Maximum Mean Discrepancy Gradient Flow

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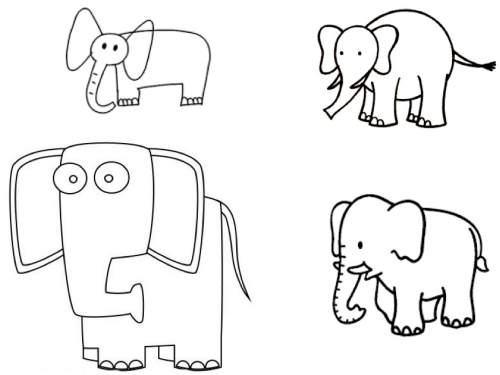
General Problem

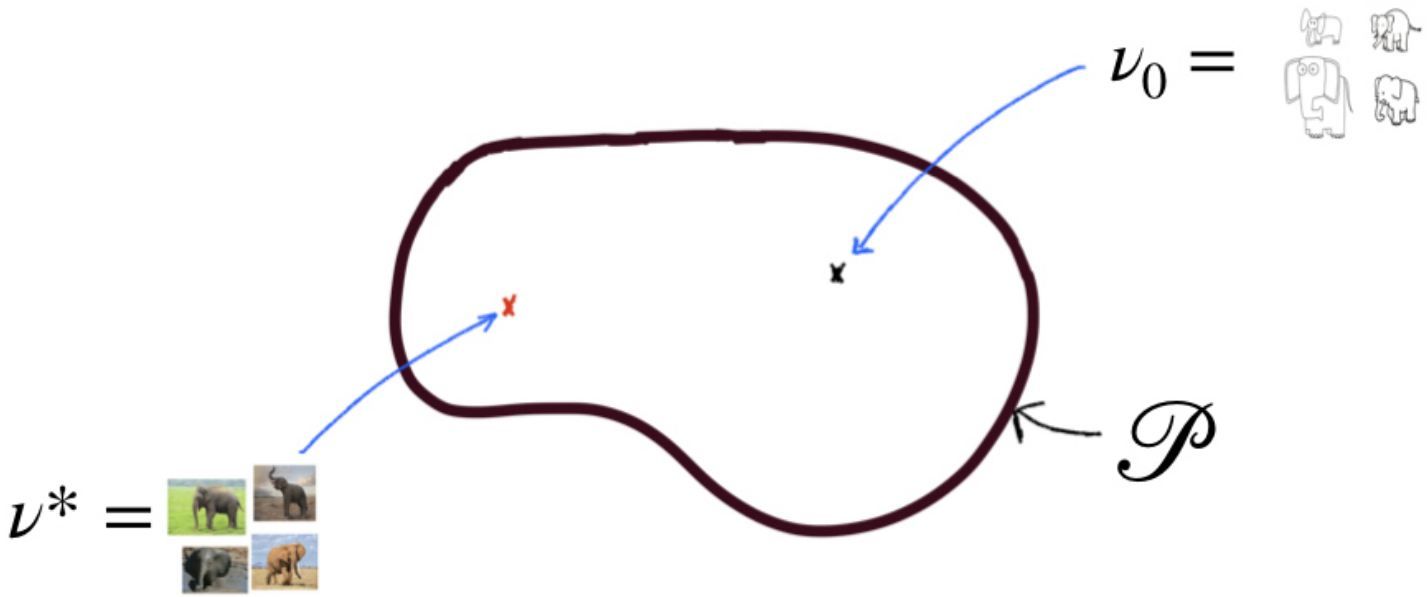
ν^*



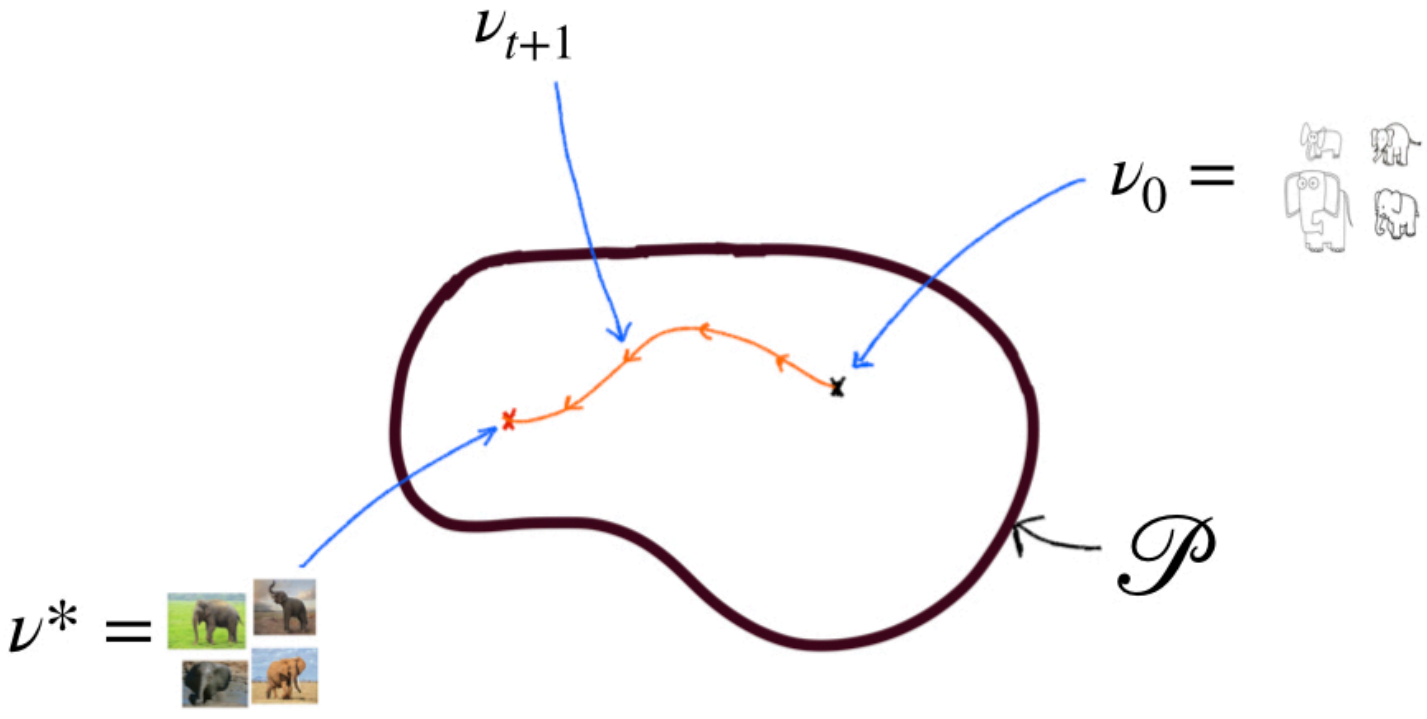
ν_0

[Goodfellow et al., 2014]

General Problem

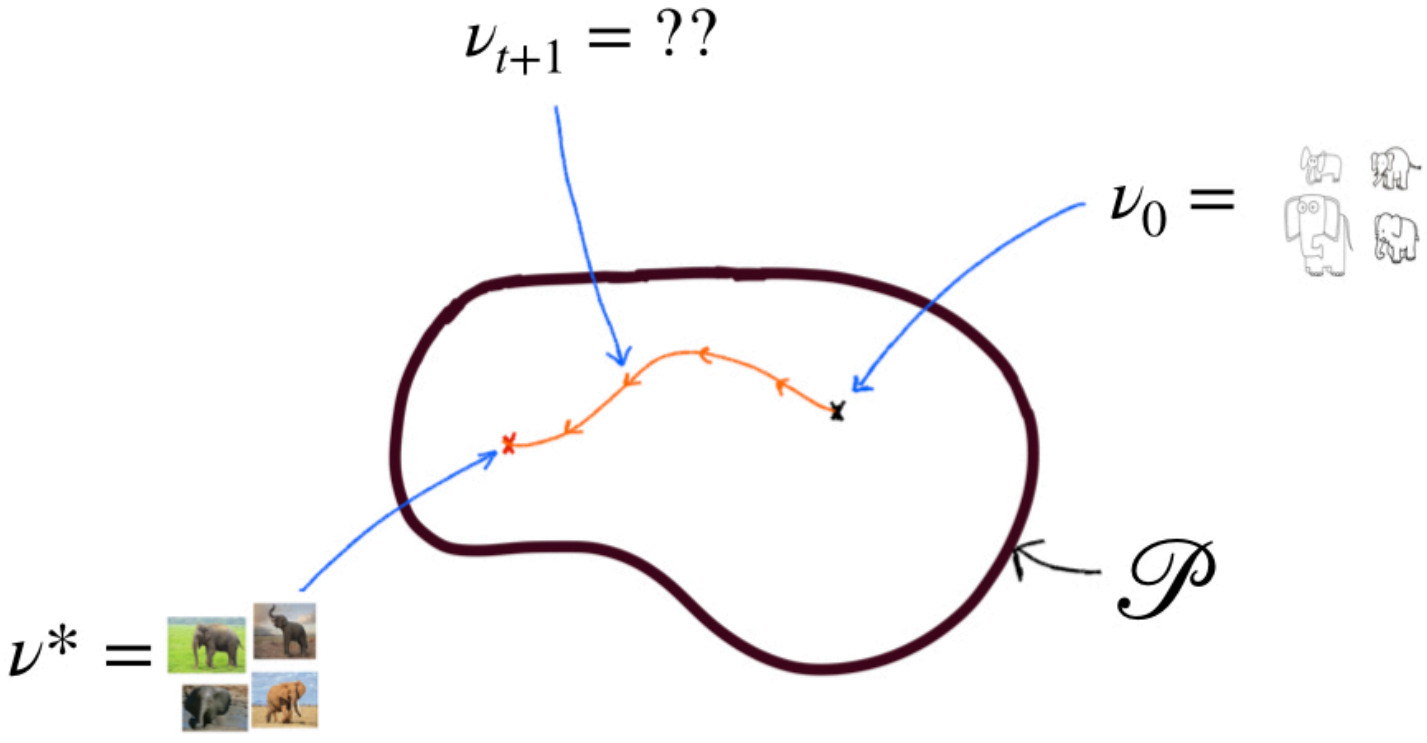


General Problem



$$\min_{\nu \in \mathscr{P}} d(\nu^*, \nu)$$

General Problem

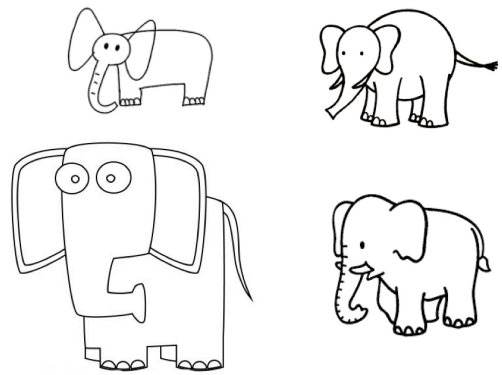


$$\min_{\nu \in \mathscr{P}} MMD(\nu^*, \nu)$$

Motivation: Implicit generative models [Goodfellow et al., 2014]

Given samples from a distribution ν^* over $\mathscr{X}$, want a model that can produce new samples from $\nu_\psi \approx \nu^*$

ν^*



ν_ψ

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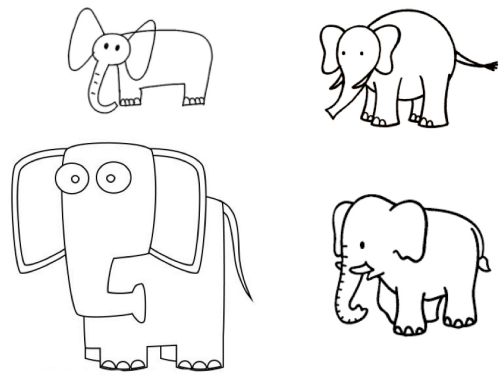
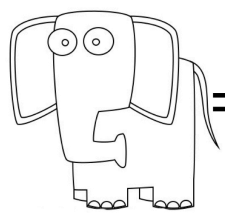


ν_ψ



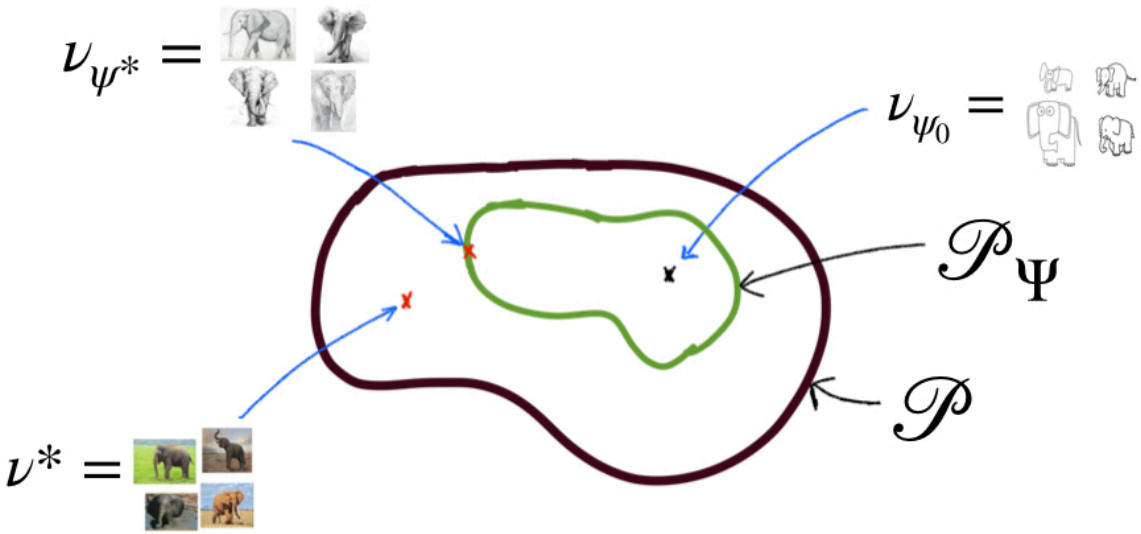
$= G_\psi(z)$

z sampled from a fixed known distribution.

[Goodfellow et al., 2014]

Implicit generative models

Learn best ν_{ψ^*} by minimizing a distance/divergence d between ν_ψ and ν^*: Constrained optimization



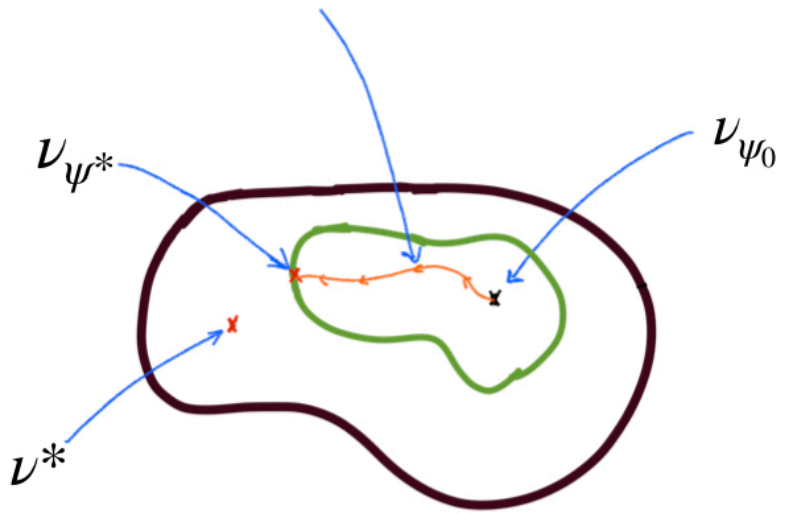
$$\min_{\nu_\psi \in \mathscr{P}_\Psi} d(\nu^*, \nu_\psi)$$

[Goodfellow et al., 2014, Nowozin et al., 2016, Arjovsky et al., 2017]

Implicit generative models

Learn best ν_{ψ^*} by minimizing a distance/divergence d between ν_ψ and ν^* : Constrained optimization

$$\nu_{\psi_{t+1}} : \psi_{t+1} = \psi_t - \gamma_t \nabla_\psi \widehat{d(\nu^*, \nu_{\psi_t})}$$



$$\min_{\nu_\psi \in \mathscr{P}_\Psi} d(\nu^*, \nu_\psi)$$

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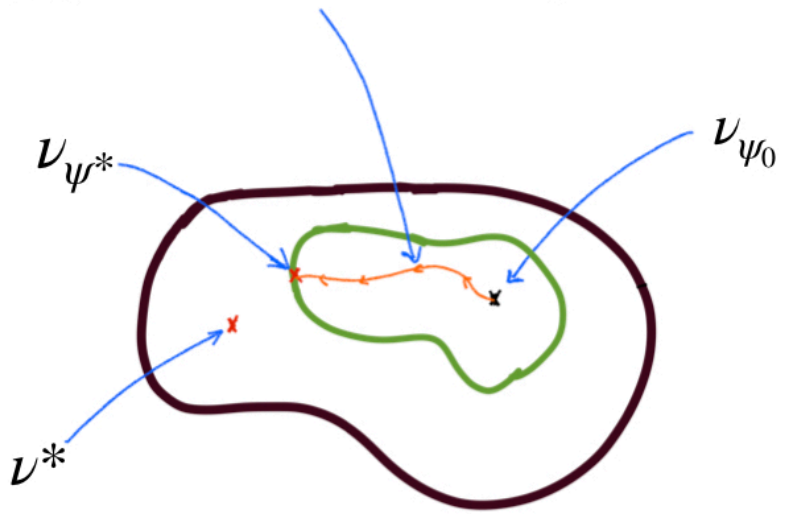
Implicit generative models

Learn best ν_{ψ^*} by minimizing a distance/divergence d between ν_ψ and ν^* : Constrained optimization

$$\nu_{\psi_{t+1}} : \psi_{t+1} = \psi_t - \gamma_t \nabla_\psi \widehat{MMD}^2(\nu^*, \nu_{\psi_t})$$

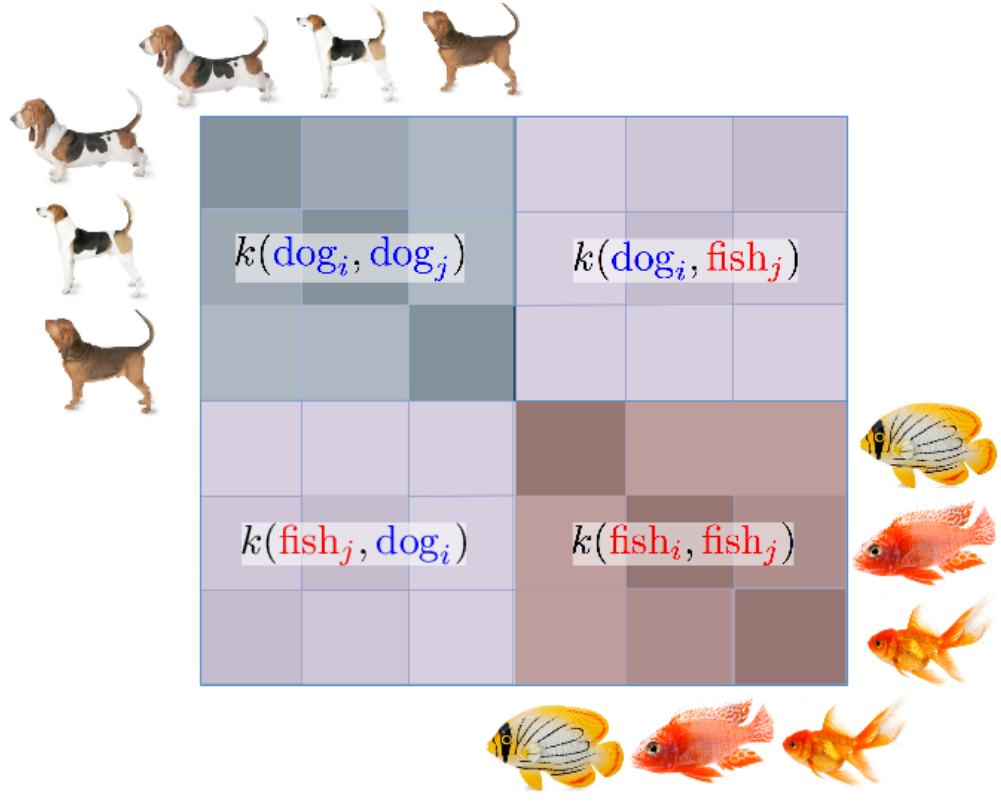


$$\min_{\nu_\psi \in \mathcal{P}_\Psi} MMD(\nu^*, \nu_\psi)$$

[Goodfellow et al., 2014, Nowozin et al., 2016, Arjovsky et al., 2017, Li et al., 2015, Bińkowski et al., 2018]

Choice of d: The Maximum Mean Discrepancy

First choose a kernel k, then compute a similarity matrix:



$$\widehat{MMD}^2 = \frac{1}{n(n-1)} \sum_{i \neq j} k(dog_i, dog_j) + \frac{1}{n(n-1)} \sum_{i \neq j} k(fish_i, fish_j) - \frac{2}{n^2} \sum_{i,j} k(dog_i, fish_j)$$

[Gretton et al., 2012]

Choice of d: The Maximum Mean Discrepancy

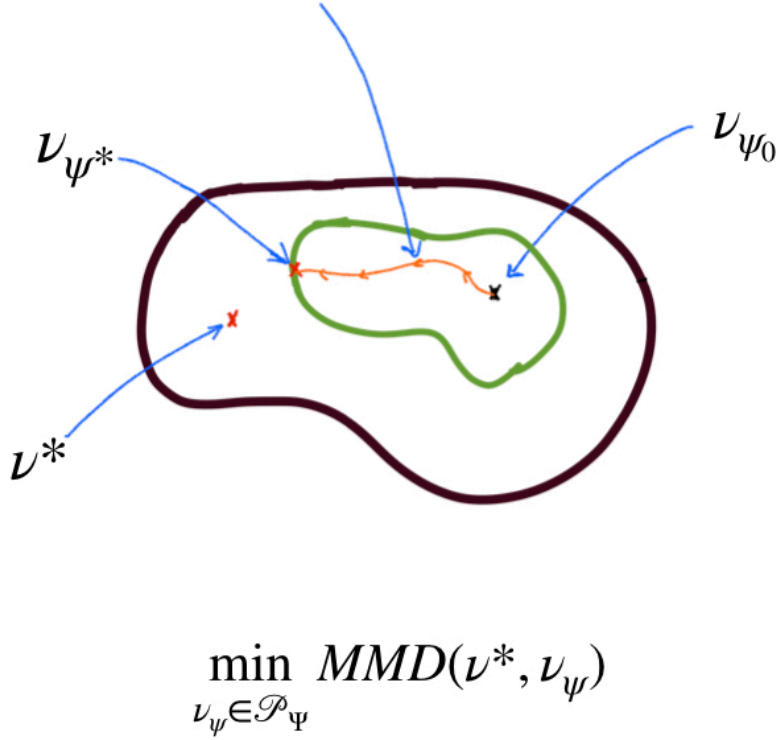
- Easy to estimate using samples
- Nice statistical guarantees [Gretton et al., 2012]
- Works well in practice[1] [Li et al., 2015, Bińkowski et al., 2018, Arbel et al., 2018]

[1] When the kernel is parameterized by a deep neural network

Implicit generative models

Guarantees that $\nu_{\psi_t} \to \nu_{\psi^*}$?

$$\nu_{\psi_{t+1}} : \psi_{t+1} = \psi_t - \gamma_t \nabla_\psi \widehat{MMD}^2(\nu^*, \nu_{\psi_t})$$



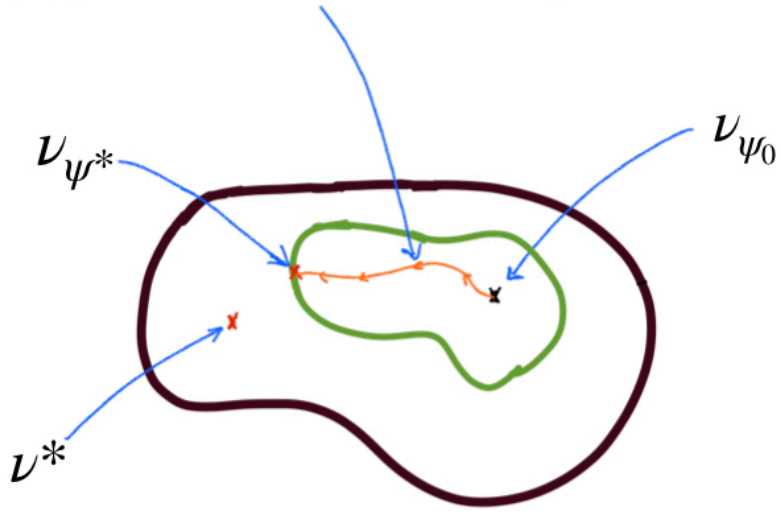
$$\min_{\nu_\psi \in \mathcal{P}_\Psi} MMD(\nu^*, \nu_\psi)$$

[Goodfellow et al., 2014, Nowozin et al., 2016, Arjovsky et al., 2017, Li et al., 2015, Bińkowski et al., 2018, Arbel et al., 2018]

Implicit generative models

Hard to say anything if $\mathscr{P}_\Psi$ is not convex.

$$\nu_{\psi_{t+1}} : \psi_{t+1} = \psi_t - \gamma_t \nabla_\psi \widehat{MMD}^2(\nu^*, \nu_{\psi_t})$$

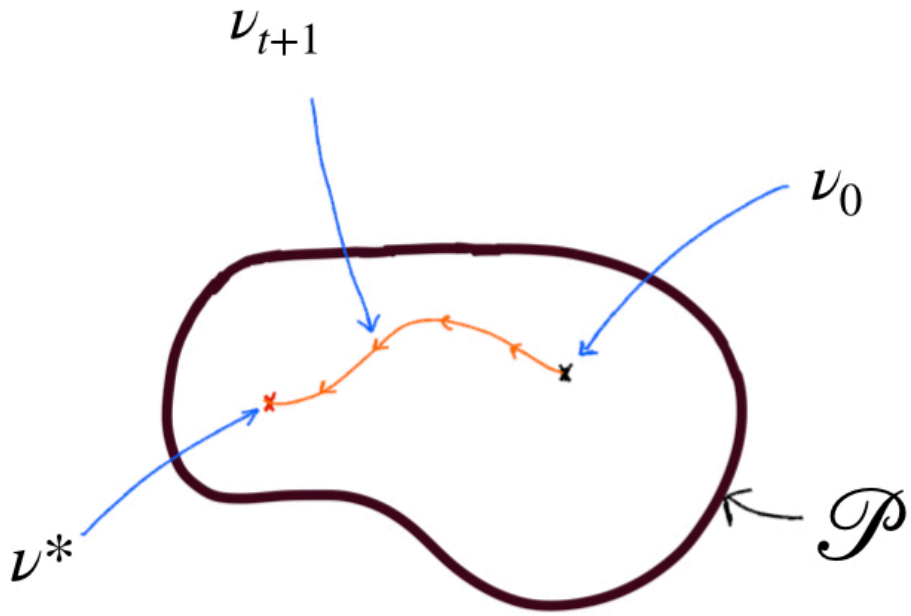


$$\min_{\nu_\psi \in \mathscr{P}_\Psi} MMD(\nu^*, \nu_\psi)$$

[Goodfellow et al., 2014, Nowozin et al., 2016, Arjovsky et al., 2017, Li et al., 2015, Bińkowski et al., 2018, Arbel et al., 2018]

Implicit generative model

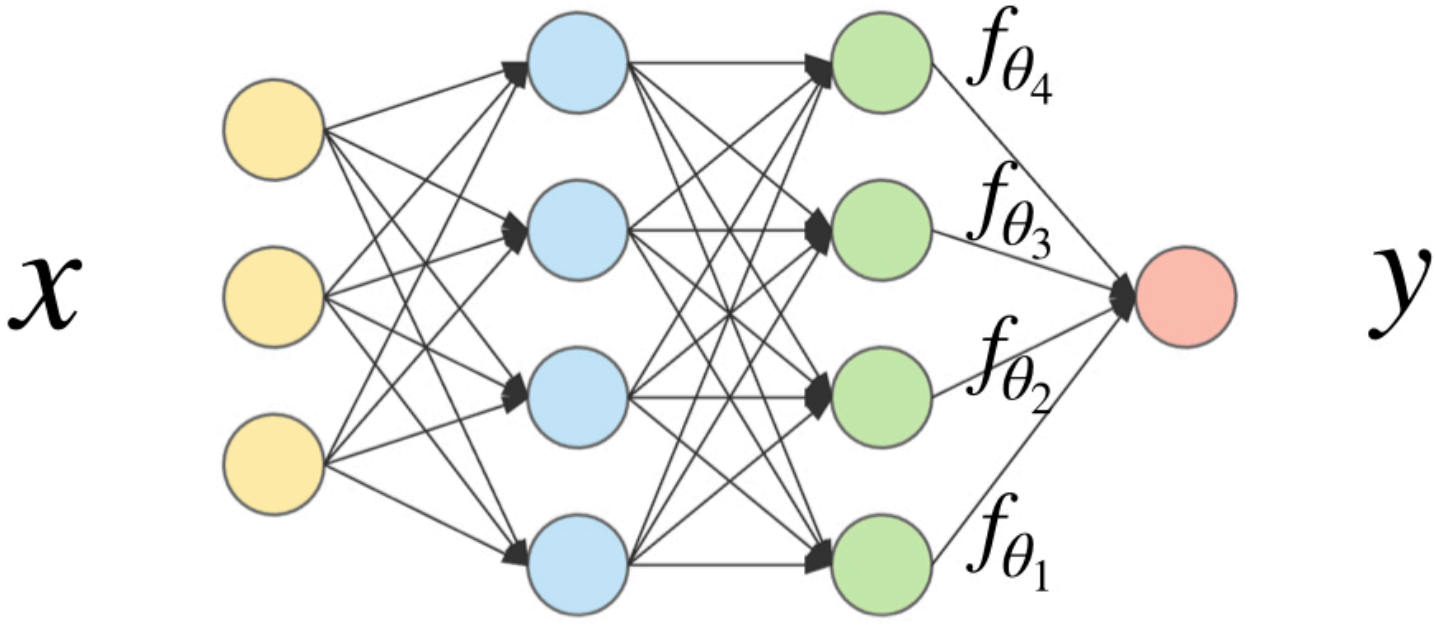
Unconstrained optimization: Replace $\mathscr{P}_\Psi$ by $\mathscr{P}$



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

Motivation: Neural Networks Optimization

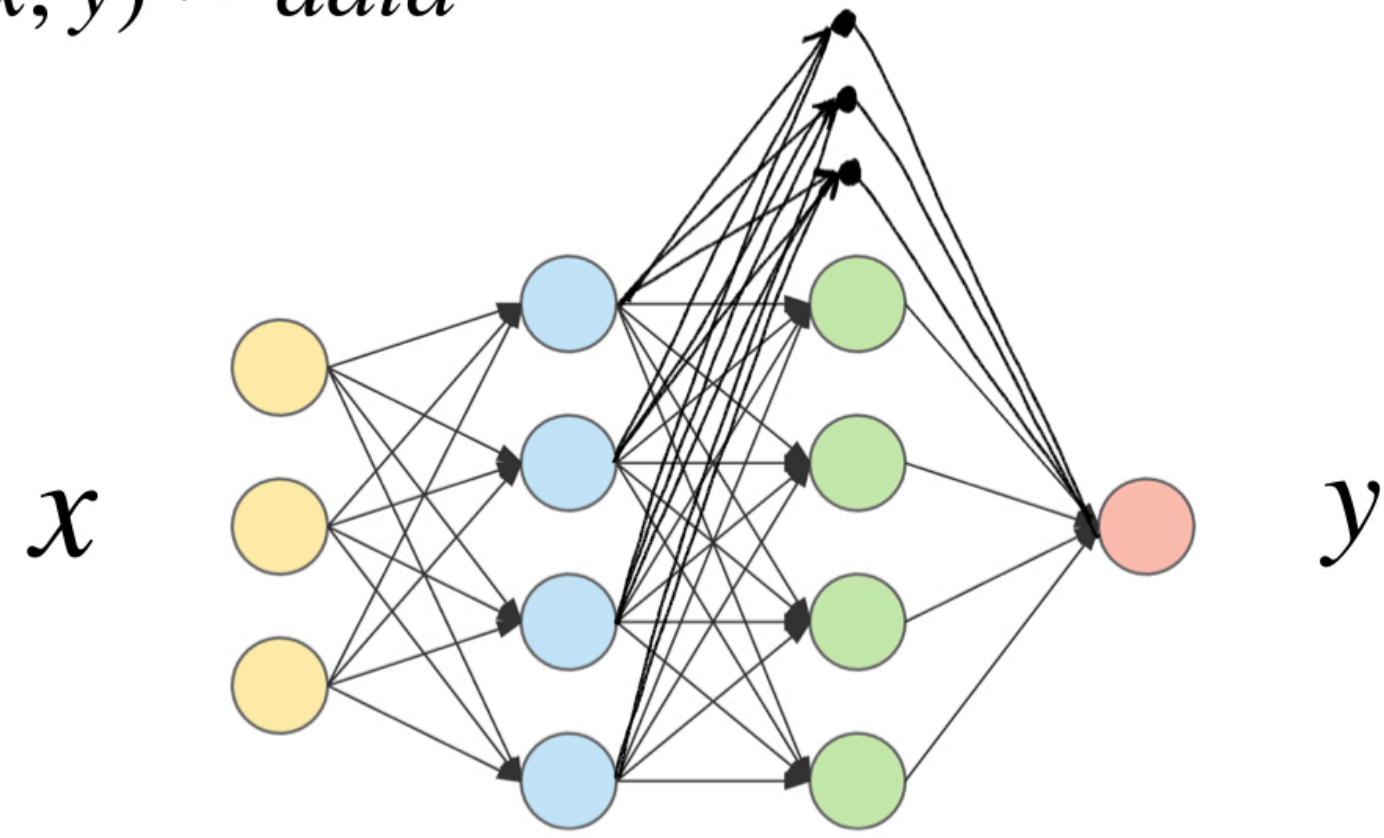
$$(x, y) \sim data$$



$$\min_{\theta_1,\ldots,\theta_N} \mathbb{E}_{data}[\|y - \frac{1}{N}\sum_{i=1}^{N} f_{\theta_i}(x)\|^2]$$

Motivation: Neural Networks Optimization

$$(x, y) \sim data$$



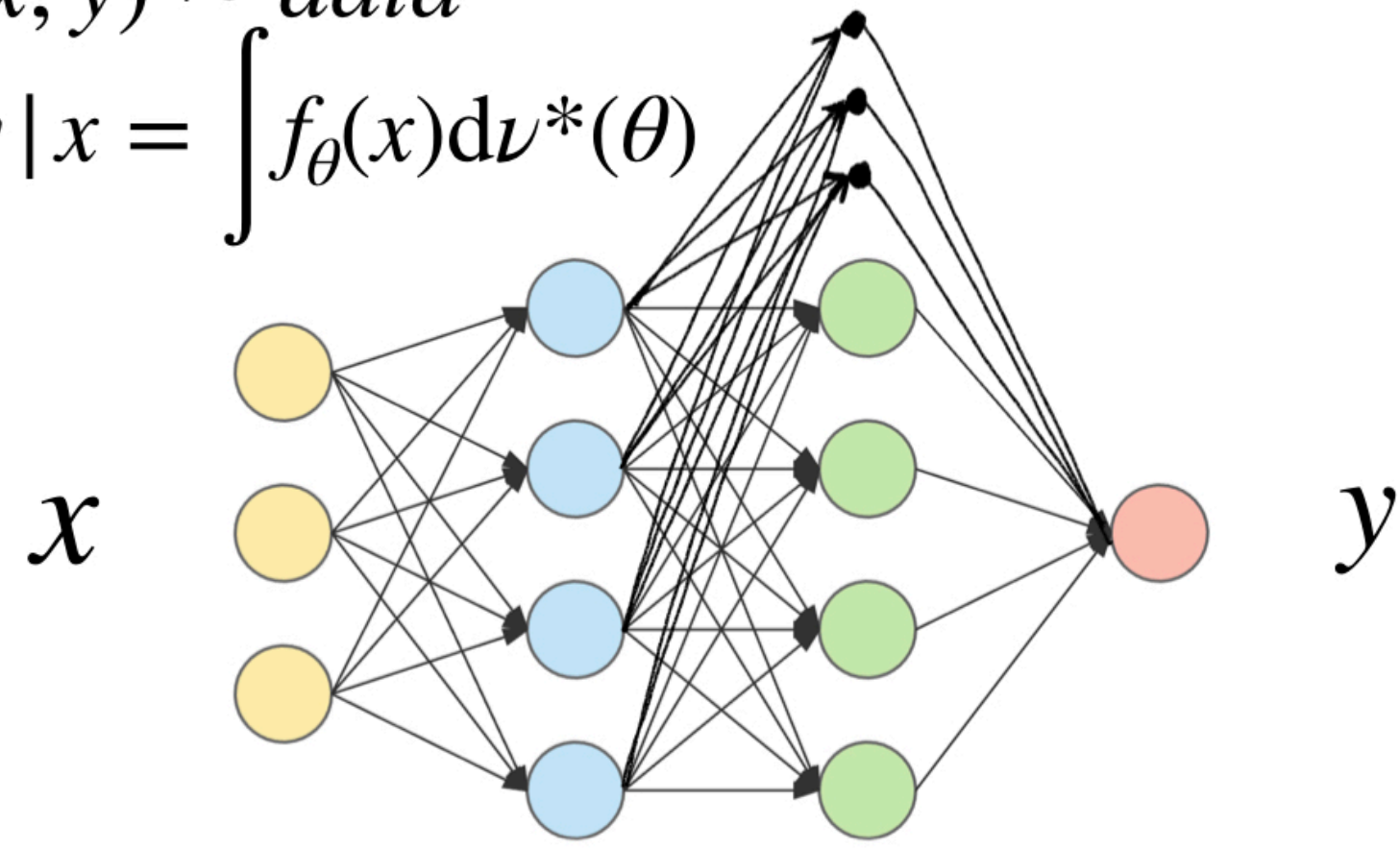
$$\min_{\nu \in \mathcal{P}} \mathbb{E}_{data}[\|y - \int f_\theta(x) \mathrm{d}\nu(\theta)\|^2]$$

[Rotskoff and Vanden-Eijnden, 2018, Chizat and Bach, 2018, Mei et al., 2018]

Motivation: Neural Networks Optimization

$$(x, y) \sim data$$

$$y \,|\, x = \int f_\theta(x) \mathrm{d}\nu^*(\theta)$$



$$\min_{\nu \in \mathcal{P}} \mathbb{E}_{data}[\|y - \int f_\theta(x) \mathrm{d}\nu(\theta)\|^2]$$

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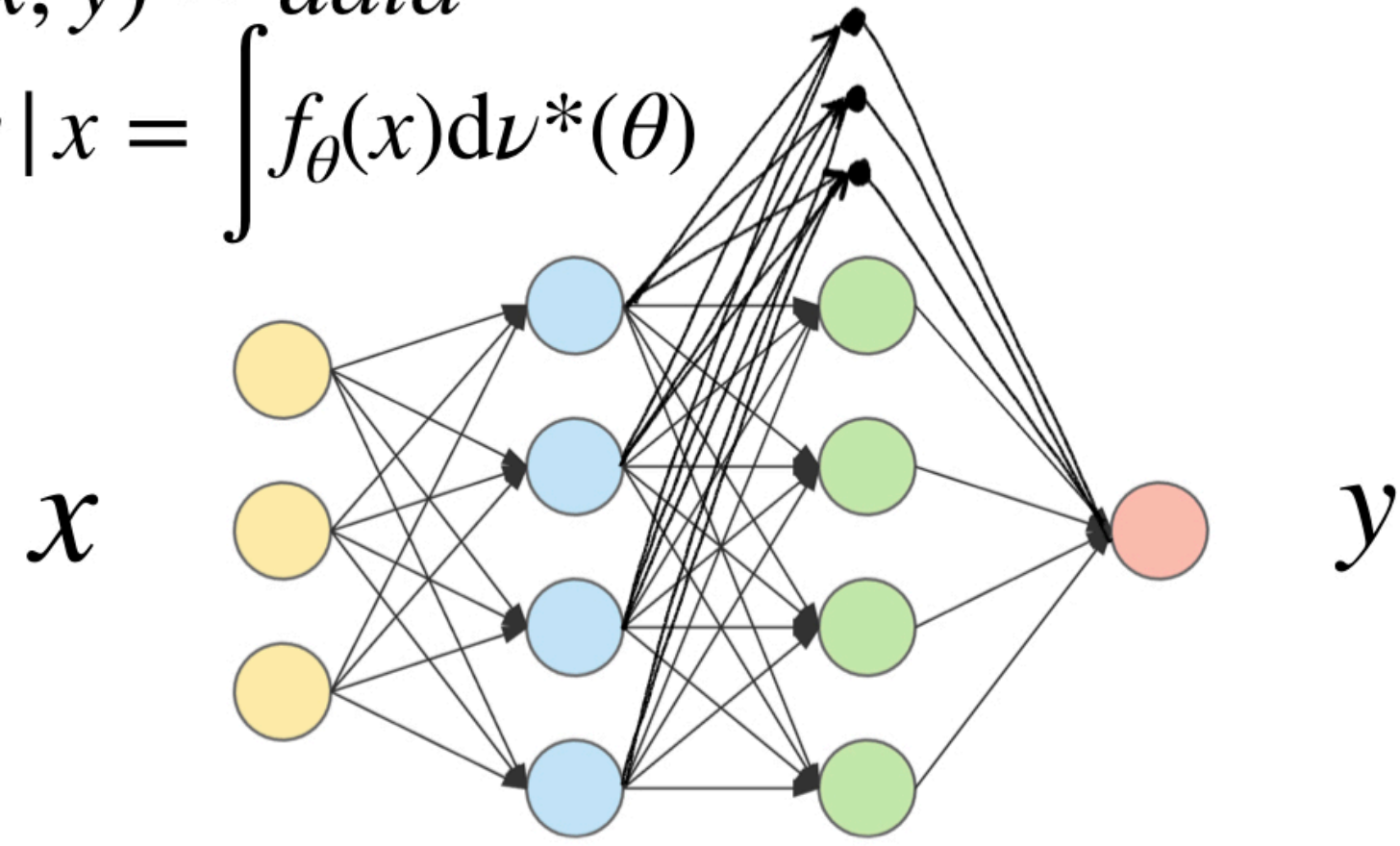

$$\min_{\nu \in \mathscr{P}} \mathbb{E}_{data}[\| \int f_\theta(x) \mathrm{d}\nu^*(\theta) - \int f_\theta(x) \mathrm{d}\nu(\theta) \|^2]$$

Motivation: Neural Networks Optimization

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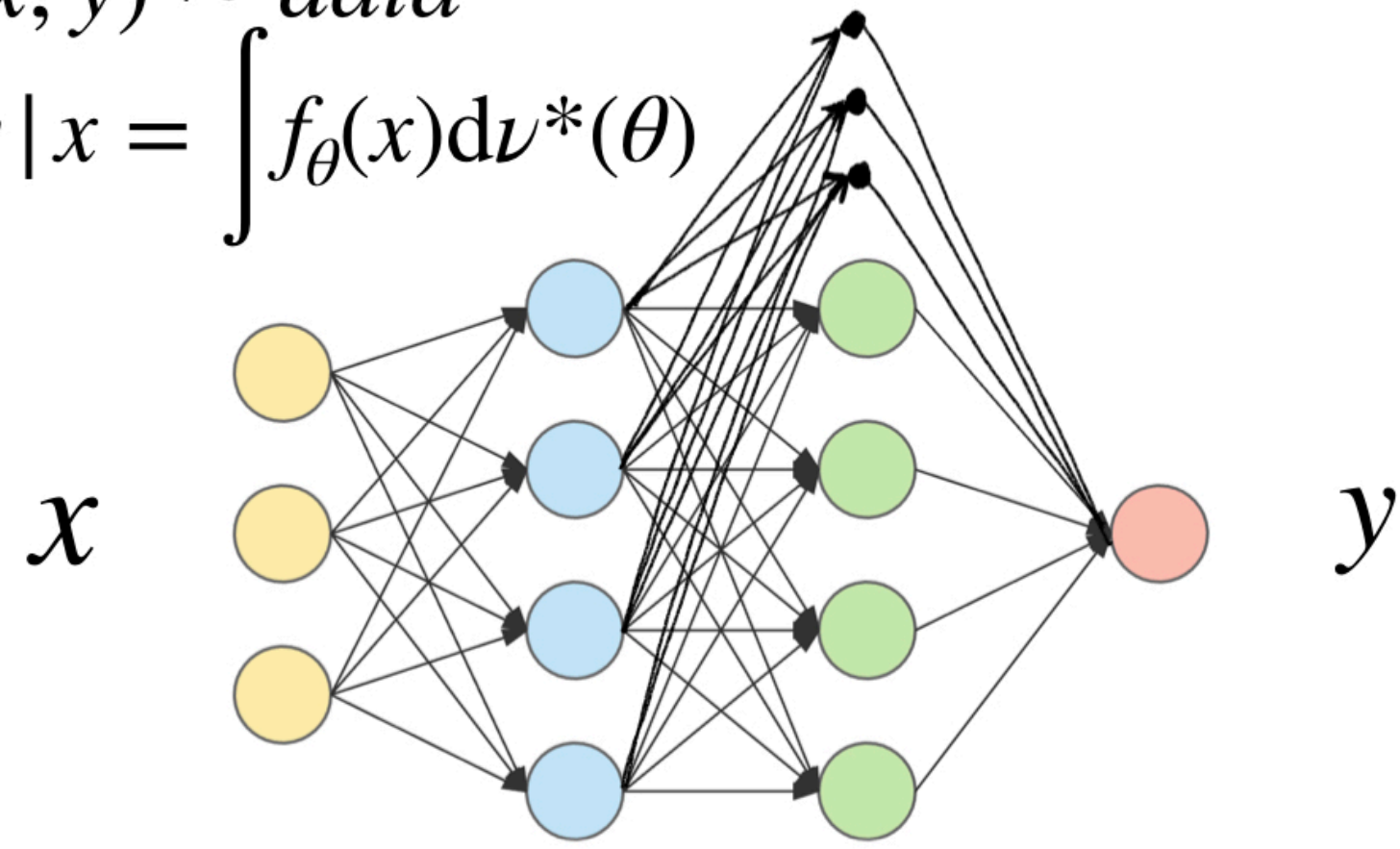
$$y \,|\, x = \int f_\theta(x) \mathrm{d}\nu^*(\theta)$$

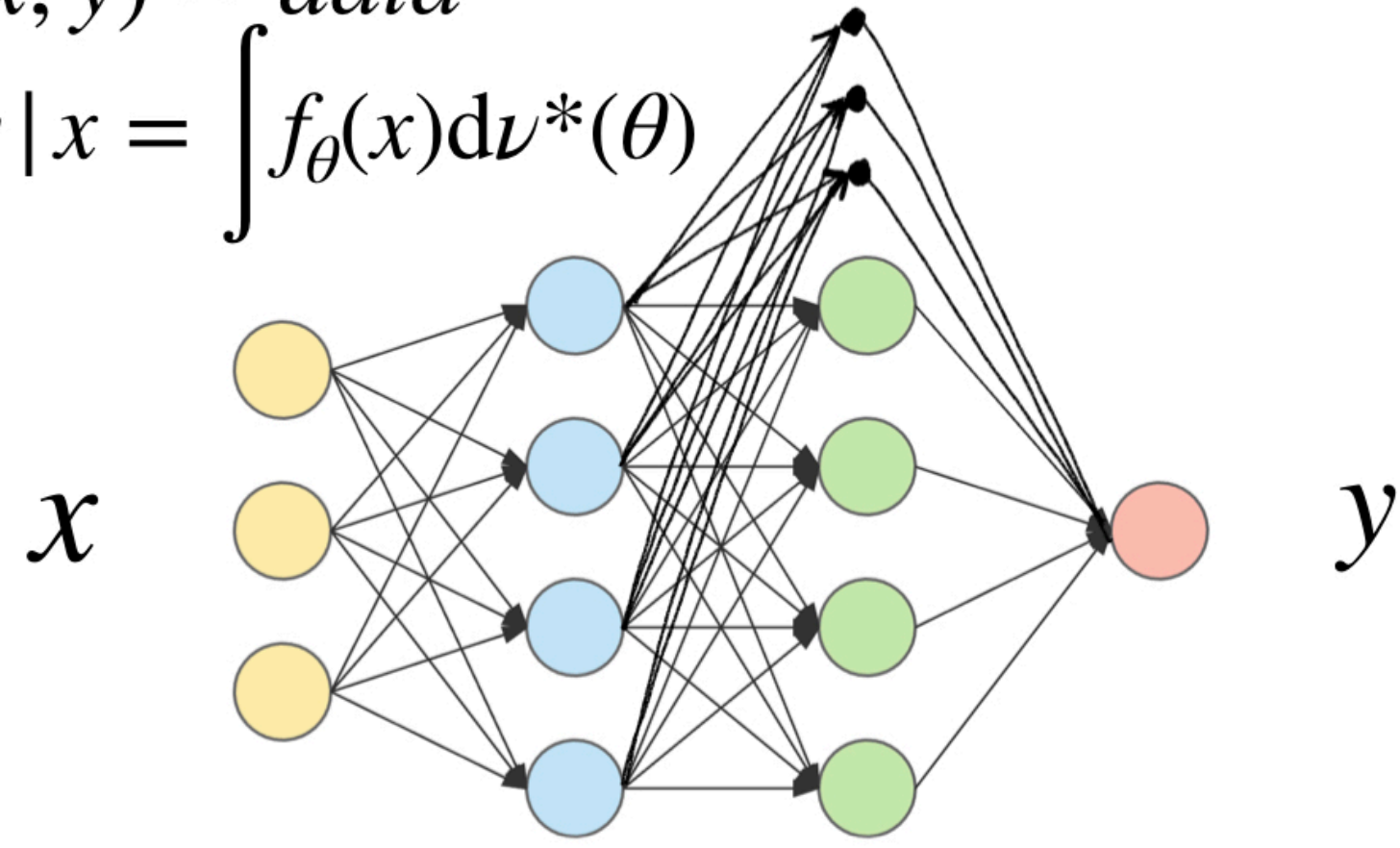


$$\min_{\nu \in \mathscr{P}} MMD^2(\nu^*, \nu)$$

Motivation: Neural Networks Optimization

$$(x, y) \sim data$$

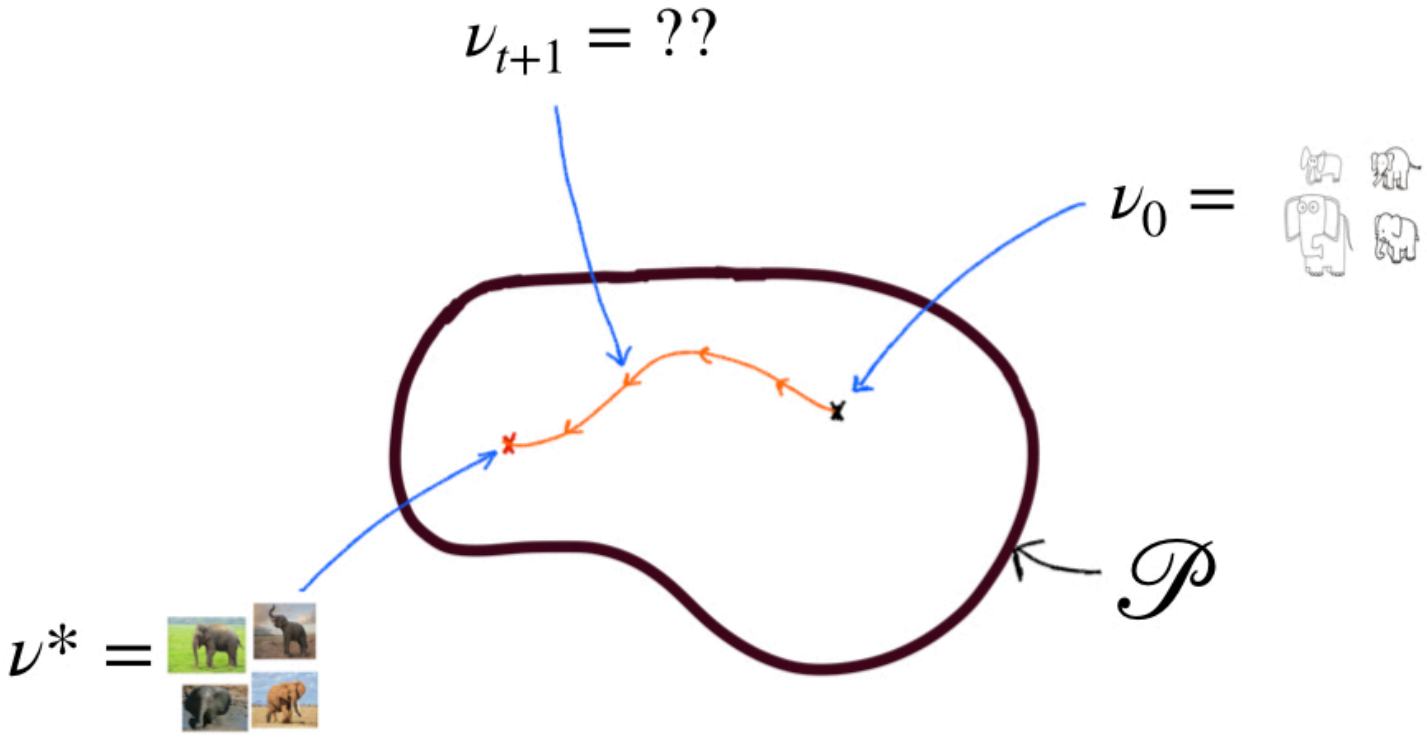
$$y \mid x = \int f_\theta(x) \mathrm{d}\nu^*(\theta)$$



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

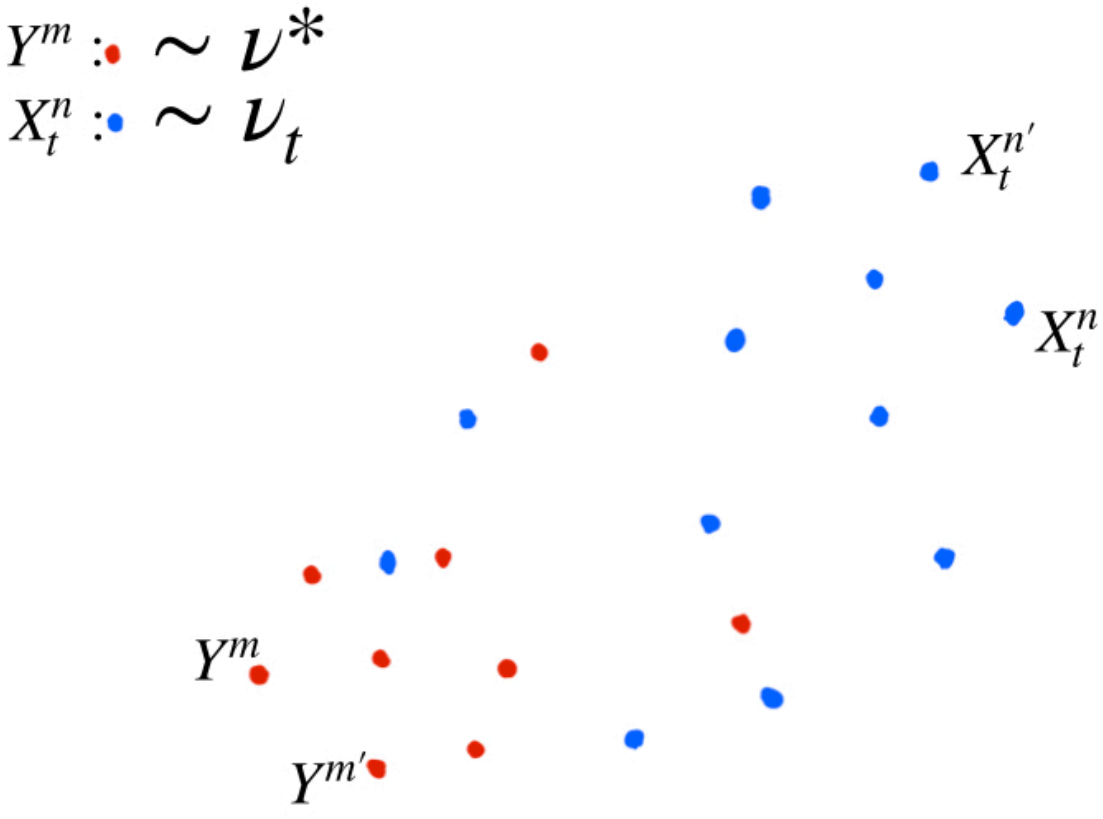
$$k(\theta, \theta') = \mathbb{E}_{data}[f_\theta(x) f_{\theta'}(x)]$$

General problem



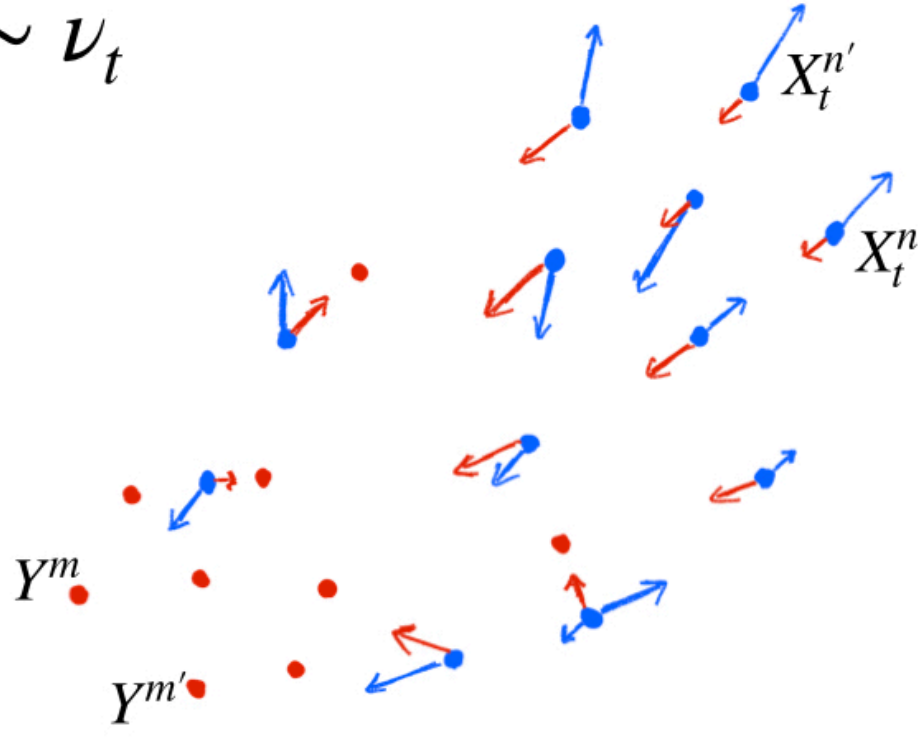
$$\min_{\nu \in \mathscr{P}} MMD(\nu^*, \nu)$$

A physical interpretation of the MMD



A physical interpretation of the MMD

$$Y^m : \sim \nu^*$$
$$X_t^n : \sim \nu_t$$



$$M\hat{M}D^2(\nu^*, \nu_t) = \underbrace{-\frac{2}{MN}\sum_{m,n} k(Y^m, X_t^n)}_{\text{confinement potential}} + \underbrace{\frac{1}{N(N-1)}\sum_{n,n'} k(X_t^n, X_t^{n'})}_{\text{interaction potential}} + \underbrace{\frac{1}{M(M-1)}\sum_{m,m'} k(Y^m, Y}_{\text{constant term}}$$

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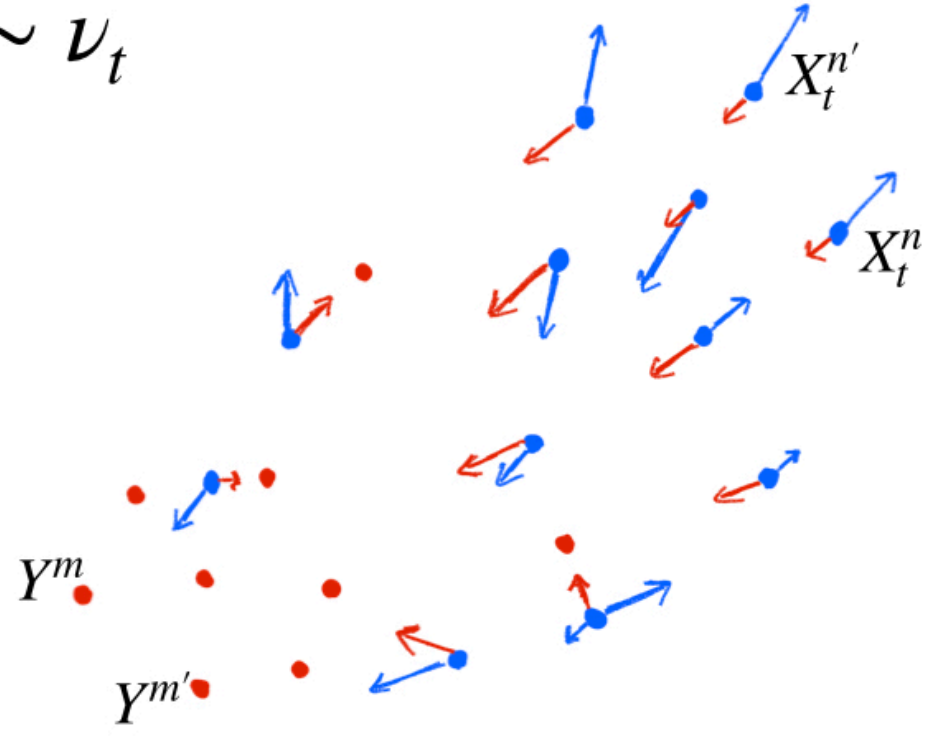
$X_t^n : \sim \nu_t$



$$\nearrow : \underbrace{\frac{1}{M}\sum_m \nabla_1 k(X_t^n, Y^m)}_{\text{confinement force}} \qquad \nearrow : \underbrace{-\frac{1}{N}\sum_{n'} \nabla_1 k(X_t^n, X_t^{n'})}_{\text{interaction force}}$$

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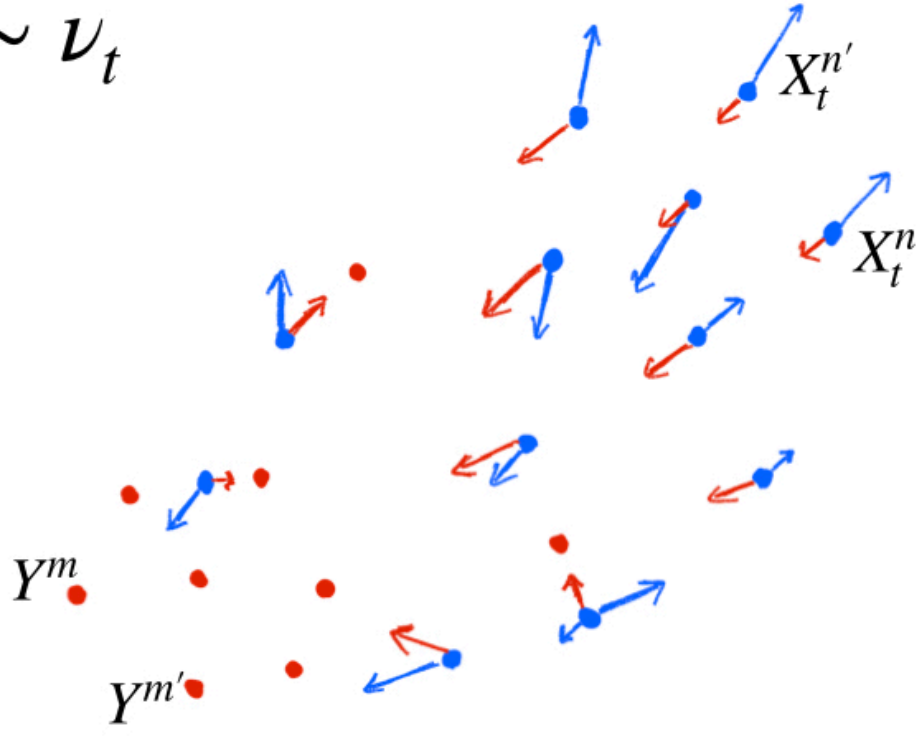
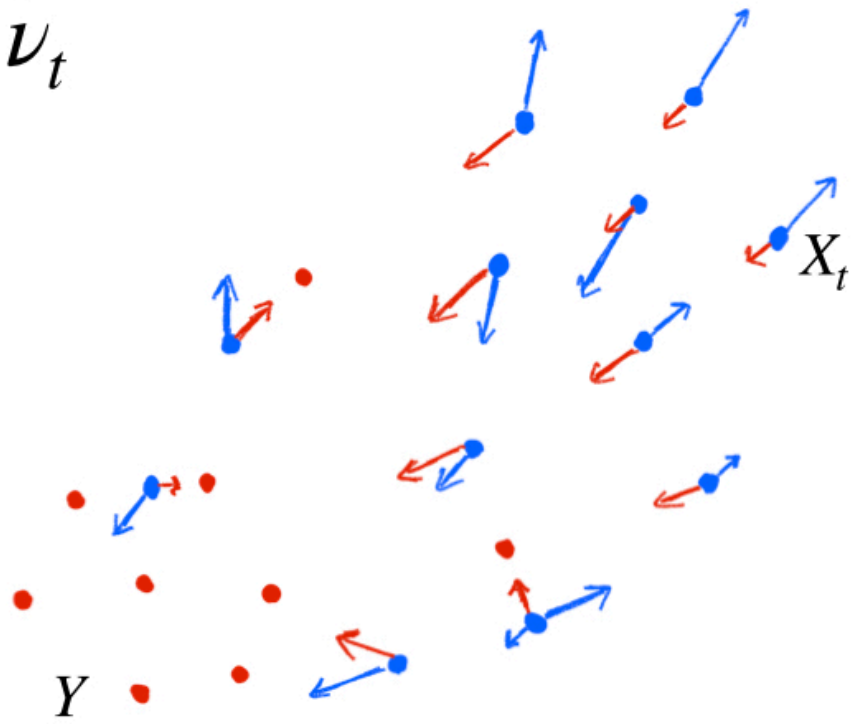


$$X_{t+1}^n = X_t^n + \gamma_t\left(\frac{1}{M}\sum_m \nabla_1 k(X_t^n, Y^m) - \frac{1}{N}\sum_{n'} \nabla_1 k(X_t^n, X_t^{n'})\right)$$

A physical interpretation of the MMD

$Y : \bullet \sim \nu^*$

$X_t : \bullet \sim \nu_t$



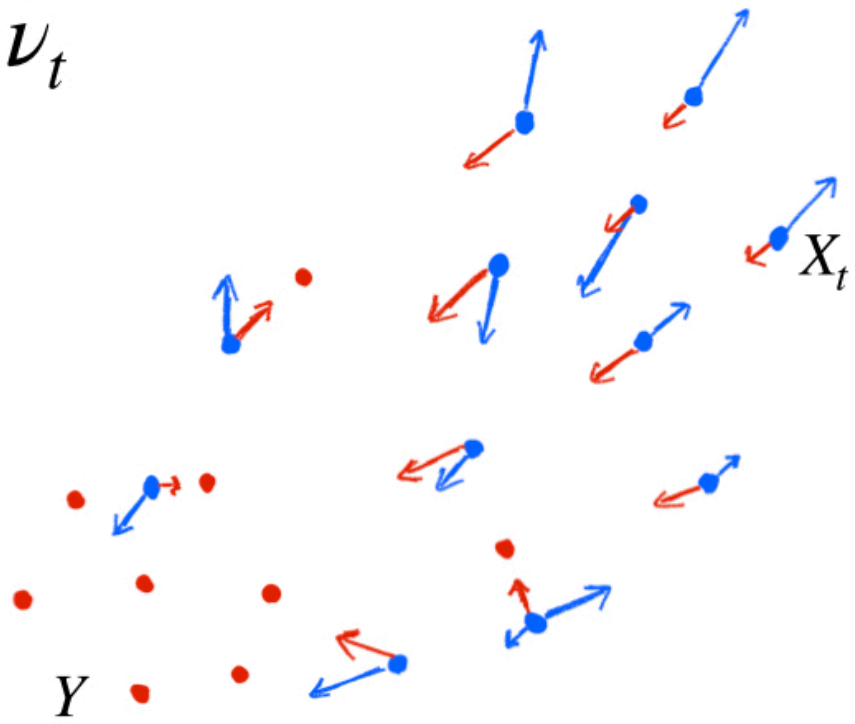
$$X_{t+1} = X_t + \gamma_t \underbrace{\left(\int \nabla_1 k(X_t, y) \mathrm{d}\nu^*(y) - \int \nabla_1 k(X_t, x_t') \mathrm{d}\nu_t(x_t') \right)}_{-\nabla f_t(X_t),}$$

f_t: **potential function**

A physical interpretation of the MMD

$Y : \bullet \sim \nu^*$

$X_t : \bullet \sim \nu_t$



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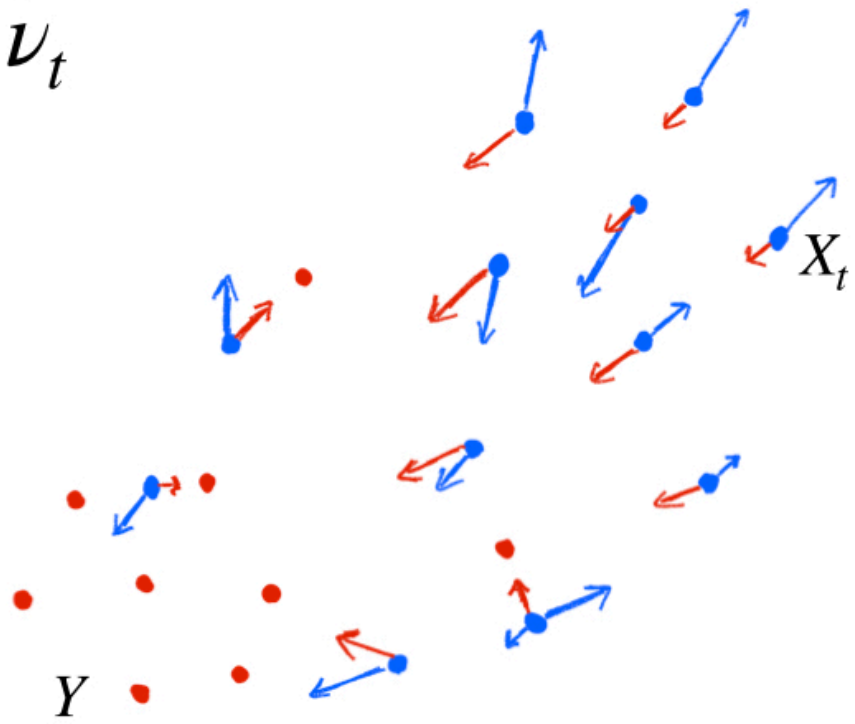

$$\nu_{t+1} : \quad X_{t+1} = X_t - \gamma_t \nabla f_t(X_t), \quad X_t \sim \nu_t$$

Descent direction

- For a small step-size γ:

$$MMD^2(\nu^*, \nu_{t+1}) - MMD^2(\nu^*, \nu_t) \leq -C\gamma \int \|\nabla f_t(x)\|^2 \, \mathrm{d}\nu_t(x)$$

Descent direction

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- ν_{t+1} : Generalized gradient descent algorithm [Villani, 2004].

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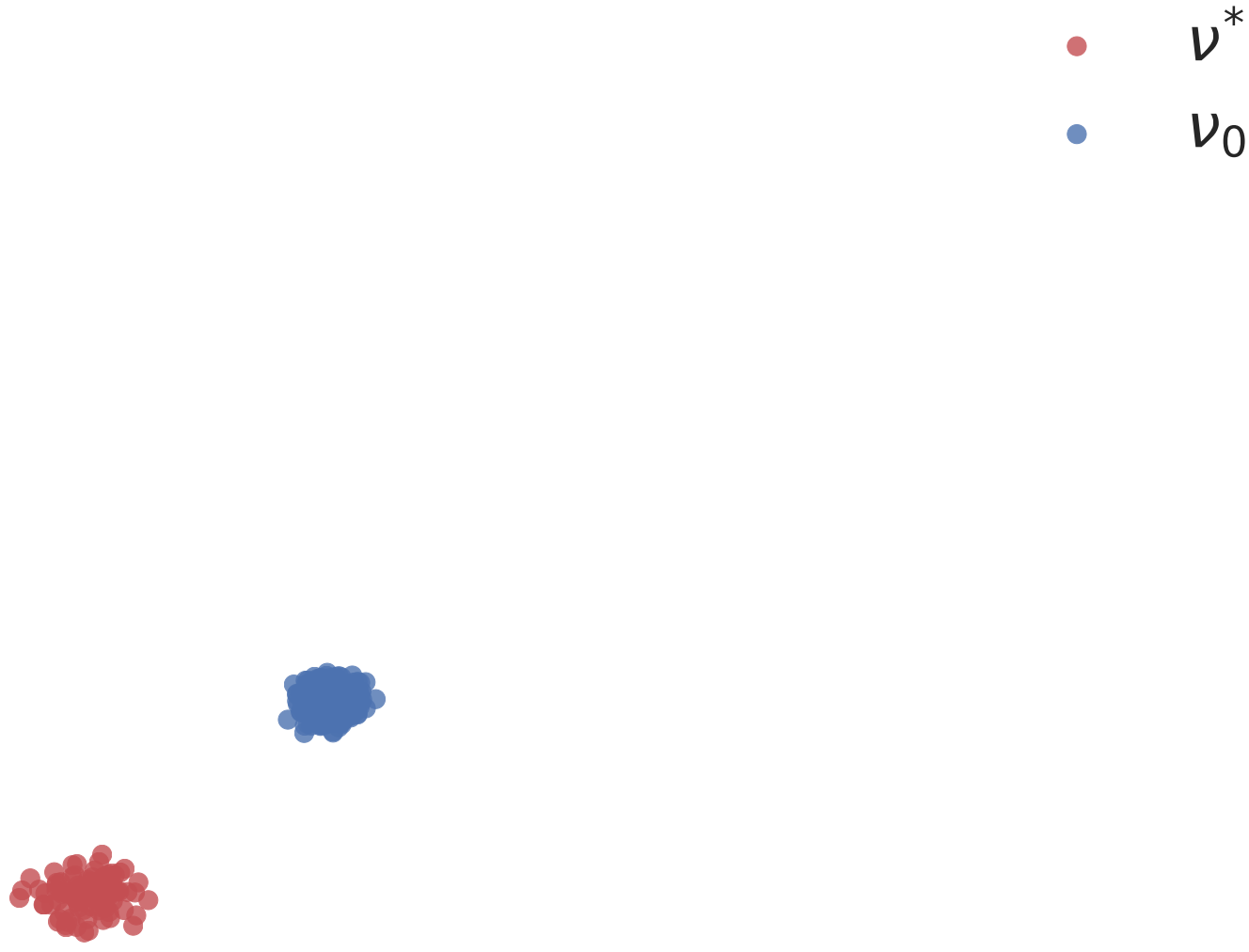
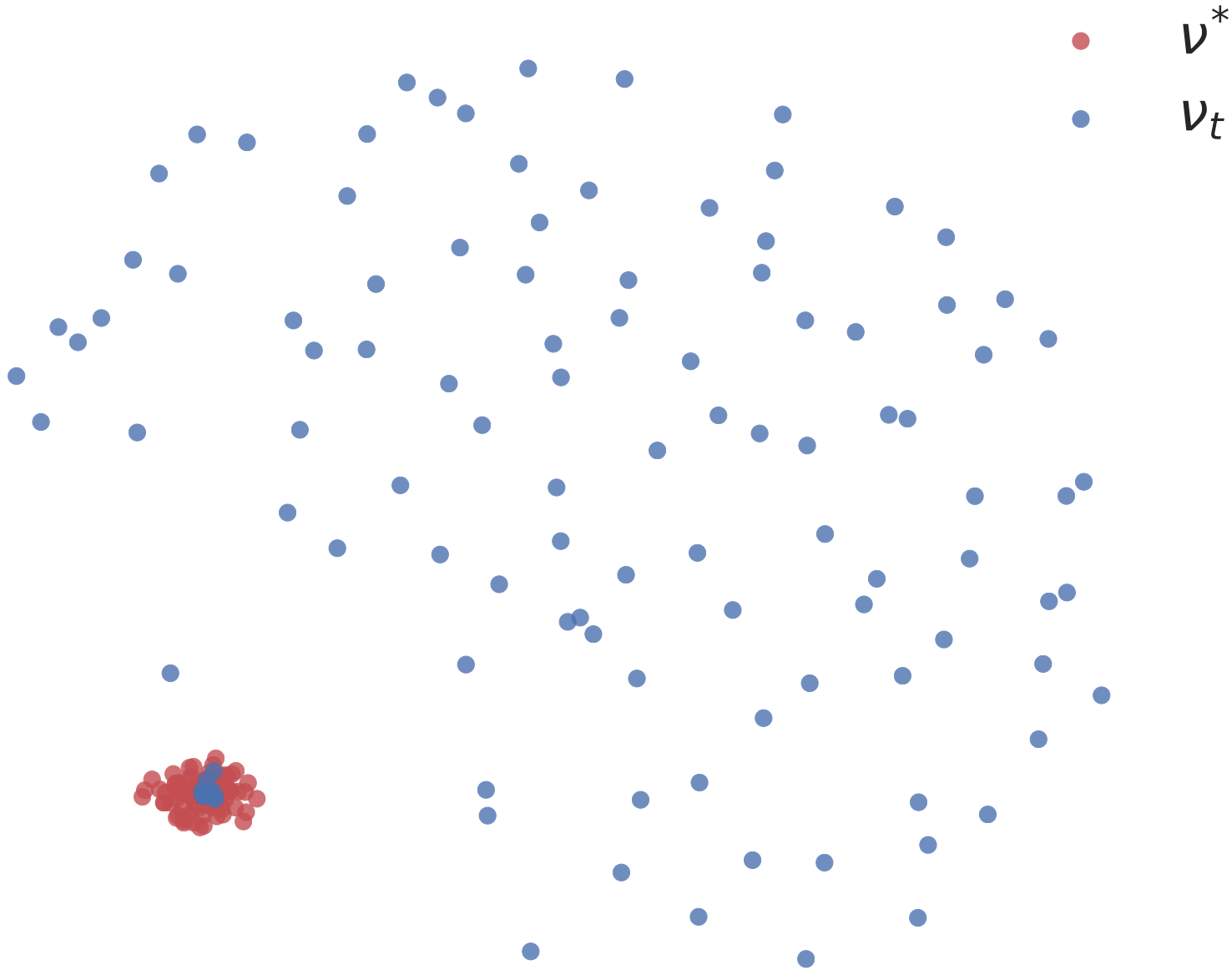
- ν_{t+1} : Generalized gradient descent algorithm [Villani, 2004].
- Convergence: $\nu_t \to \nu^*$?

Convergence: Failure case

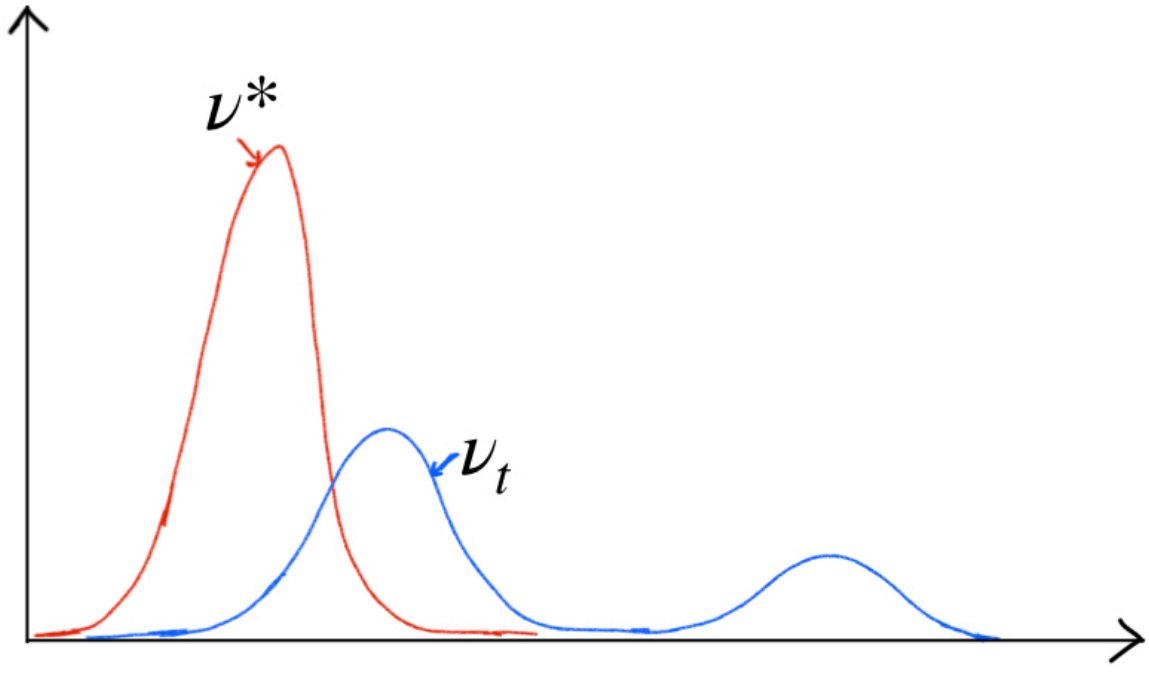


Convergence: Failure case



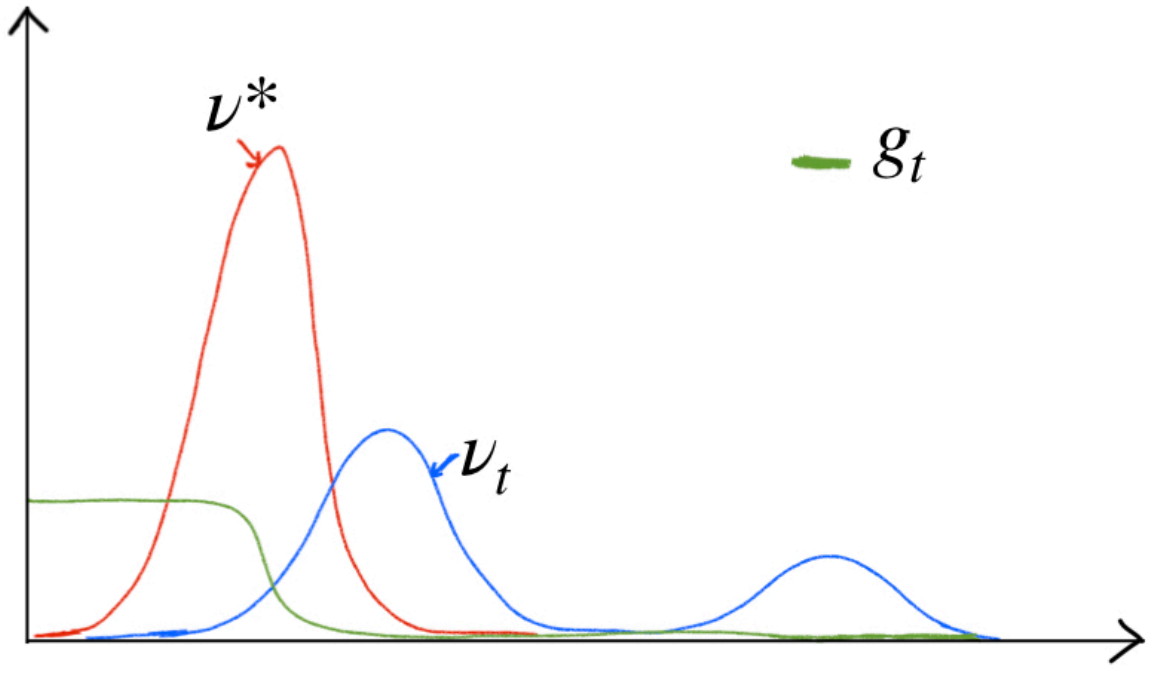
A criterion for convergence

Similar to a 'mode collapse'



A criterion for convergence

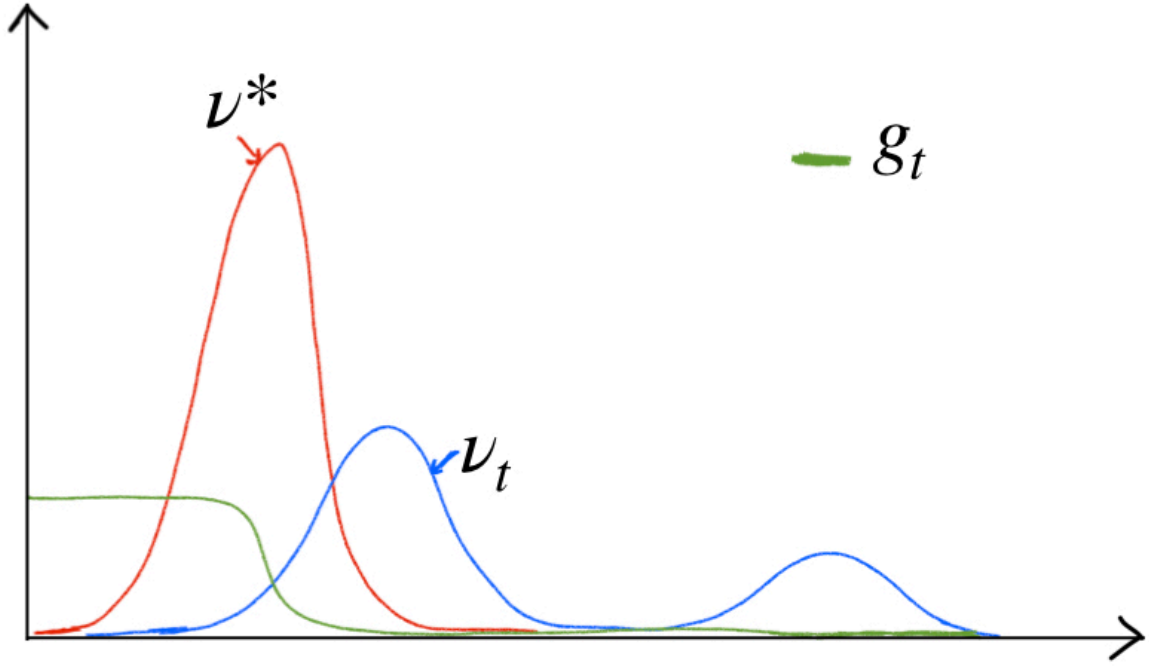
Similar to a 'mode collapse': Can construct g_t to be 'flat' on the support of ν_t



$$\int \|\nabla g_t(x)\|^2 \, d\nu_t(x) \leq 1$$

A criterion for convergence

Similar to a 'mode collapse': Can construct g_t to be 'flat' on the support of ν_t, and still witnesses the difference between ν^* and ν_t

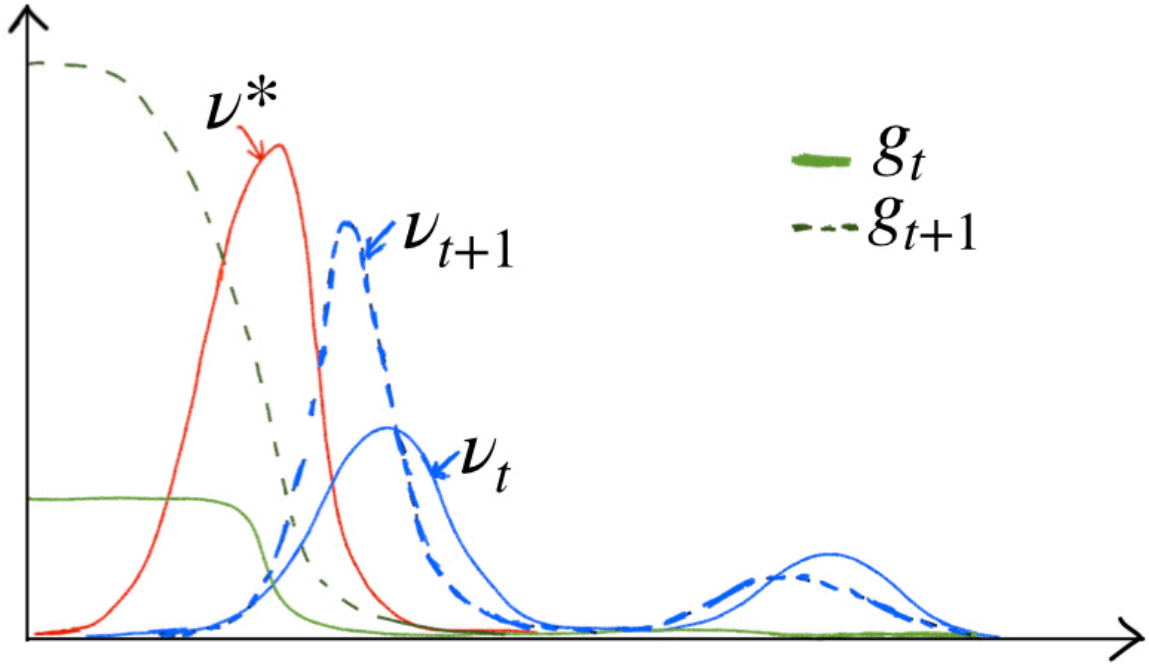


$$\int \|\nabla g_t(x)\|^2 \, d\nu_t(x) \leq 1$$

$$\left| \int g_t(x) d\nu^*(x) - \int g_t(x) d\nu_t(x) \right| > Ct^2$$

A criterion for convergence

Similar to a 'mode collapse': Can construct g_t to be 'flat' on the support of ν_t, and still witnesses the difference between ν^* and ν_t



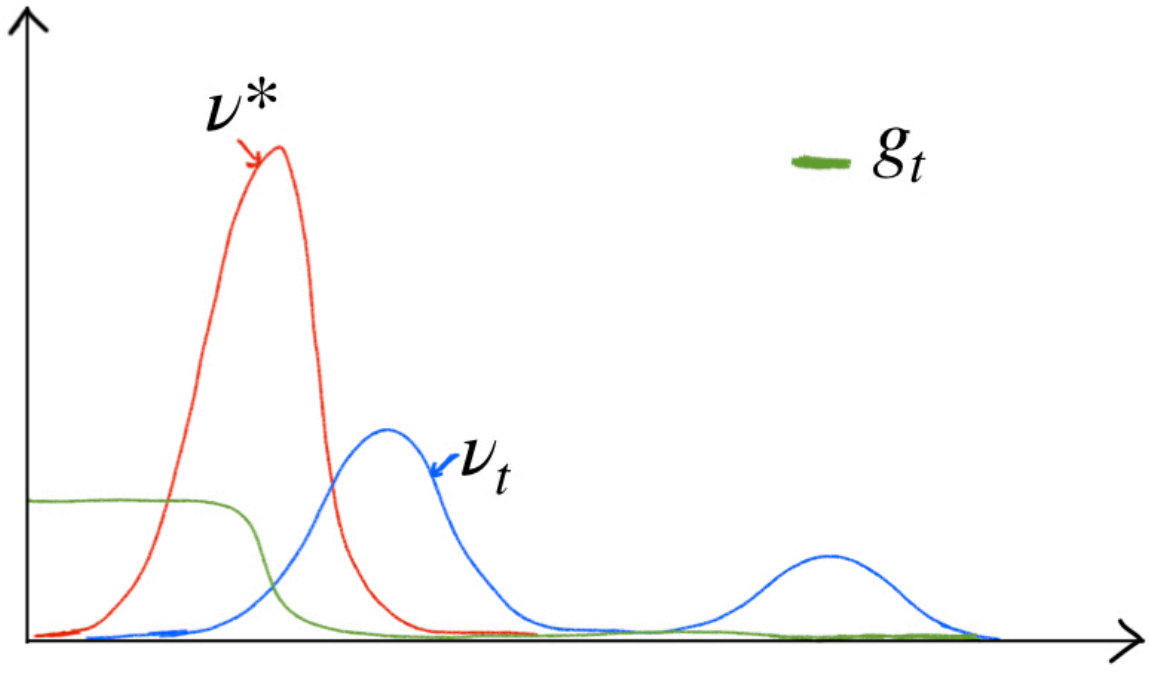
$$\int \|\nabla g_{t+1}(x)\|^2 \, d\nu_{t+1}(x) \leq 1$$

$$\left| \int g_{t+1}(x) d\nu^*(x) - \int g_{t+1}(x) d\nu_{t+1}(x) \right| > C(t+1)^2$$

A criterion for convergence: Negative Sobolev distance

Define:

$S(\nu^*|\nu_t) = \sup_{g,\int \|\nabla g(x)\|^2 \mathrm{d}\nu_t(x)\leq 1} |\int g(x)\,\mathrm{d}\nu^*(x) - \int g(x)\,\mathrm{d}\nu_t(x)|$



$$\int \|\nabla g_t(x)\|^2 \, d\,\nu_t(x) \leq 1$$

$$S(\nu^* \,|\, \nu_t) \geq |\int g_t(x) d\,\nu^*(x) - \int g_t(x) d\,\nu_t(x)\,| > Ct^2$$

A criterion for convergence: Negative Sobolev distance

- Assume that $S(\nu^*|\nu_t) \leq C$ for all t, then

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

A criterion for convergence: Negative Sobolev distance

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

- Depends on the whole sequence ν_t: Hard to verify in general
- Can be checked for simple exemples.

Noise Injection

- Failure case when $\nabla f_t(x) \simeq 0$ on the support of ν_t but $\|\nabla f_t(x)\| \gg 1$ outside of it:

$$X_{t+1} = X_t - \gamma \nabla f_t(X_t) \simeq X_t$$

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

$$X_{t+1} = X_t - \gamma \nabla f_t(X_t + \beta_t u_t); \qquad X_t \sim \mu_t$$

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- Similar to *continuation methods* [Chaudhari et al., 2017, Hazan et al., 2015]
- But extended to interacting particles.

Noise Injection

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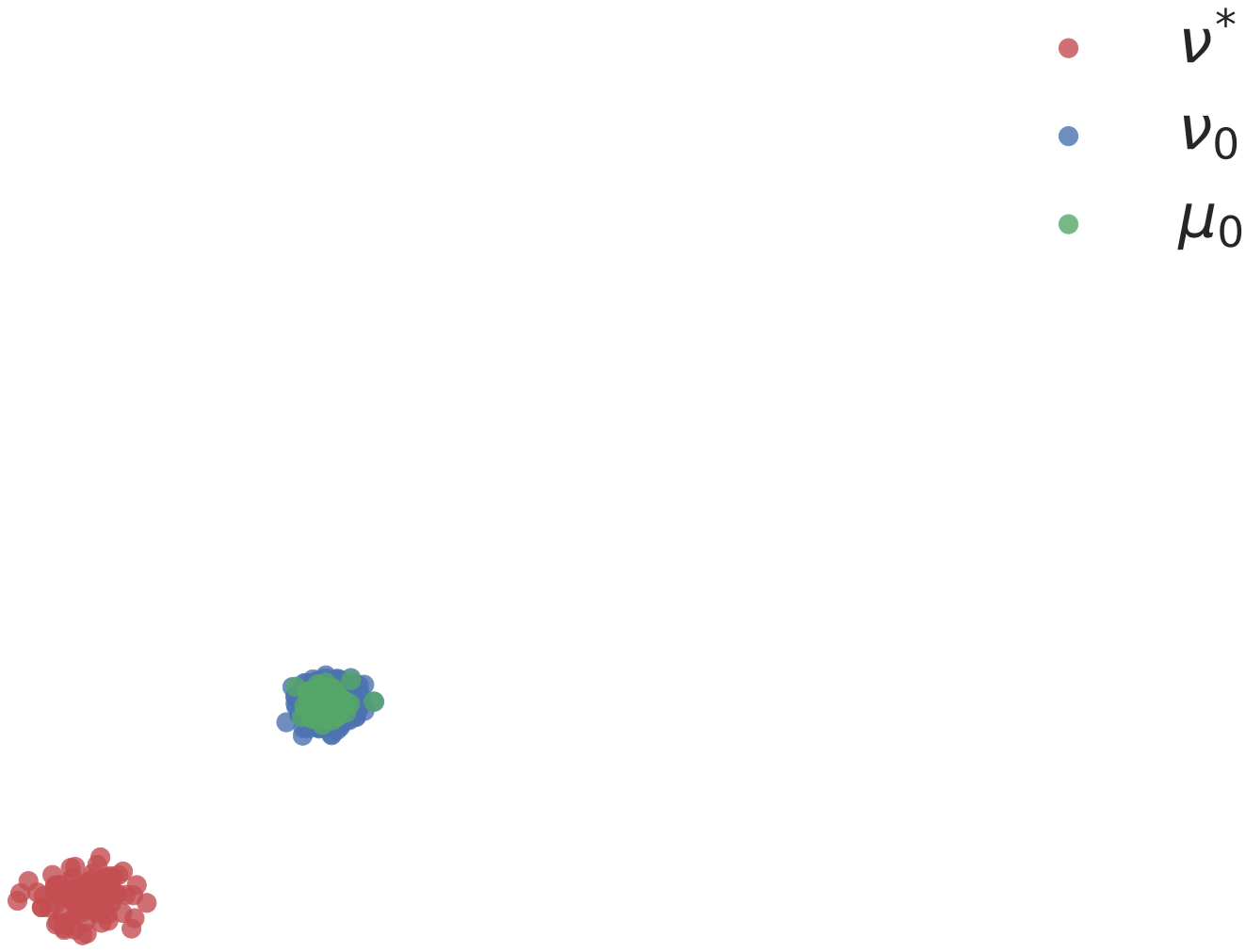
$$X_{t+1} = X_t - \gamma \nabla f_t(X_t + \beta_t u_t); \qquad X_t \sim \mu_t \tag{1}$$

- Different from entropic regularization [Mei et al., 2018]

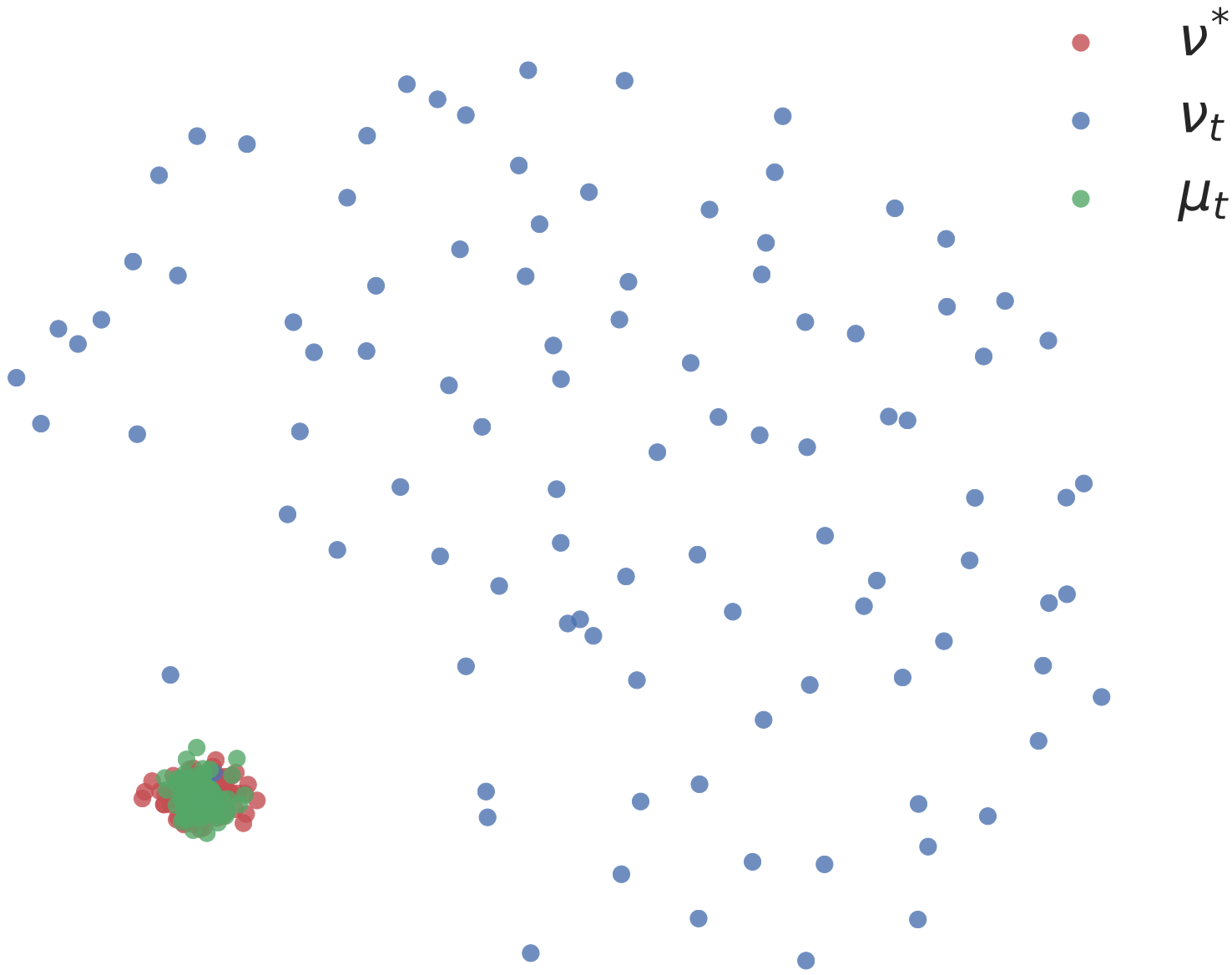
$$X_{t+1} = X_t - \gamma \nabla f_t(X_t) + \beta_t u_t \tag{2}$$

Noise Injection: Experiments



Noise Injection: Experiments

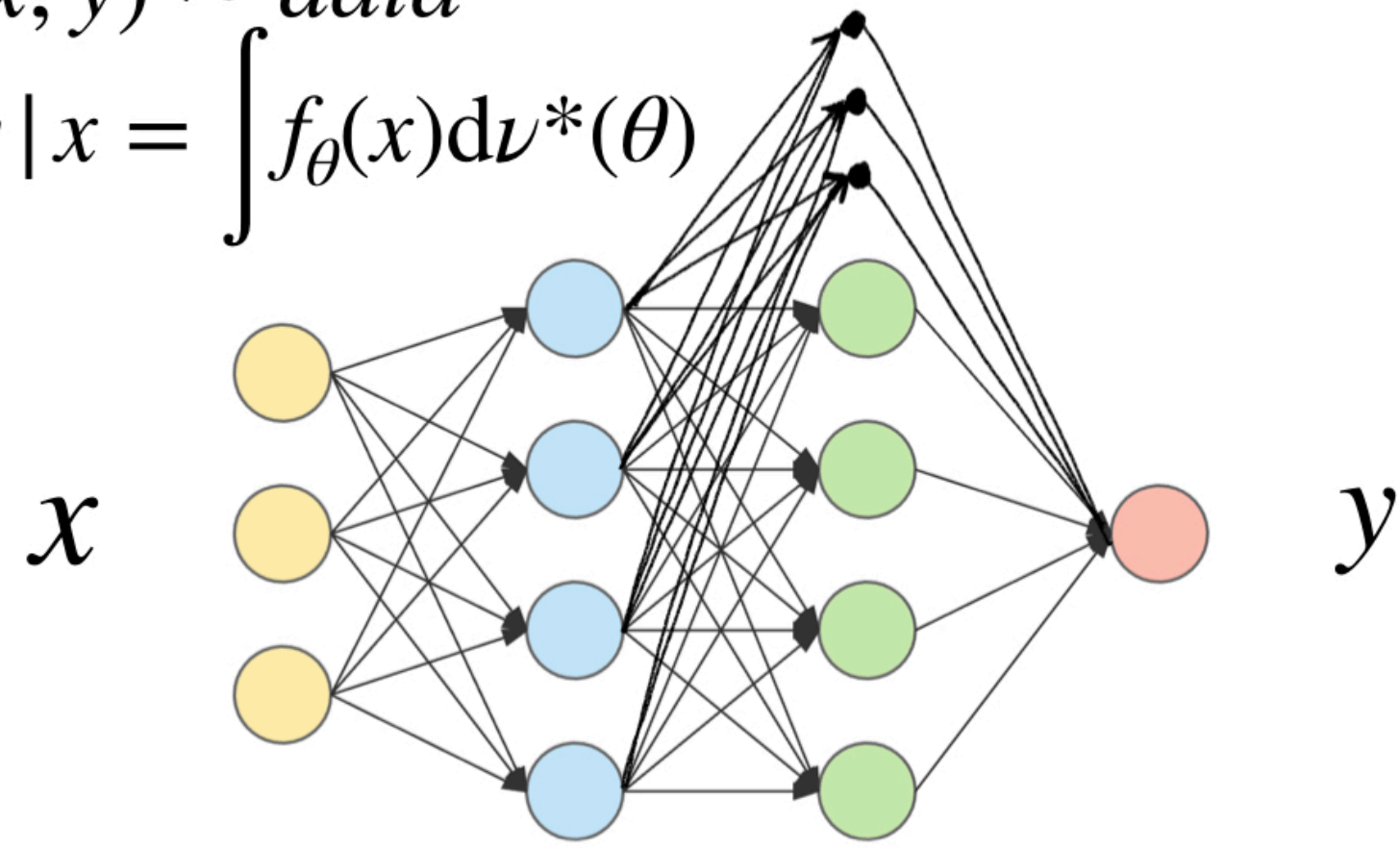
It works in practice:



Noise Injection: Experiments

$$(x, y) \sim data$$

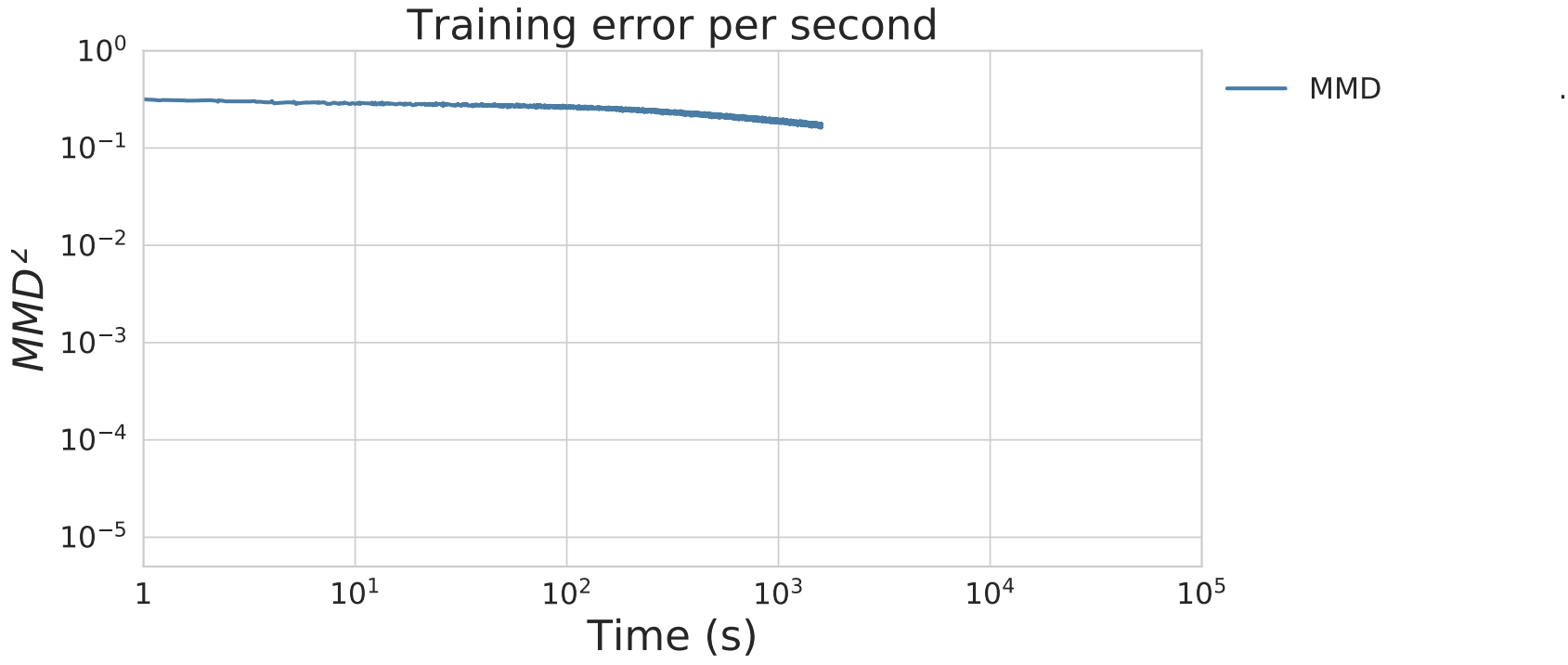
$$y \mid x = \int f_\theta(x) \mathrm{d}\nu^*(\theta)$$



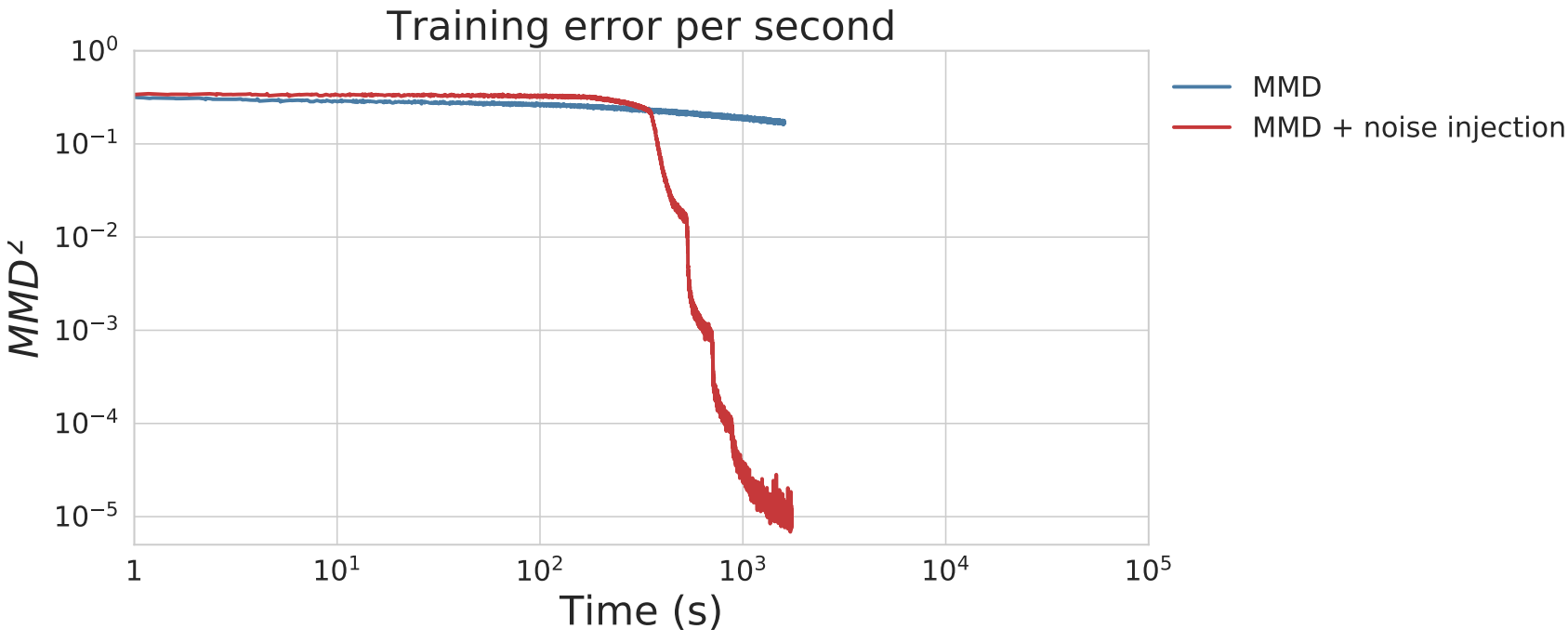
$$\min_{\nu \in \mathcal{P}} MMD^2(\nu^*, \nu)$$

$$k(\theta, \theta') = \mathbb{E}_{data}[f_\theta(x) f_{\theta'}(x)]$$

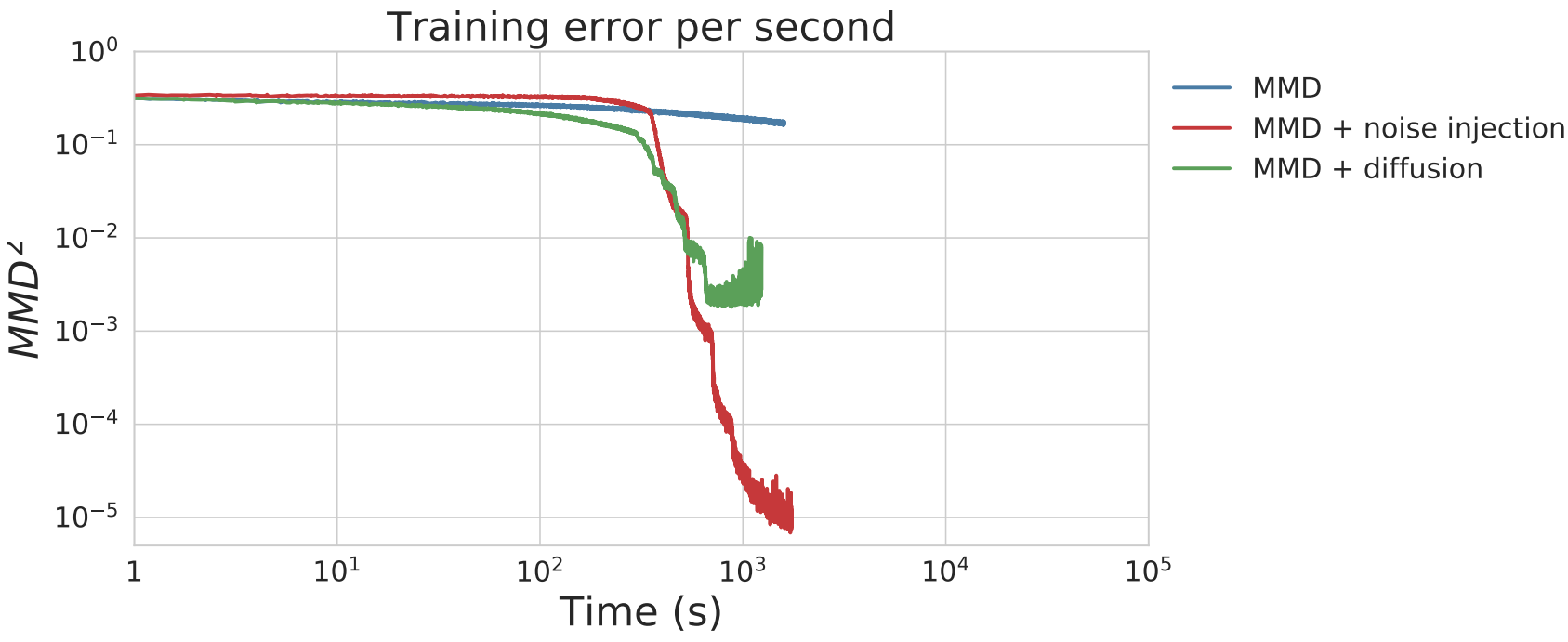
Noise Injection: Experiments



Noise Injection: Experiments

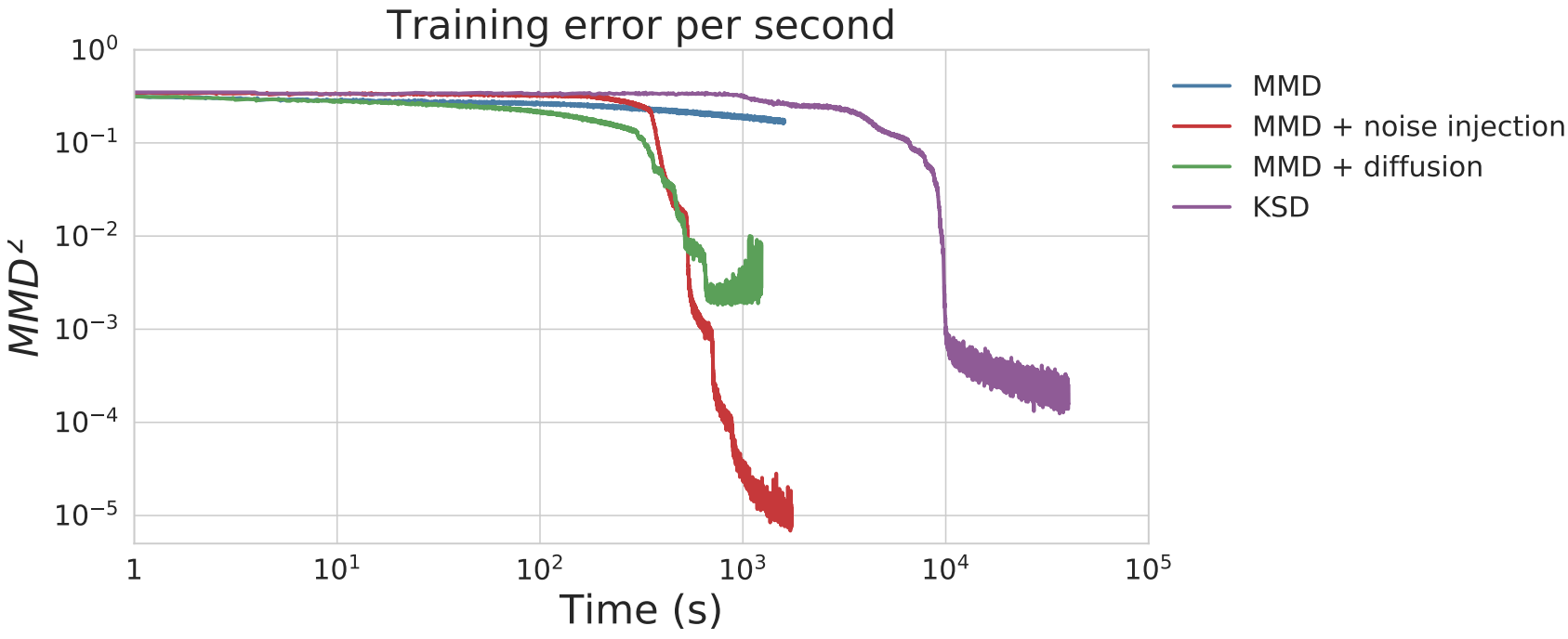


Noise Injection: Experiments



MMD + diffusion: [Mei et al., 2018]

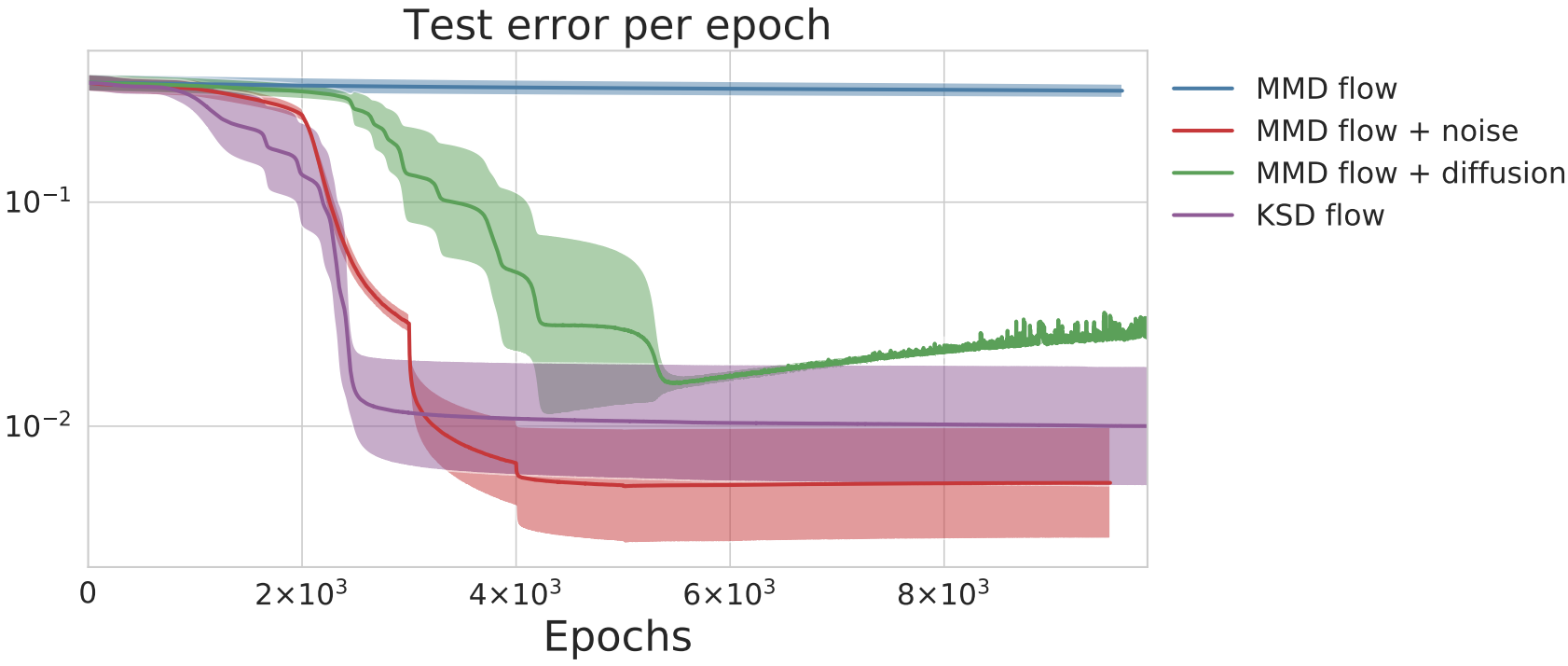
Noise Injection: Experiments



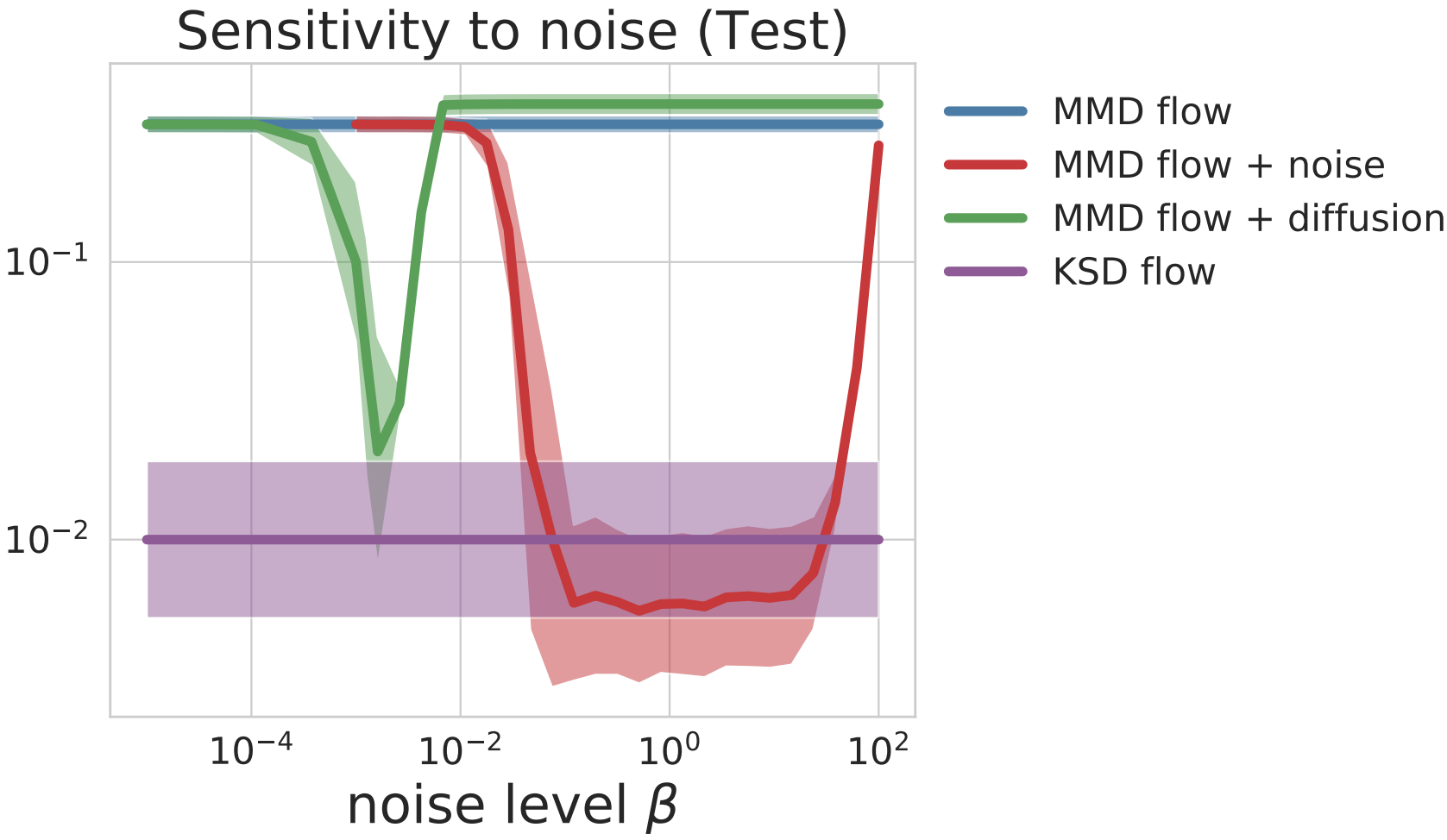
MMD + diffusion: [Mei et al., 2018]

KSD: [Mroueh, 2018]

Noise Injection: Experiments



Noise Injection: Experiments



Conclusion

Contributions:

- Analyzed a simple algorithm to optimize the MMD based on interacting particles.
- Provided a convergence criterion for the algorithm.
- Proposed an extension to the noise injection algorithm for interacting particles.

Future work:

- A convergence criterion independent from the whole trajectory.
- Stronger guarantees for the convergence of the noise injection algorithm.

Take home message

When you are stuck, add noise!!

Thank you!

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