),$
 $(w_i, \theta_i) \in \mathbb{R} \times \mathbb{R}^d$
 $\phi_{Z_i} : \text{non linearity}$

► Example:

$$\phi_Z(x) = wg(ax + b)$$

where $g : \mathbb{R} \rightarrow \mathbb{R}$

(sigmoid

$g(z) = 1/(1 + e^{-z})$, ReLU

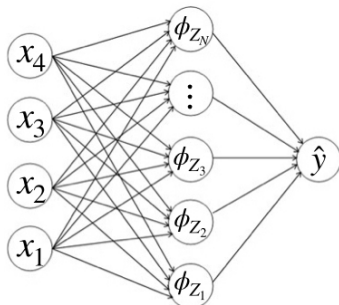
($g(z) = \max(0, z)$...)

General problem

Finite dimensional **non-convex** optimization (regression setting):

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

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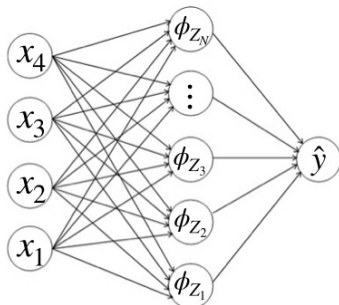
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► Optimization using gradient descent (GD):

$$\mathbf{z}_i^{t+1} = \mathbf{z}_i^t - \gamma \nabla_{\mathbf{z}_i} \mathcal{L} \left(\frac{1}{N} \sum_{i=1}^N \delta_{\mathbf{z}_i^t} \right)$$

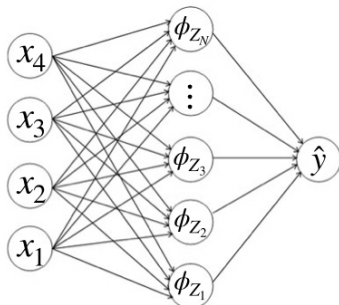
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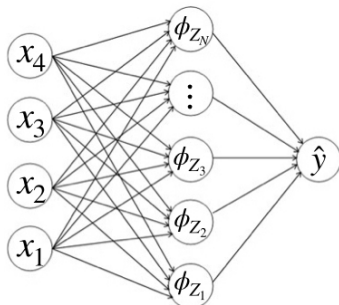
- Hard to describe the dynamics of GD!

General problem

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$(x, y) \sim data$



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

- Optimization using gradient descent (GD):

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

- Hard to describe the dynamics of GD!
- Idea: look at the distribution of the Z_i 's

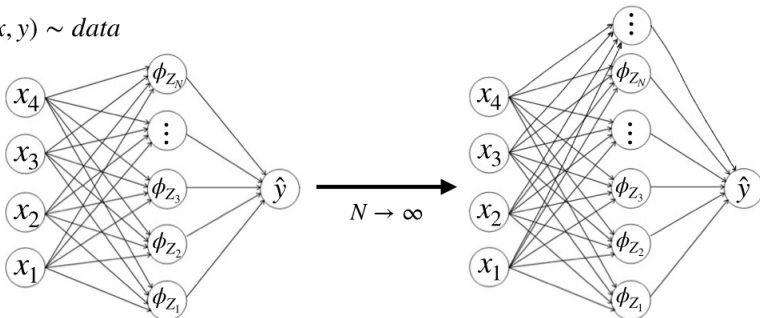
General problem

Infinite dimensional **convex** optimization [Chizat and Bach, 2018],

[Mei et al., 2018]:

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

$(x, y) \sim \text{data}$



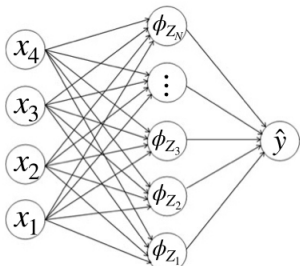
$$\min_{Z_1, \dots, Z_N} \mathbb{E}_{\text{data}} \left[\|y - \frac{1}{N} \sum_{i=1}^N \phi_{Z_i}(x)\|^2 \right] \xrightarrow{N \rightarrow \infty} \min_{\nu \in \mathcal{P}} \mathbb{E}_{\text{data}} \left[\|y - \mathbb{E}_{Z \sim \nu} [\phi_Z(x)]\|^2 \right]$$

General problem

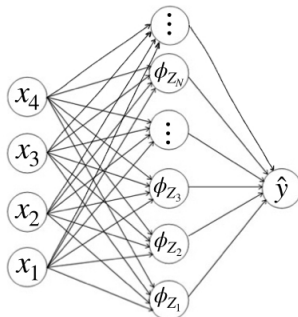
- **Global convergence of Gradient descent**¹ when $N \rightarrow \infty$ and $\phi_Z(x)$ of the form:

$$\phi_Z(x) = wg(x, \theta), \quad Z = (w, \theta)$$

$(x, y) \sim \text{data}$



$N \rightarrow \infty$



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

$N \rightarrow \infty$

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

¹[Rotskoff and Vanden-Eijnden, 2018, Chizat and Bach, 2018]

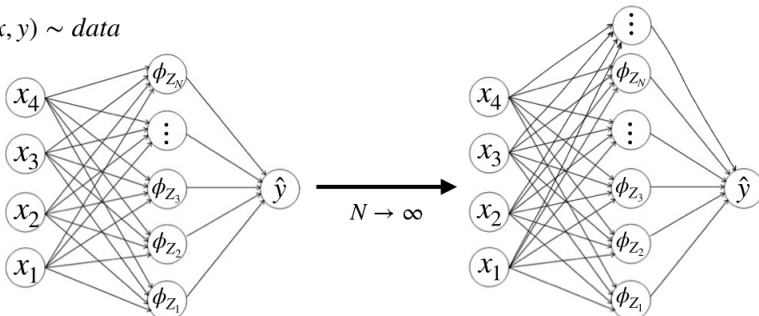
General problem

- **Global convergence of Gradient descent¹** when $N \rightarrow \infty$ and $\phi_Z(x)$ of the form:

$$\phi_Z(x) = wg(x, \theta), \quad Z = (w, \theta)$$

- Interested in more general form for $\phi_Z(x)$.

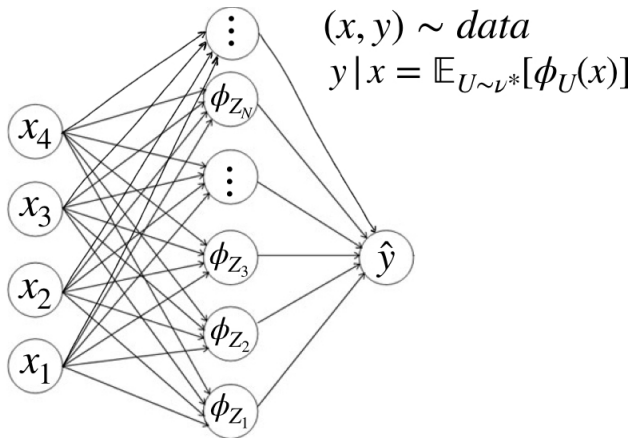
$(x, y) \sim \text{data}$



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

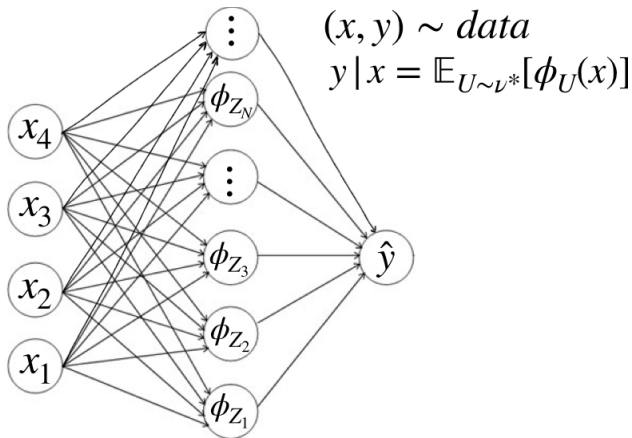
¹[Rotskoff and Vanden-Eijnden, 2018, Chizat and Bach, 2018]

Minimization of the MMD: the well-specified case



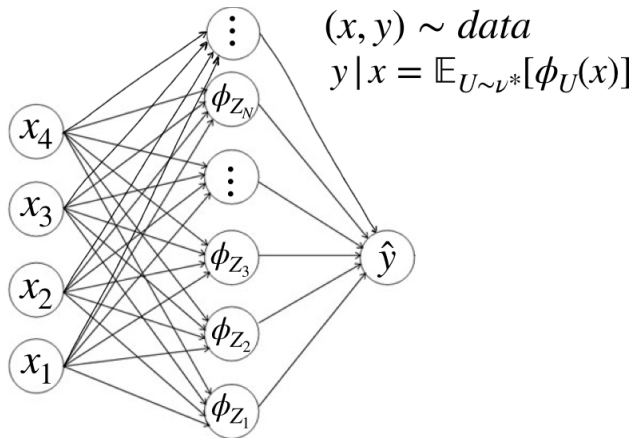
$$\min_{\nu \in \mathcal{P}} \mathbb{E}_{data} [\|y - \mathbb{E}_{Z \sim \nu} [\phi_Z(x)]\|^2]$$

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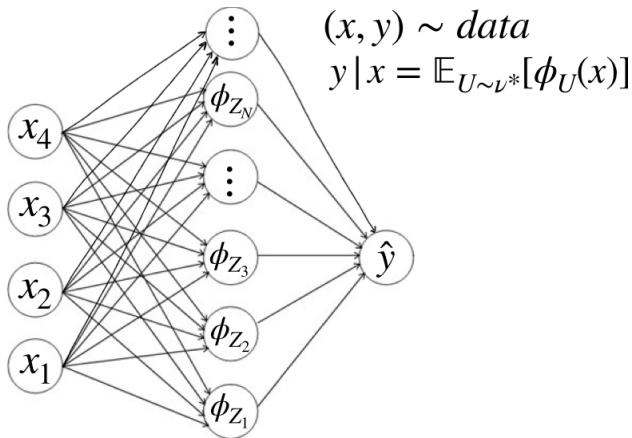
$$\min_{\nu \in \mathcal{P}} \mathbb{E}_{data} [\|\mathbb{E}_{U \sim \nu^*}[\phi_U(x)] - \mathbb{E}_{Z \sim \nu}[\phi_Z(x)]\|^2]$$

Minimization of the MMD: the well-specified case



$$\min_{\nu \in \mathcal{P}} \mathbb{E}_{\substack{U \sim \nu^* \\ U' \sim \nu^*}} [k(U, U')] + \mathbb{E}_{\substack{Z \sim \nu \\ Z' \sim \nu}} [k(Z, Z')] - 2 \mathbb{E}_{\substack{U \sim \nu^* \\ Z' \sim \nu}} [k(U, Z)]$$

Minimization of the MMD: the well-specified case

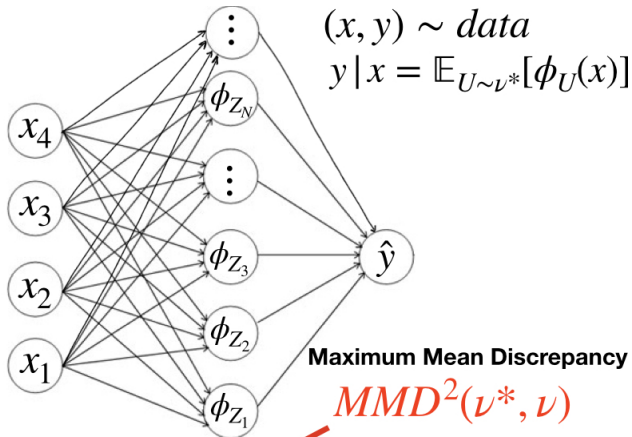


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$U' \sim \nu^* \qquad Z' \sim \nu \qquad Z' \sim \nu$

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

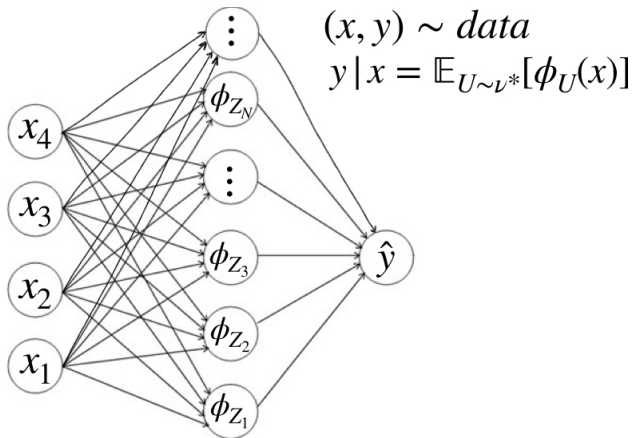
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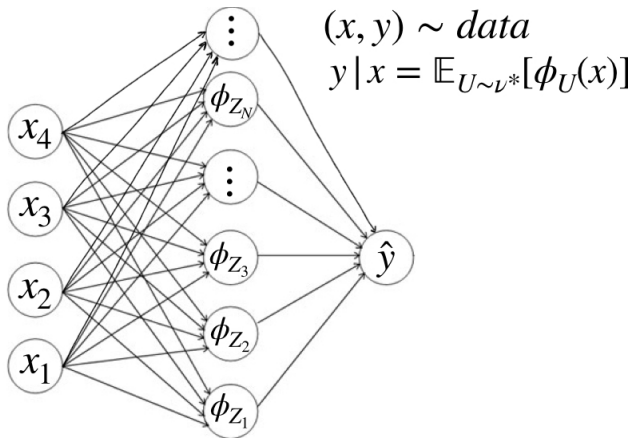
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$$\min_{\nu \in \mathcal{P}} MMD^2(\nu^*, \nu)$$

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Minimization of the MMD: the well-specified case



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

MMD Gradient Flow

- ▶ The optimization over the parameters of a neural network can be seen as a minimization of the MMD on $\mathcal{P}$ in the population limit ($N \rightarrow \infty$).

$$\min_{\nu} \text{MMD}^2(\nu, \nu^*)$$

$$\nu_{t+1} \approx \nu_t - \gamma \nabla_{\nu_t} \text{MMD}^2(\nu_t, \nu^*)$$

- ▶ Gradient descent dynamics in this setting takes the form of a PDE (gradient flow on $\mathcal{P}$)
- ▶ Powerful tool to analyze dynamics and possibly alterate them

Outline

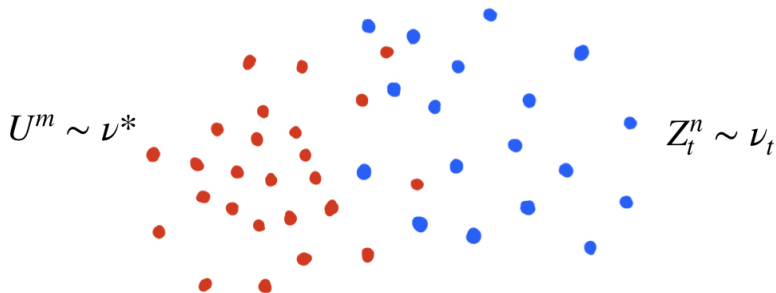
Background and motivation

Wasserstein gradient flow of the MMD

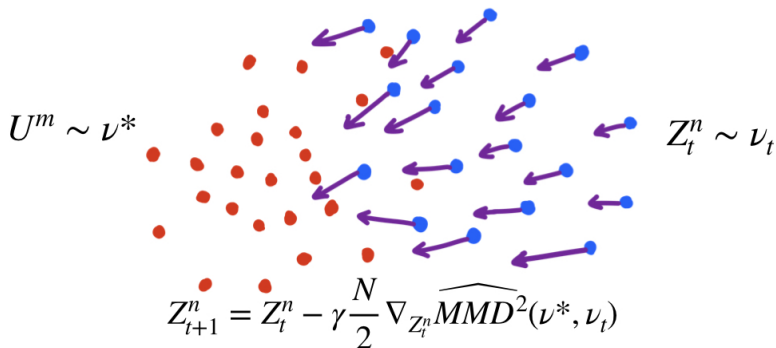
Convergence properties of the MMD gradient flow

A noise-injection algorithm for better convergence

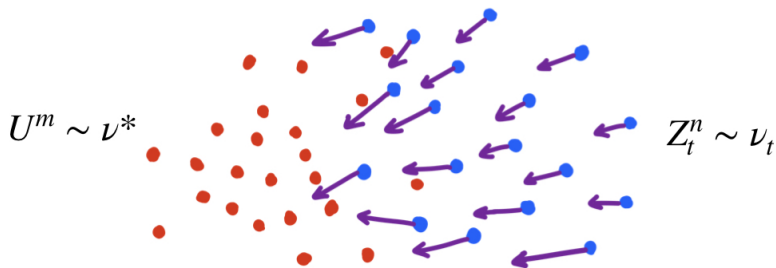
Gradient descent of the MMD



Gradient descent of the MMD



Gradient descent of the MMD



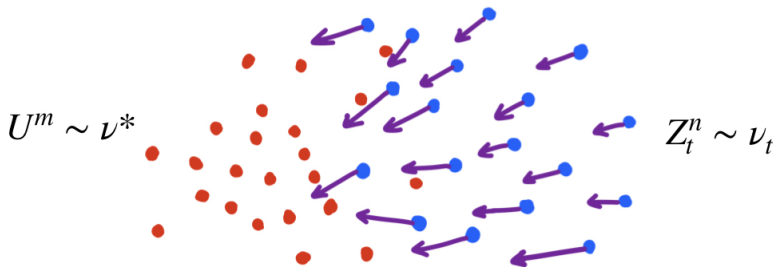
$$Z_{t+1}^n = Z_t^n - \gamma \frac{N}{2} \nabla_{Z_t^n} \widehat{MMD^2}(\nu^*, \nu_t)$$

$$\frac{N}{2} \nabla_{Z_t^n} \widehat{MMD^2}(\nu^*, \nu_t) = \frac{1}{N-1} \sum_{n' \neq n} \partial_1 k(Z_t^n, Z_t^{n'}) - \frac{1}{M} \sum_{m=1}^M \partial_1 k(Z_t^n, U^m)$$

$$\downarrow N, M \rightarrow \infty$$

$$\nabla_{Z_t} \left(\mathbb{E}_{Z' \sim \nu_t} [k(Z_t, Z')] - \mathbb{E}_{U \sim \nu^*} [k(Z_t, U)] \right)$$

Gradient descent of the MMD

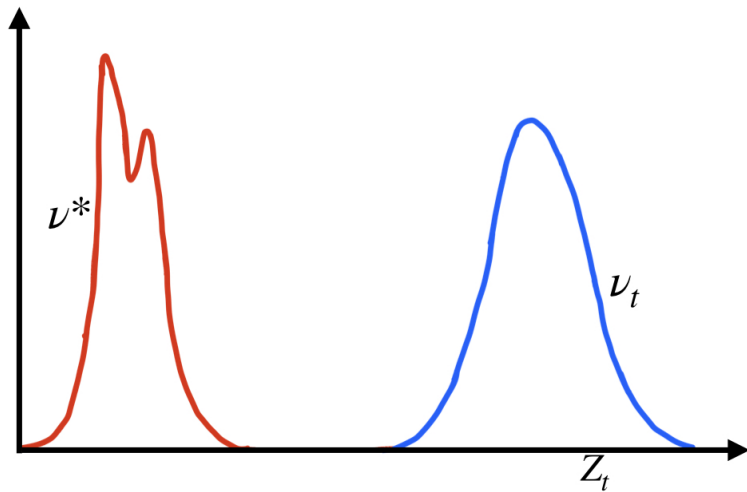


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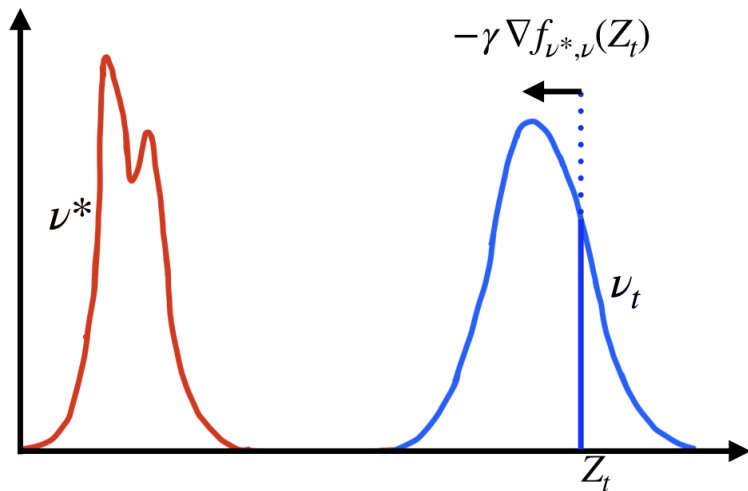
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$$\begin{aligned} & \downarrow N, M \rightarrow \infty \\ & \nabla_{Z_t} \left(\underbrace{\mathbb{E}_{Z' \sim \nu_t} [k(Z_t, Z')] - \mathbb{E}_{U \sim \nu^*} [k(Z_t, U)]}_{f_{\nu^*, \nu_t}(Z_t)} \right) \end{aligned}$$

Wasserstein gradient descent

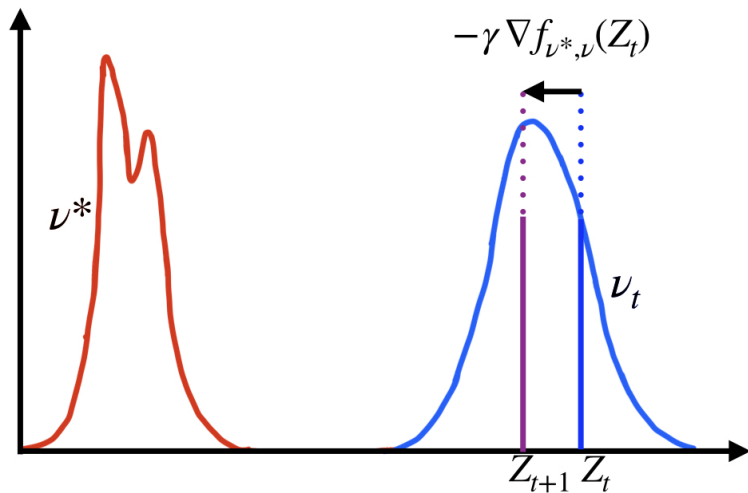


Wasserstein gradient descent



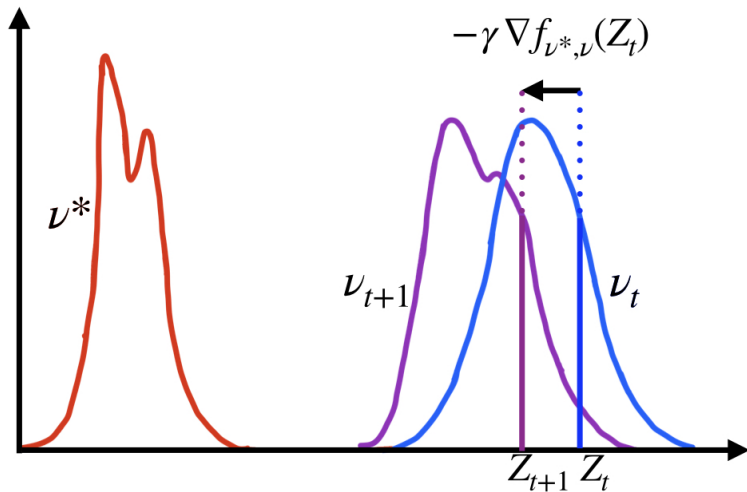
$$f_{\nu^*, \nu_t}(Z_t) = \mathbb{E}_{Z' \sim \nu_t}[k(Z_t, Z')] - \mathbb{E}_{U \sim \nu^*}[k(Z_t, U)]$$

Wasserstein gradient descent



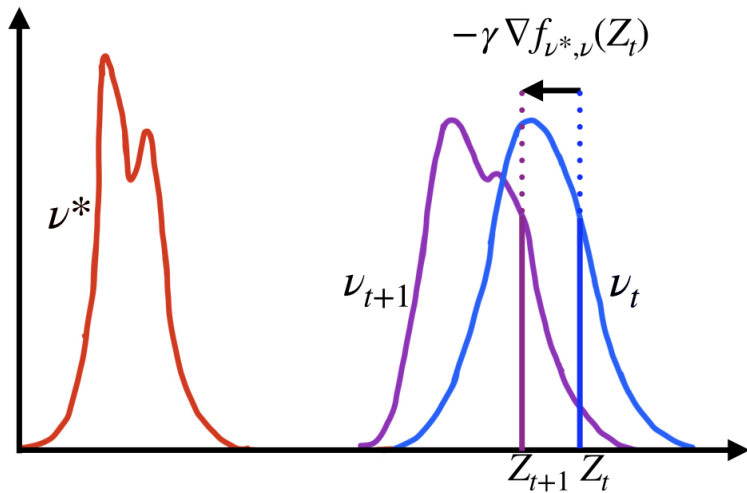
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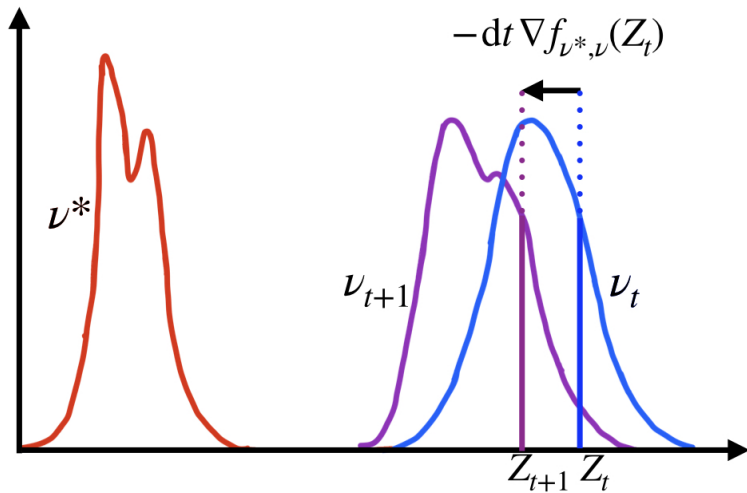


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Wasserstein gradient descent



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

Wasserstein gradient flow

- ▶ Continuous time equation: Mc-Kean Vlasov dynamics ²

$$\frac{dZ_t}{dt} = -\nabla_{Z_t} f_{\nu^*, \nu_t}(Z_t), \quad Z_t \sim \nu_t$$

²[Kac, 1956]

³[Otto, 2001, Villani, 2004, Ambrosio et al., 2004]

Wasserstein gradient flow

- ▶ Continuous time equation: Mc-Kean Vlasov dynamics ²

$$\frac{dZ_t}{dt} = -\nabla_{Z_t} f_{\nu^*, \nu_t}(Z_t), \quad Z_t \sim \nu_t$$

- ▶ Equivalent to a PDE in ν_t :

$$\partial_t \nu_t = \operatorname{div}(\nu_t \nabla f_{\nu^*, \nu_t})$$

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Wasserstein gradient flow

- ▶ Continuous time equation: Mc-Kean Vlasov dynamics²

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- ▶ Equivalent to a PDE in ν_t :

$$\partial_t \nu_t = \operatorname{div}(\nu_t \nabla f_{\nu^*, \nu_t})$$

- ▶ Interpretation as a gradient flow in probability space³, a curve $\nu : [0, \infty] \rightarrow \mathcal{P}$:

$$\partial_t \nu_t = -\nabla_{\nu_t} \mathcal{L}(\nu_t) \quad \mathcal{L}(\nu) := \frac{1}{2} \operatorname{MMD}^2(\nu^*, \nu)$$

can be obtained as the limit when $\tau \rightarrow 0$ of:

$$\nu_{t+1} \in \arg \min_{\nu \in \mathcal{P}} \mathcal{L}(\nu) + \frac{1}{2\tau} W_2^2(\nu, \nu_t).$$

²[Kac, 1956]

³[Otto, 2001, Villani, 2004, Ambrosio et al., 2004]

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Wasserstein gradient flow of the MMD

Convergence properties of the MMD gradient flow

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Convergence of gradient flows and convexity

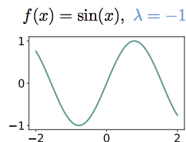
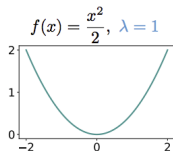
In a **euclidean** setting, a gradient flow of a differentiable function $f : \mathbb{R}^d \rightarrow \mathbb{R}$ is a curve $x : [0, \infty] \rightarrow \mathbb{R}^d$:

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

Existence, uniqueness results on gradient flows rely on the notion of **convexity**.

A function f defined on $\mathbb{R}^d$ is λ -convex if for any $x, y \in \mathbb{R}^d$ and $t \in [0, 1]$:

$$f((1-t)x + ty) \leq (1-t)f(x) + tf(y) - t(1-t)\frac{\lambda}{2}|x-y|^2$$



When $\lambda > 0$: any gradient flow x_t converges to a unique $x^* = \operatorname{argmin}_x f(x)$ when $t \rightarrow \infty$.

Convergence of the MMD (W2-)gradient flow

In the **W2** setting, a gradient flow of a functional $\mathcal{L} : \mathcal{P} \rightarrow \mathbb{R}$ is a curve $\nu : [0, \infty] \rightarrow \mathcal{P}$ that satisfies:

$$\frac{d\nu_t}{dt} = -\nabla_{\nu_t} \mathcal{L}(\nu_t)$$

Existence, uniqueness results on gradient flows on $\mathcal{P}$ rely on the notion of **convexity**, wrt W2 geodesic curves.

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$$\mathcal{L}(\rho(t)) \leq (1-t)\mathcal{L}(\rho(0)) + t\mathcal{L}(\rho(1)) - t(1-t)\frac{\lambda}{2}d(\rho(0), \rho(1))^2$$

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Our finding: The MMD is λ -convex with $\lambda < 0$.

Too bad... $\lambda > 0$ would have guaranteed that all gradient flows of $\mathcal{L}$ would converge the **unique** minimizer of $\mathcal{L}$ [Carrillo et al., 2006]

Second strategy - Obtain a Łojasiewicz inequality

$$\frac{d\mathcal{L}(\nu_t)}{dt} \leq -C\mathcal{L}(\nu_t)^2$$

Applying Gronwall's lemma results in: $\mathcal{L}(\nu_t) = \mathcal{O}(\frac{1}{t})$.

Second strategy - Obtain a Lojasiewicz inequality

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► on the right, it's the **RKHS norm**:

$$\begin{aligned}\mathcal{L}(\nu_t) &= \frac{1}{2} \text{MMD}^2(\nu^*, \nu_t) \\ &= \frac{1}{2} \int k(U, U) d\nu^*(U) d\nu^*(U) + \frac{1}{2} \int k(Z, Z) d\nu_t(Z) d\nu_t(Z) \\ &\quad - \int k(U, Z) d\nu^*(U) d\nu_t(Z) \\ &= \frac{1}{2} \|f_{\nu^*, \nu_t}\|_{\mathcal{H}}^2\end{aligned}$$

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► on the left we have the **weighted Sobolev semi-norm**:

$$\frac{d\mathcal{L}(\nu_t)}{dt} = - \int \|\nabla f_{\nu^*, \nu_t}(x)\|^2 d\nu_t(x) = -\|f_{\nu^*, \nu_t}\|_{\dot{H}(\nu_t)}^2$$

Since:

$$\partial_t \nu_t = \operatorname{div}(\nu_t \nabla f_{\nu^*, \nu_t})$$

A criterion for convergence

Define the weighted Negative Sobolev norm:

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

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It can be shown that:

$$\|f_{\nu^*, \nu_t}\|_{\mathcal{H}}^2 \leq \|f_{\nu^*, \nu_t}\|_{\dot{H}(\nu_t)} \|\nu^* - \nu_t\|_{\dot{H}^{-1}(\nu_t)}$$

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Assume that $\|\nu_t - \nu^*\|_{\dot{H}^{-1}(\nu_t)} \leq C$ for all t , then

$$MMD^2(\nu^*, \nu_t) \leq \frac{1}{MMD^2(\nu^*, \nu_0) + 4C^{-1}t}$$

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It can be shown that:

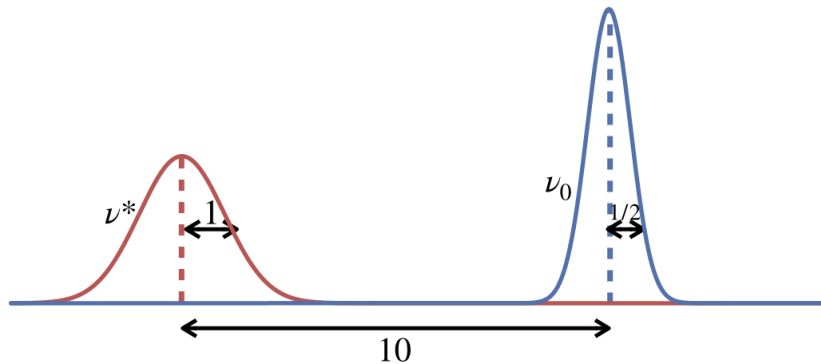
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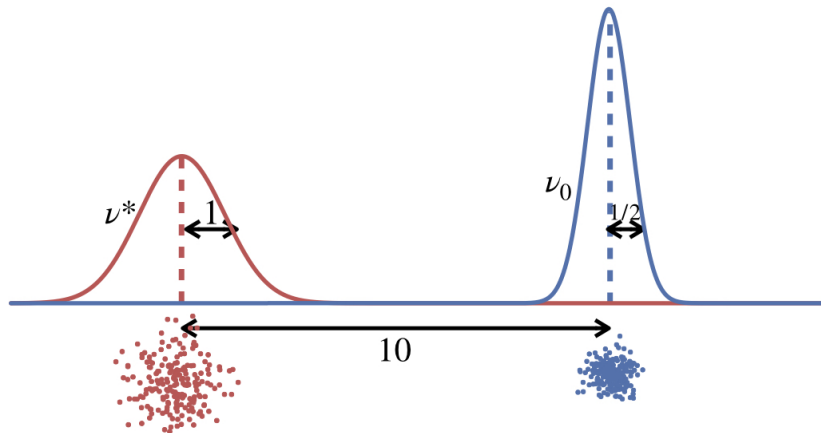
$$MMD^2(\nu^*, \nu_t) \leq \frac{1}{MMD^2(\nu^*, \nu_0) + 4C^{-1}t}$$

Problem: Depends on the whole sequence ν_t ; Hard to verify in general [Peyre, 2018]; and we've seen failure cases in practice.

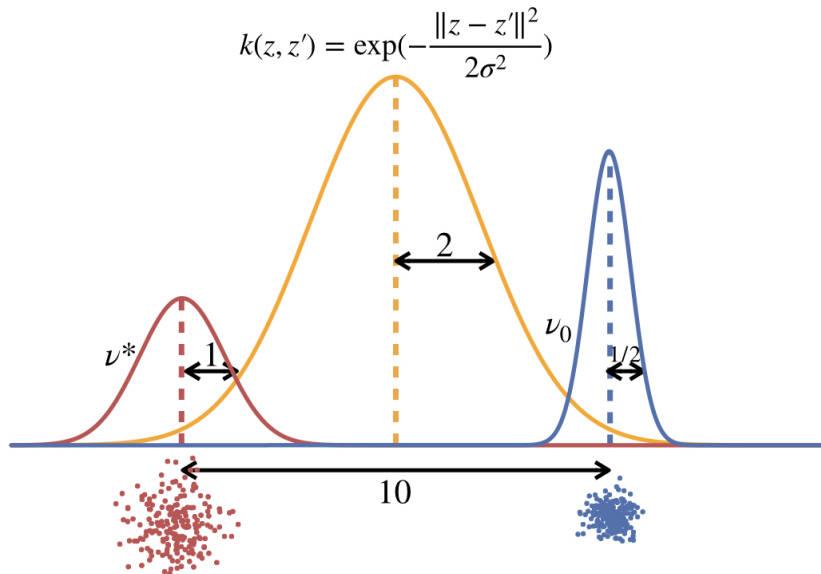
Convergence: Failure case



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Outline

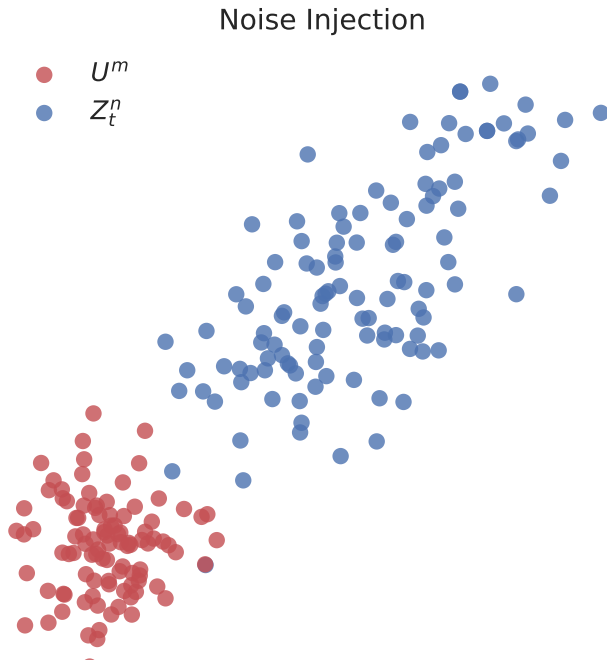
Background and motivation

Wasserstein gradient flow of the MMD

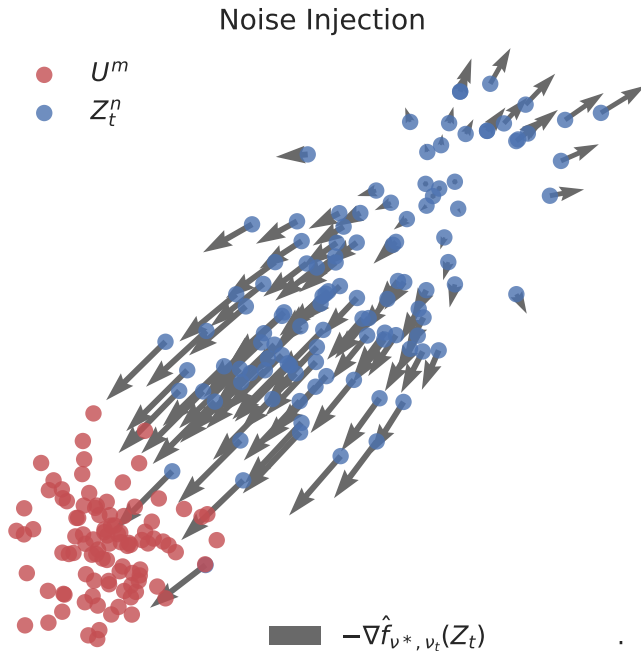
Convergence properties of the MMD gradient flow

A noise-injection algorithm for better convergence

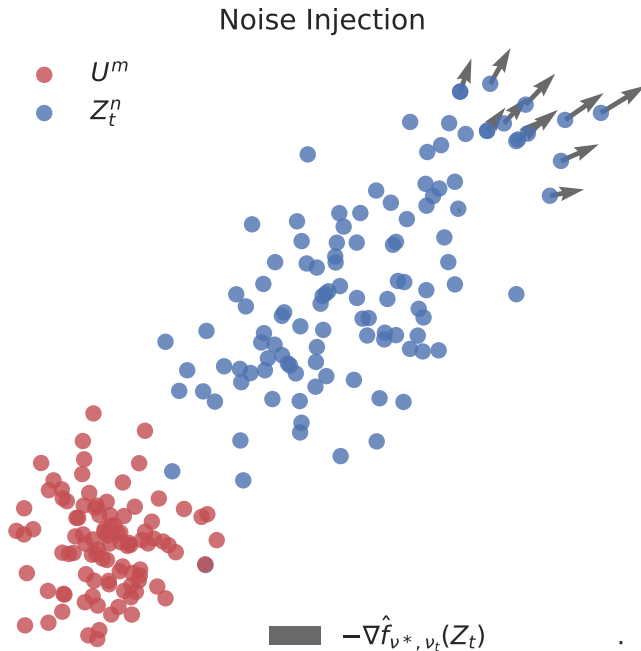
Noise Injection



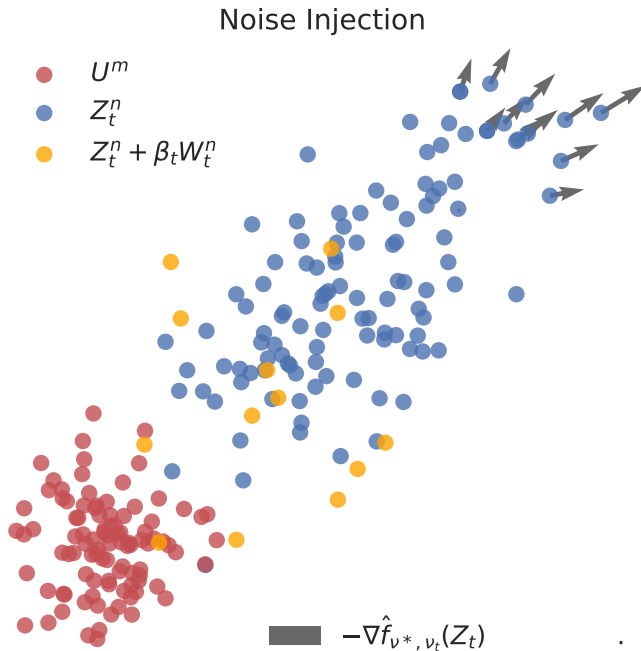
Noise Injection



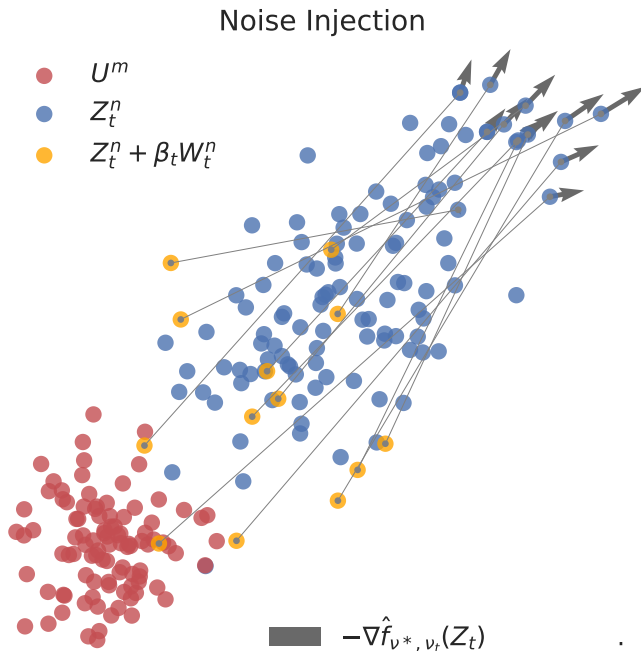
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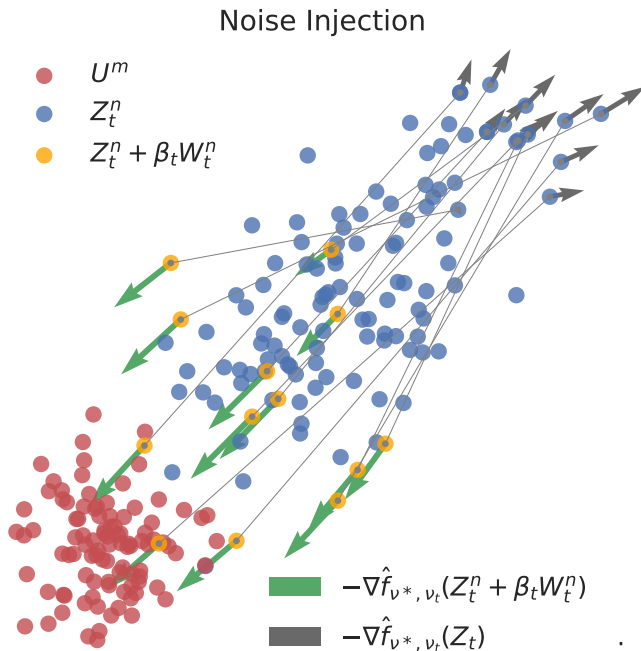
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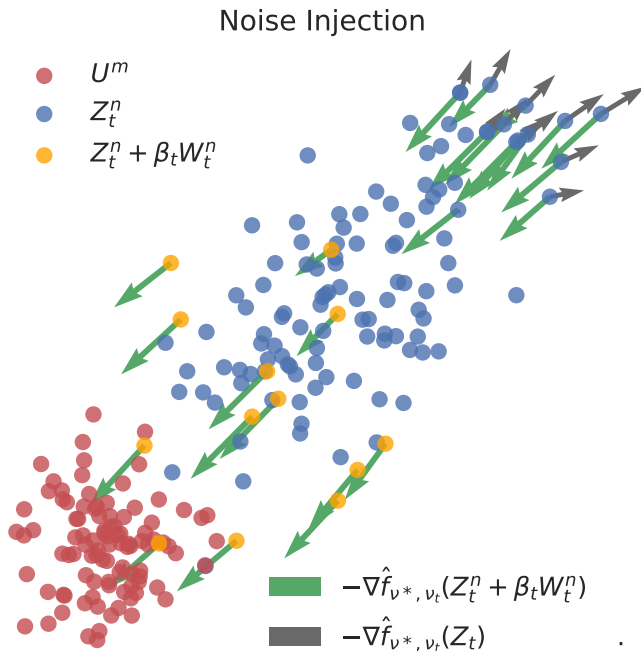
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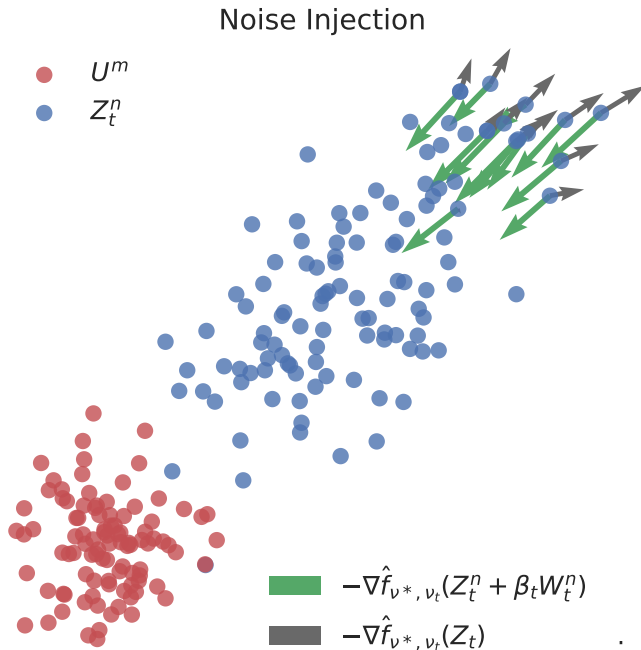
Noise Injection



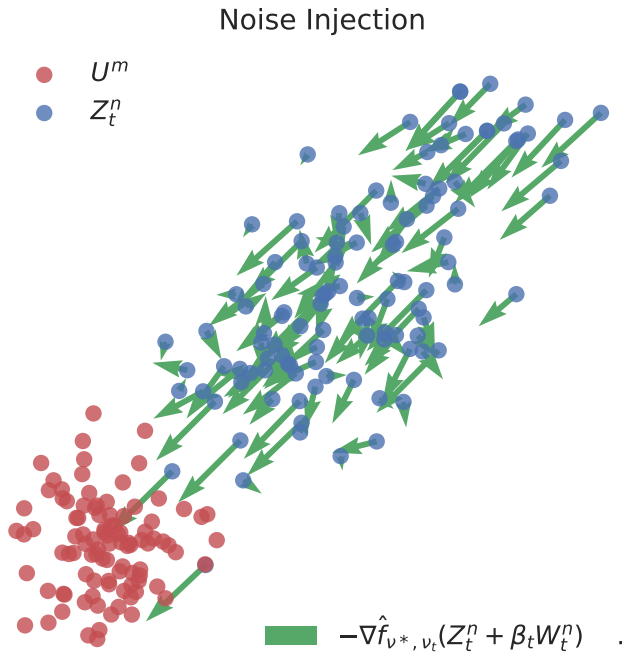
Noise Injection



Noise Injection



Noise Injection



Noise Injection: Experiments

Noise Injection

- ▶ The condition we exhibited for global convergence may not hold and $(\mathcal{L}(\nu_t))_t$ might be stuck at a local minima.

$$\begin{aligned}\frac{d\mathcal{L}(\nu_t)}{dt} &= - \int \|\nabla f_{\nu^*, \nu_t}(x)\|^2 d\nu_t(x) \text{ at equilibrium} \\ &\implies \int \|\nabla f_{\nu^*, \nu^\infty}(x)\|^2 d\nu^\infty(x) = 0\end{aligned}$$

If ν^∞ positive everywhere this implies $f_{\nu^*, \nu^\infty} = cte = 0$ as soon as $\mathcal{H}$ does not contain non-zero constant functions. But ν^∞ might be singular...

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

Noise Injection

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

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

⁴[Chaudhari et al., 2017, Hazan et al., 2016]

⁵[Duchi et al., 2012]

⁶[Mei et al., 2018]

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- ▶ Similar to *continuation methods*⁴ or *randomized smoothing*⁵, but extended to interacting particles.
- ▶ Different from adding noise outside ("diffusion")

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

which corresponds to an entropic regularization of the original loss ⁶.

⁴[Chaudhari et al., 2017, Hazan et al., 2016]

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Noise Injection: Theory (discrete time)

Tradeoff for β_t

- ▶ Large β_t : ν_{t+1} not a descent direction anymore:
 $MMD^2(\nu^*, \nu_{t+1}) > MMD^2(\nu^*, \nu_t)$

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Need β_t such that:

$$\beta_t^2 MMD^2(\nu_t) \leq C_k \mathbb{E}_{\substack{X_t \sim \nu_t \\ U_t \sim \mathcal{N}(0,1)}} [\|\nabla f_t(X_t + \beta_t U_t)\|^2] \quad (1)$$

and:

$$\sum_{t=1}^T \beta_t^2 \rightarrow \infty$$

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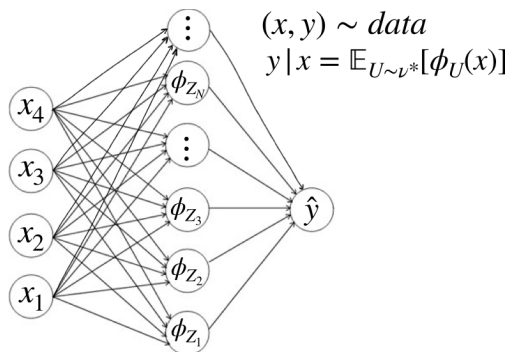
$$\sum_{t=1}^T \beta_t^2 \rightarrow \infty$$

Then

$$MMD^2(\nu^*, \nu_T) \leq MMD^2(\nu^*, \nu_0) e^{-C_k \gamma (1 - \gamma C'_k) \sum_{t=1}^T \beta_t^2}$$

Noise Injection: Student-Teacher network

Recall the supervised learning problem in the well specified case:



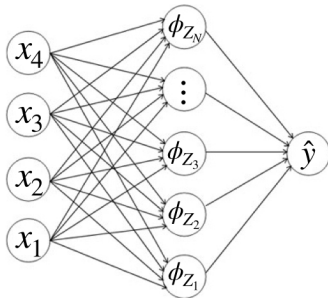
$$\min_{\nu \in \mathcal{P}} \mathbb{E}_{data} [\|y - \mathbb{E}_{Z \sim \nu}[\phi_Z(x)]\|^2]$$

Noise Injection: Student-Teacher network

Example of the Student-Teacher network:

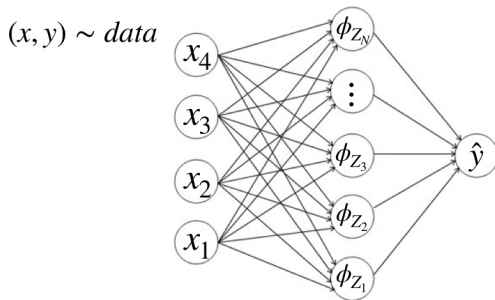
- ▶ the output of the Teacher network is deterministic and given by $y = \int \phi_Z(x) d\nu^*(Z)$ where $\nu^* = \frac{1}{M} \sum_{j=1}^M \delta_{U^m}$
- ▶ Student network parametrized by $\nu_0 = \frac{1}{N} \sum_{n=1}^N \delta_{Z_0^n}$ tries to learn the mapping $x \mapsto \int \phi_Z(x) d\nu^*(Z)$.

$(x, y) \sim \text{data}$



$$\min_{Z_1, \dots, Z_N} \mathbb{E}_{\text{data}} \left[\left\| \frac{1}{M} \sum_m \phi_{U^m}(x) - \frac{1}{N} \sum_{n=1}^N \phi_{Z_n}(x) \right\|^2 \right]$$

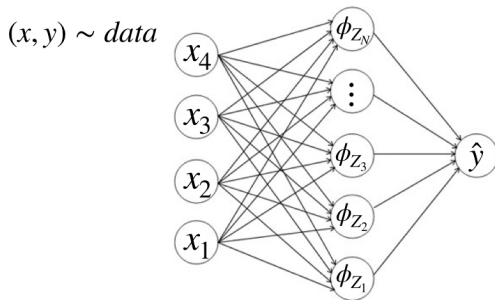
Noise Injection: Student-Teacher network



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

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

Noise Injection: Student-Teacher network



$$\min_{Z_1, \dots, Z_N} \mathbb{E}_{data} \left[\left\| \frac{1}{M} \sum_m \phi_{U^m}(x) - \frac{1}{N} \sum_{n=1}^N \phi_{Z^n}(x) \right\|^2 \right]$$
$$\hat{k}(Z, Z') = \frac{1}{B} \sum_{b=1}^B \phi_Z(x_b) \phi_{Z'}(x_b)$$

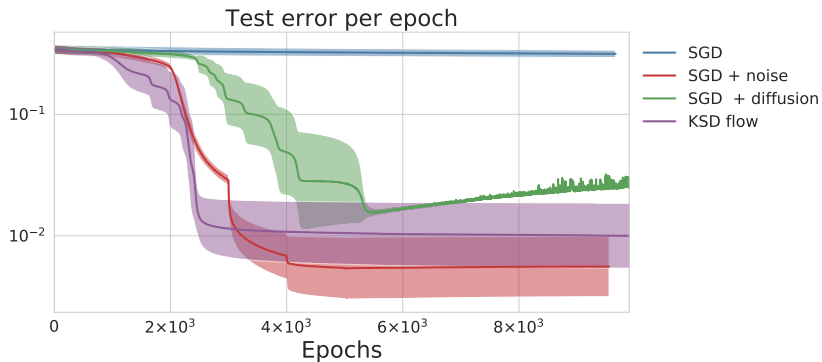
Noise Injection: Experiments

Methods:

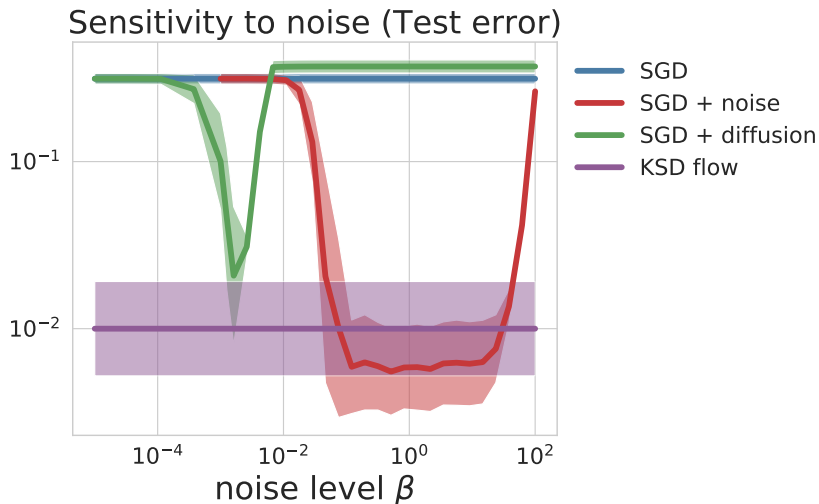
- ▶ SGD
- ▶ SGD + Noise injection
- ▶ SGD + diffusion
- ▶ KSD ⁷: SGD using the Negative Sobolev distance $\nu \mapsto \|\nu - \nu^*\|_{\dot{H}^{-1}(\nu)}$ as a loss function: also decreases the MMD.

⁷[Mroueh et al., 2019]

Noise Injection: Experiments



Noise Injection: Experiments



Conclusion

Contributions:

- ▶ Provided a convergence criterion for the Wasserstein gradient flow of the MMD.
- ▶ Studying the gradient flow and its time/space discretizations helps understand the convergence when training big neural networks
- ▶ Proposed a perturbation of the dynamics with a noise injection and showed its effectiveness on simple examples.

Openings:

- ▶ A criterion for convergence that is independent from the whole optimization trajectory.
- ▶ Stronger guarantees for the convergence for the noise injection algorithm.

Thank you!



Ambrosio, L., Gigli, N., and Savaré, G. (2004).

Gradient flows with metric and differentiable structures, and applications to the Wasserstein space.

Atti della Accademia Nazionale dei Lincei. Classe di Scienze Fisiche, Matematiche e Naturali. Rendiconti Lincei. Matematica e Applicazioni, 15(3-4):327–343.



Carrillo, J. A., McCann, R. J., and Villani, C. (2006).

Contractions in the 2-wasserstein length space and thermalization of granular media.

Archive for Rational Mechanics and Analysis, 179(2):217–263.



Chaudhari, P., Osher, S., Soatto, S., and Carlier, G. (2017).

Deep Relaxation: partial differential equations for optimizing deep neural networks.

arXiv:1704.04932 [cs, math].



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

On the global convergence of gradient descent for

The sample-based approximate scheme

How can we simulate

$$X_{n+1} = X_n - \gamma \nabla f_{\mu, \nu_n}(X_n + \beta_n U_n), \quad n \geq 0?$$

It depends on:

- ▶ the current distribution $\nu_n \implies$ approximate it by the empirical distribution of a system of N interacting particles
- ▶ the target distribution $\mu \implies$ replace it by the empirical distribution of the M samples that we have access to ($\hat{\mu}$)

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$\implies$ **create a system of interacting particles**

$$\hat{\nu}_{n+1} \left\{ \begin{array}{l} X_{n+1}^1 = X_n^1 - \gamma \nabla f_{\hat{\mu}, \hat{\nu}_n}(X_n^1 + \beta_n U_n^1) \\ \dots \\ X_{n+1}^N = X_n^N - \gamma \nabla f_{\hat{\mu}, \hat{\nu}_n}(X_n^N + \beta_n U_n^N) \end{array} \right.$$

Theoretical guarantees

(Propagation of chaos type of result)

Theorem

Let $n \geq 0$ and $T > 0$. Let ν_n and $\hat{\nu}_n$ defined by the (theoretical) Euler-scheme and the practical algorithm. Suppose $\|\nabla k\|_{Lip} = L$ and that $\beta_n < B$ for all n , for some $B > 0$. Then for any $\frac{T}{\gamma} \geq n$:

$$\mathbb{E}[W_2(\hat{\nu}_n, \nu_n)] \leq \frac{C_1(\nu_0, B, T, L)}{\sqrt{N}} + \frac{C_2(\mu, T, L)}{\sqrt{M}}$$

where N is the number of interacting particles and M is the number of samples from the target distribution.