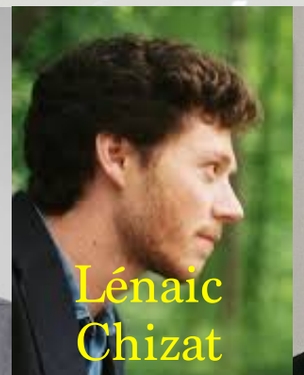
Scaling Optimal Transport to High Dimensional Learning

Gabriel Peyré

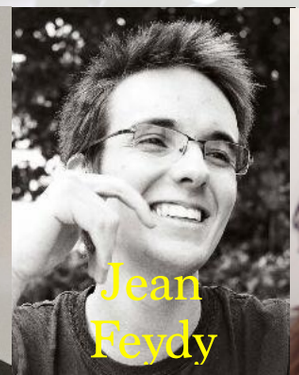
Joint works with:


Shun'ichi Amari

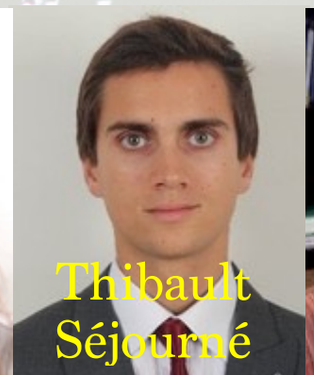

Francis Bach


Lénaic Chizat


Marco Cuturi


Jean Feydy

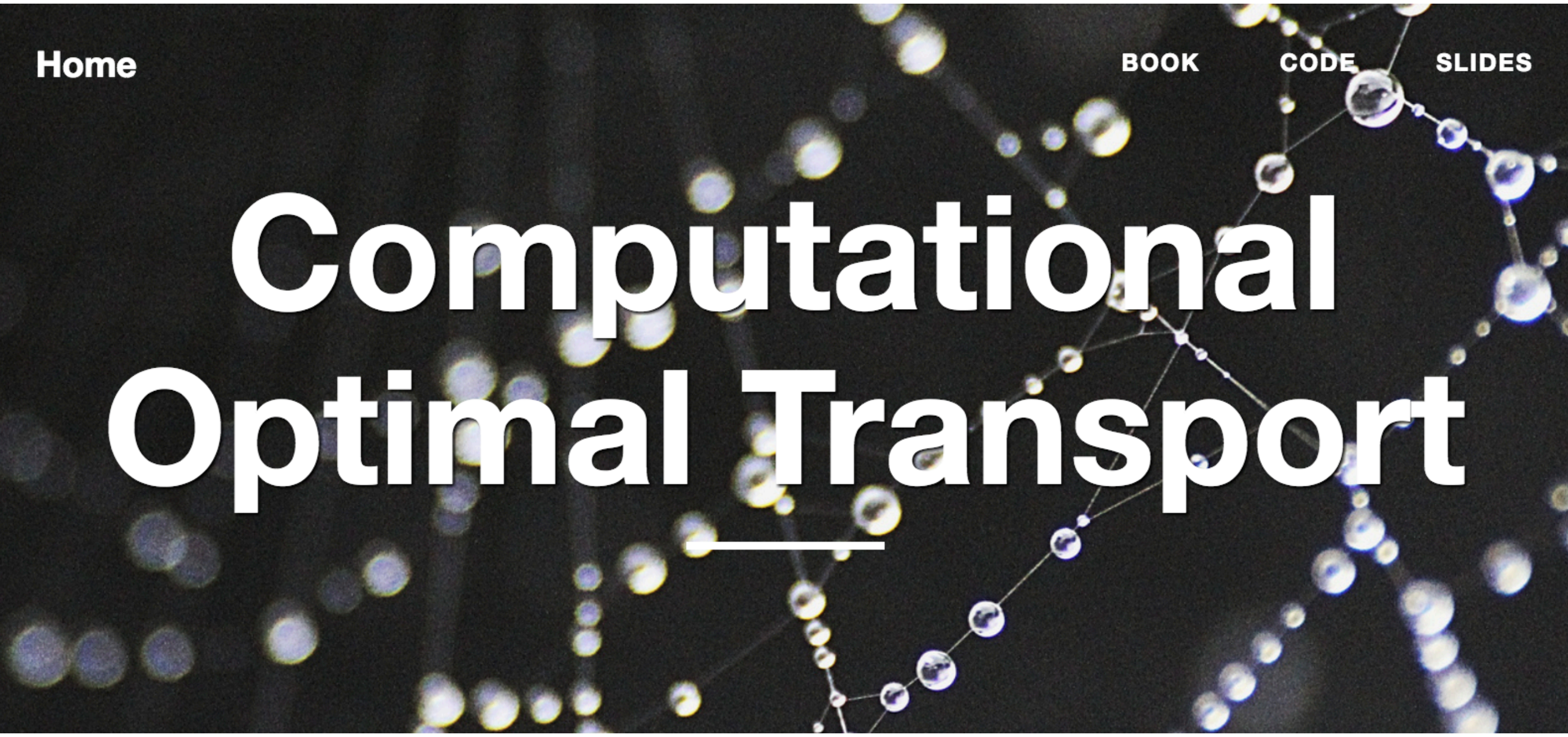

Aude Genevay


Thibault Séjourné


Alain Trouvé


François-Xavier Vialard

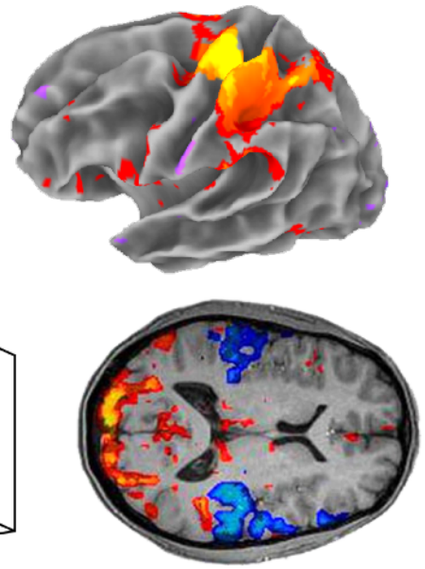
https://optimaltransport.github.io

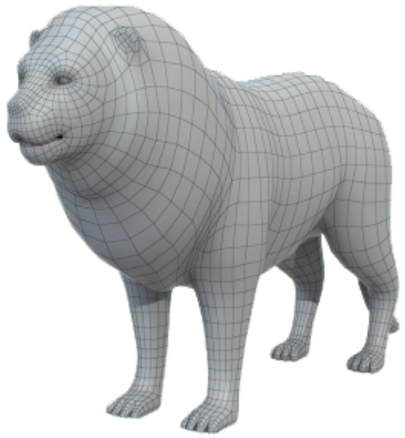


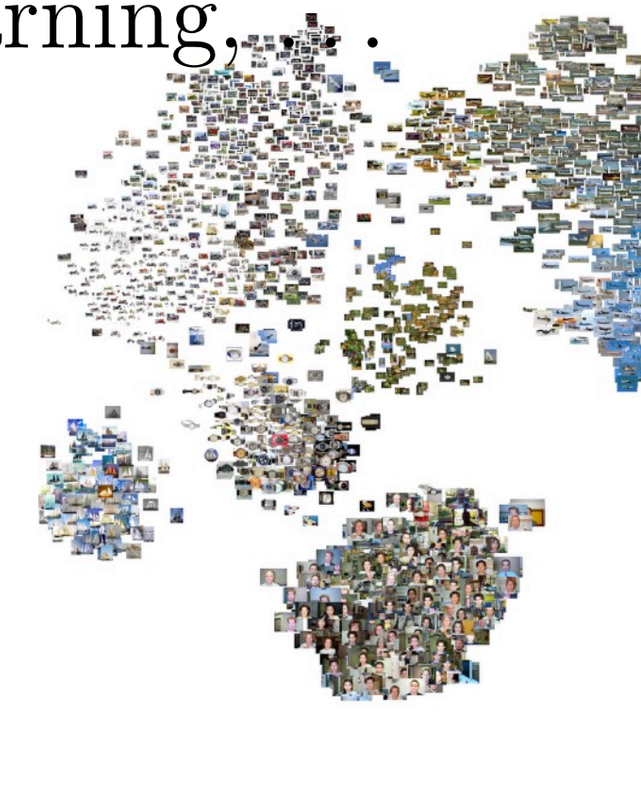
Probability Distributions in Data Sciences

Probability distributions and histograms

$\rightarrow$ images, vision, graphics and machine learning, . . .







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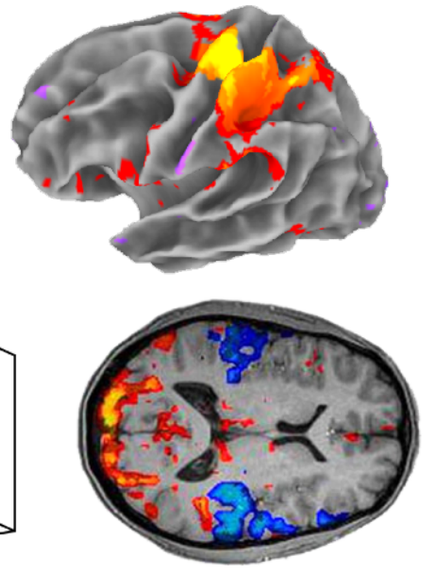
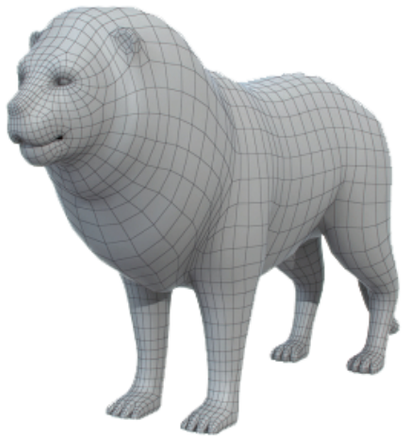
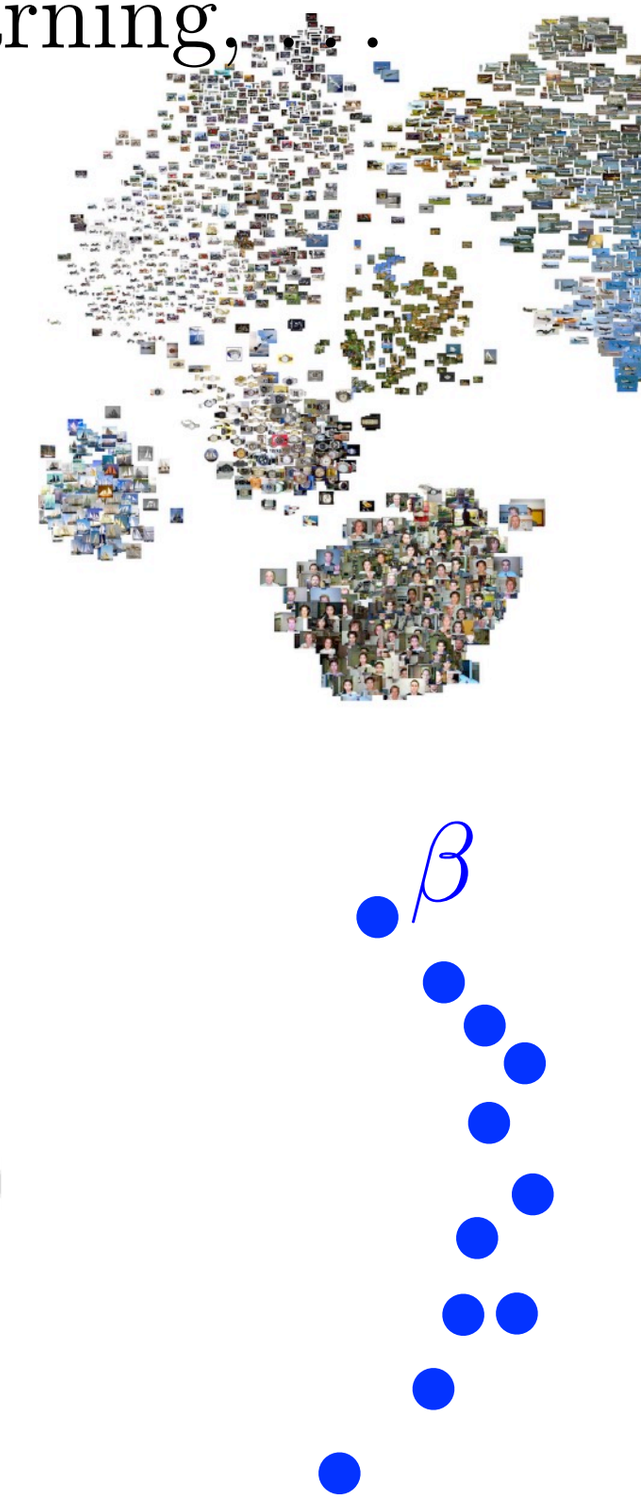


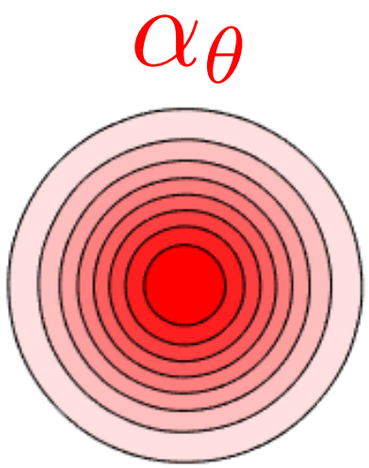




Unsupervised learning

Observations: $\beta \stackrel{\text{def.}}{=} \frac{1}{n} \sum_{i=1}^{n} \delta_{x_i}$

Parametric model: $\theta \mapsto \alpha_\theta$



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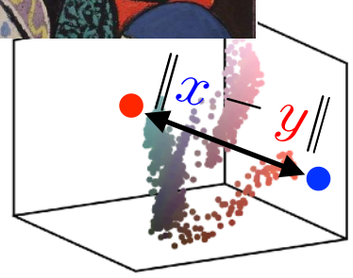

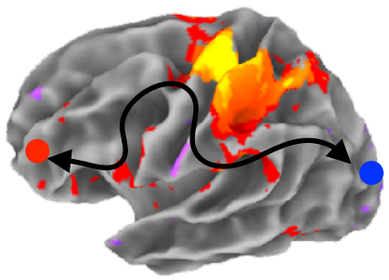

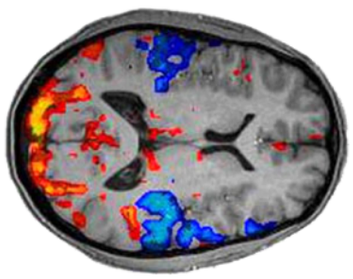

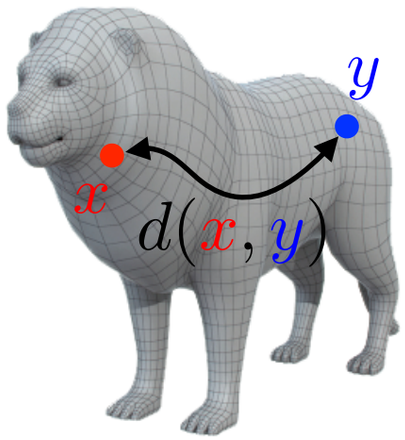

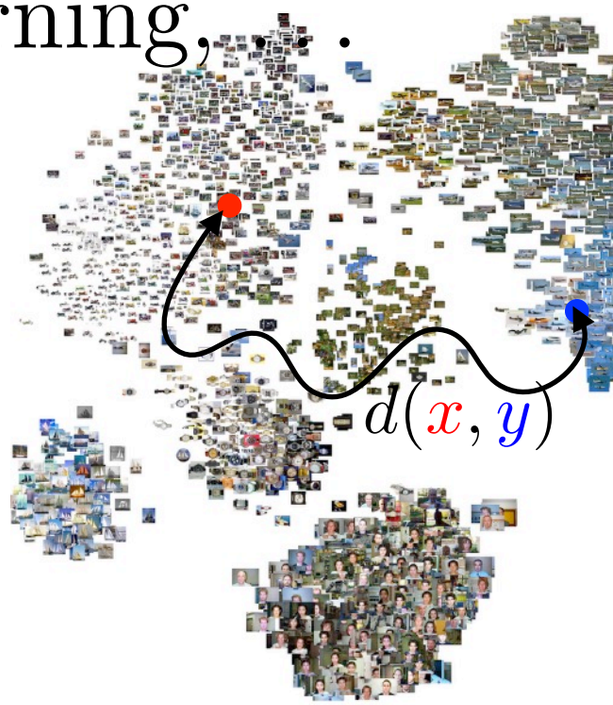

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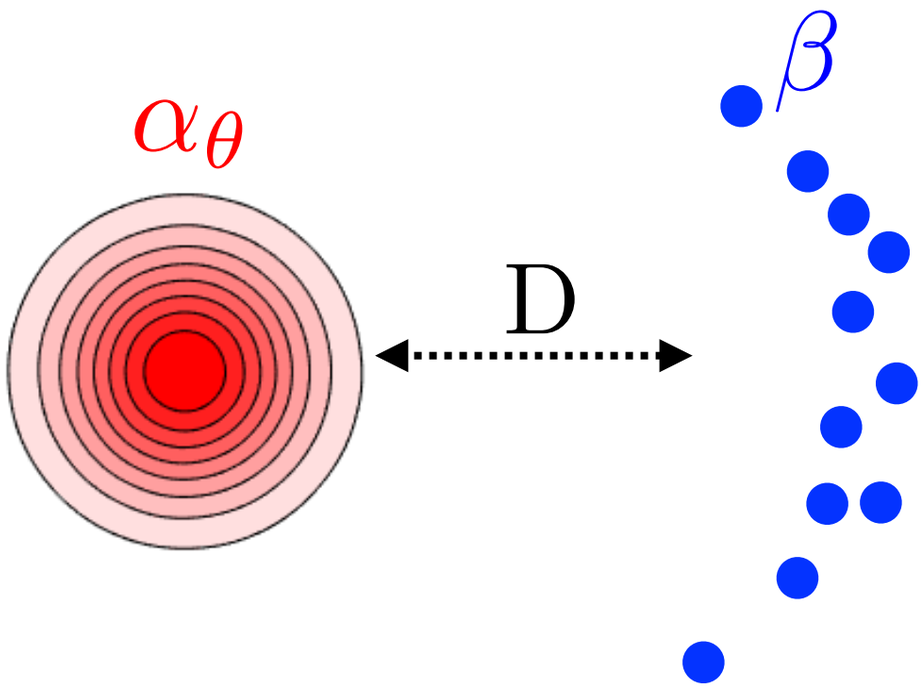
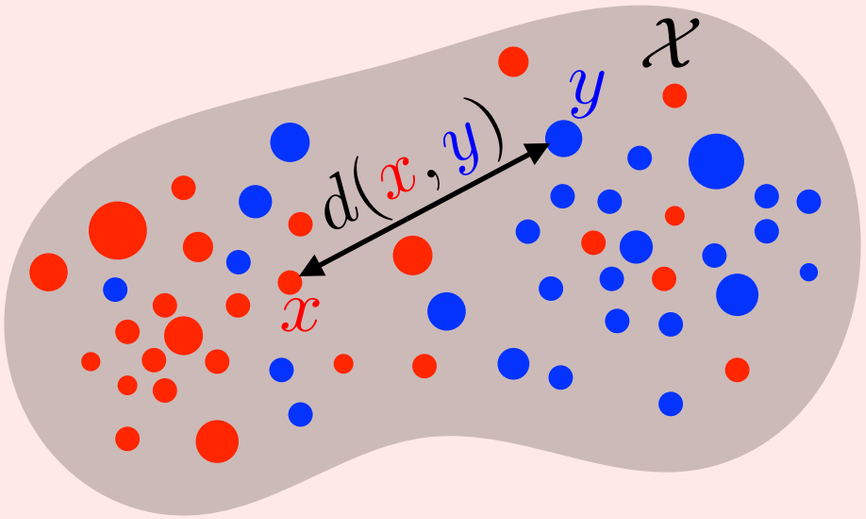
Parametric model: $\theta \mapsto \alpha_\theta$

Density fitting: $\min_\theta \mathrm{D}(\alpha_\theta, \beta)$

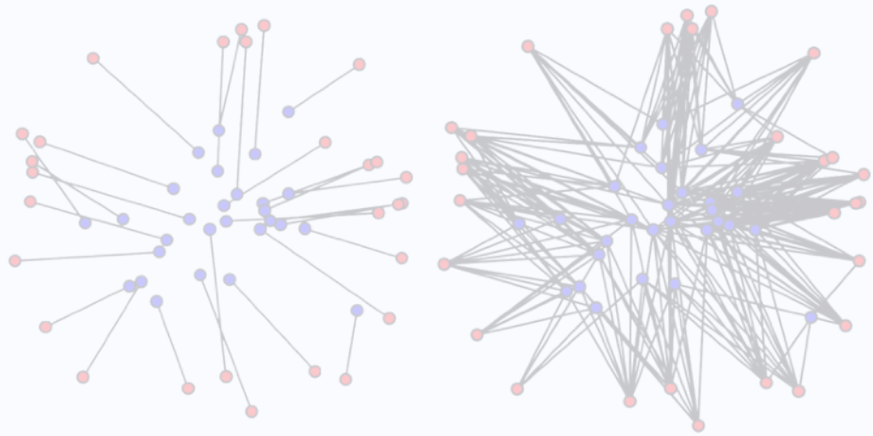
$\rightarrow$ takes into account a metric d.



1. Optimal Transport

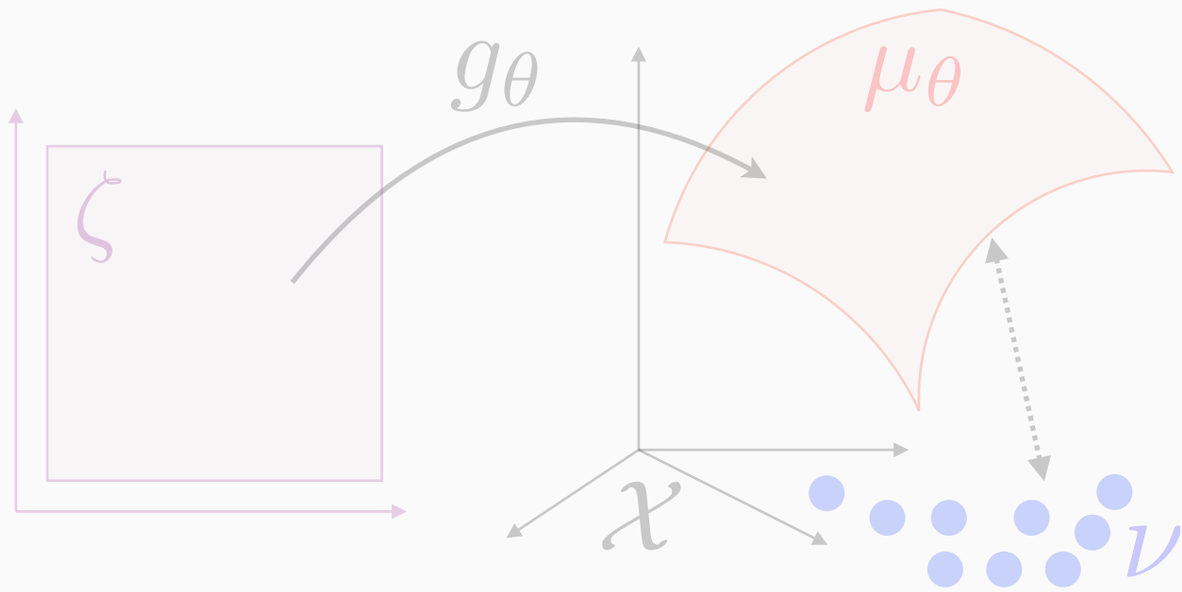


2. Entropic Regularization



3. Sinkhorn Divergences

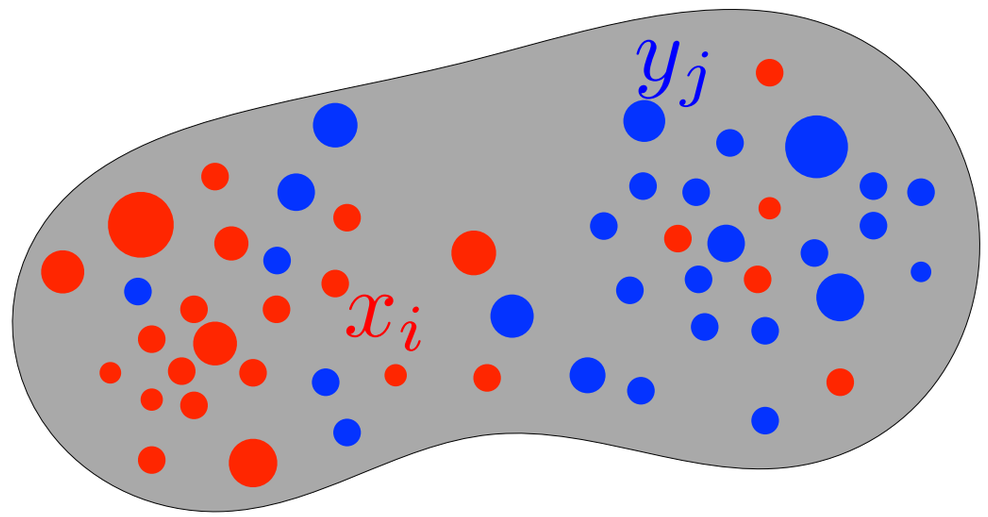
4. Application to Generative Models



Kantorovitch's Formulation

Input distributions

$\alpha = \sum_{i=1}^{n} \mathbf{a}_i \delta_{x_i} \quad \beta = \sum_{j=1}^{m} \mathbf{b}_j \delta_{y_j}$



Points $(x_i)_i$, $(y_j)_j$

Weights $\mathbf{a}_i \geqslant 0$, $\mathbf{b}_j \geqslant 0$.

$\sum_{i=1}^{n} \mathbf{a}_i = \sum_{j=1}^{m} \mathbf{b}_j = 1$

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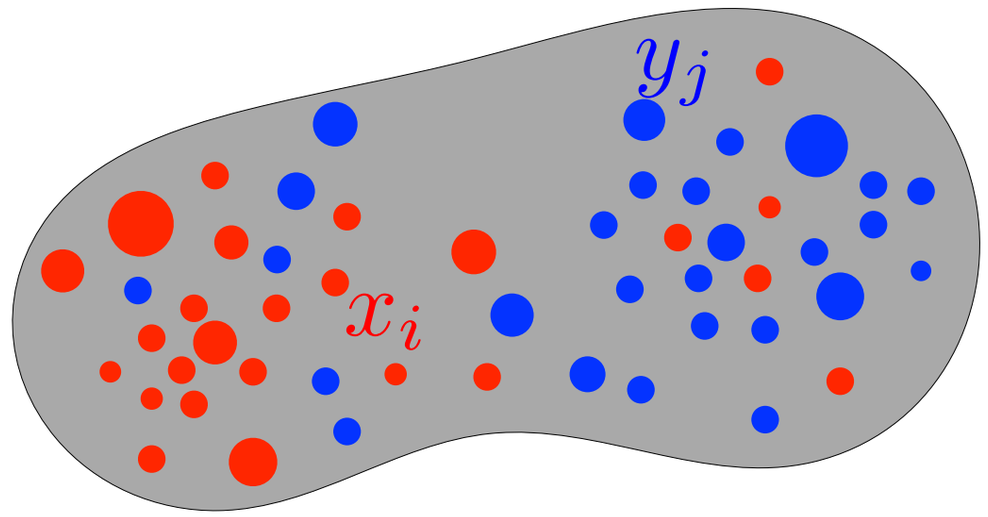

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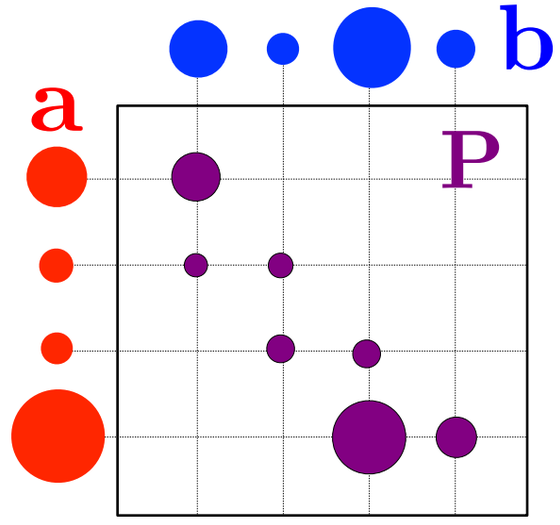
Couplings:

$$\mathbf{U}(\mathbf{a}, \mathbf{b}) \stackrel{\text{def.}}{=} \left\{ \mathbf{P} \in \mathbb{R}_+^{n \times m} \;;\; \mathbf{P}\mathbb{1}_m = \mathbf{a}, \mathbf{P}^\top \mathbb{1}_n = \mathbf{b} \right\}$$



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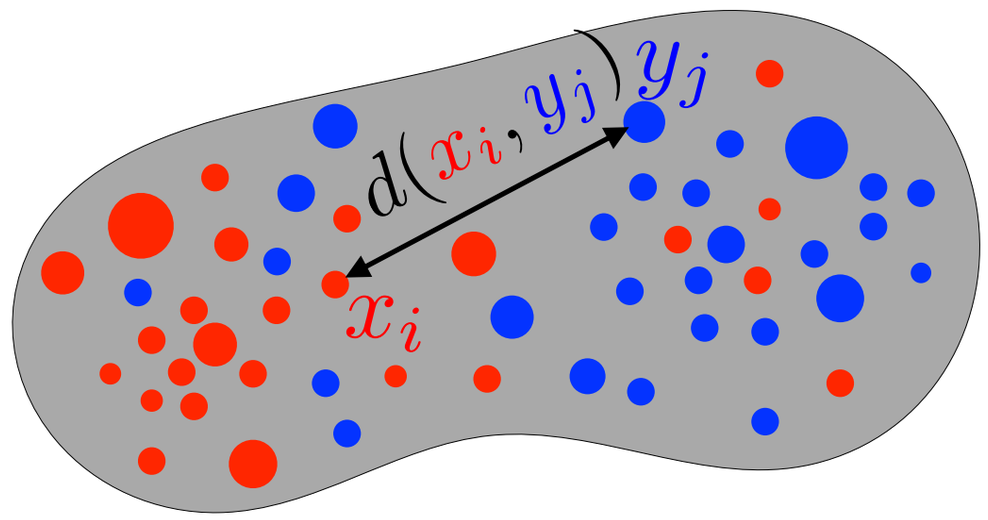

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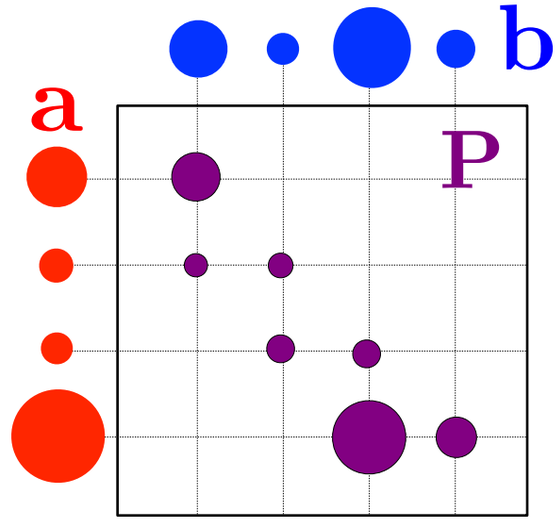

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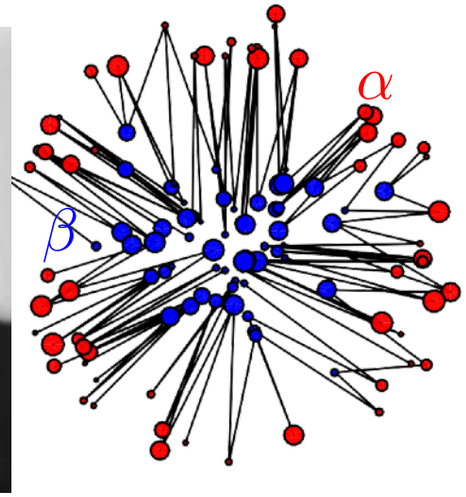
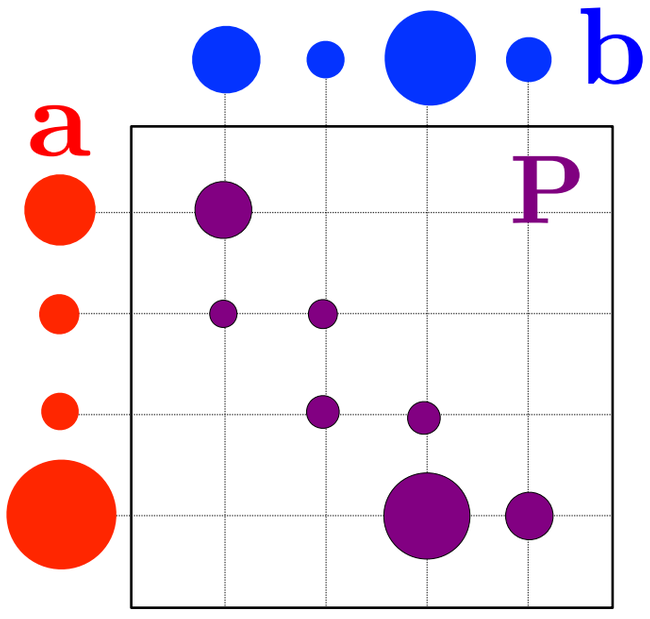
[Kantorovich 1942]

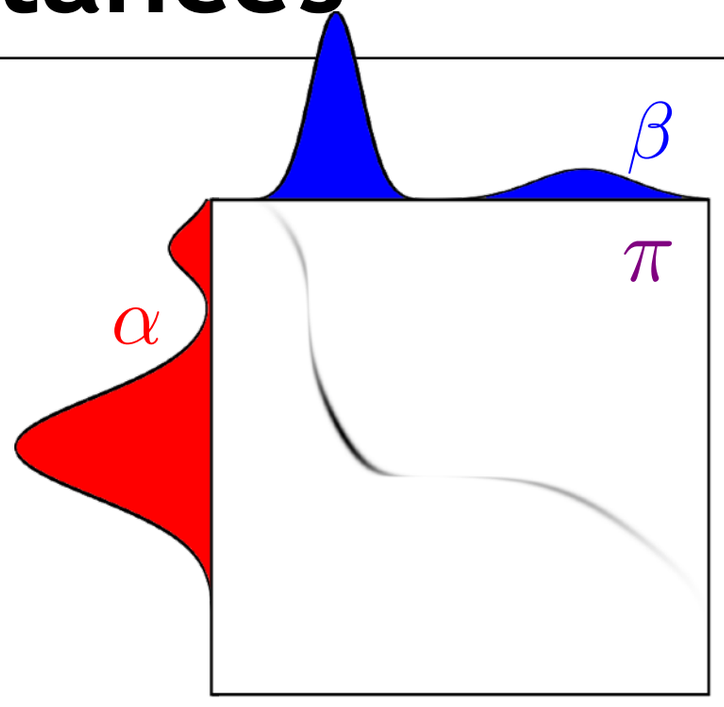
$$\min \left\{ \sum_{i,j} d(x_i, y_j)^p \mathbf{P}_{i,j} \;;\; \mathbf{P} \in \mathbf{U}(\mathbf{a}, \mathbf{b}) \right\}$$



Optimal Transport Distances

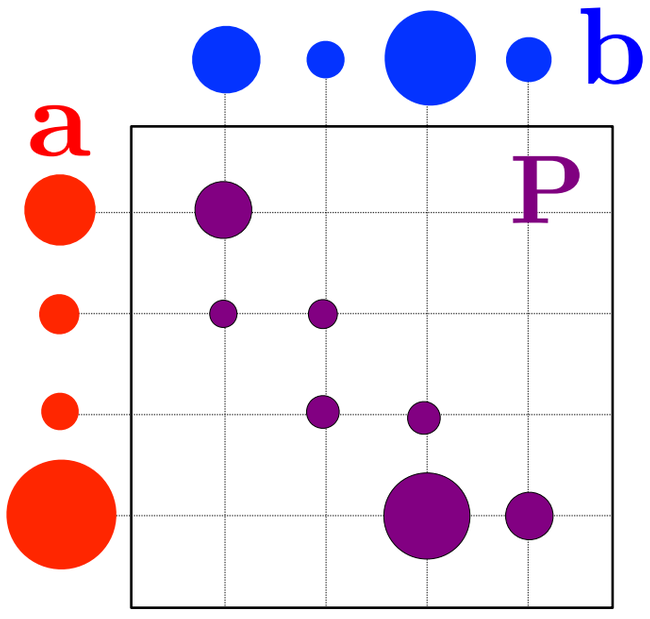


$$\pi = \sum_{i,j} \mathbf{P}_{i,j} \delta_{x_i, y_j}$$



$$\mathrm{W}_p(\alpha,\beta)^p \stackrel{\text{def.}}{=} \min_{\pi \in \mathcal{M}_+^1(\mathcal{X}^2)} \left\{ \int_{\mathcal{X}^2} d(x,y)^p \mathrm{d}\pi(x,y) \;;\; \pi_1 = \alpha, \pi_2 = \beta \right\}$$

Optimal Transport Distances



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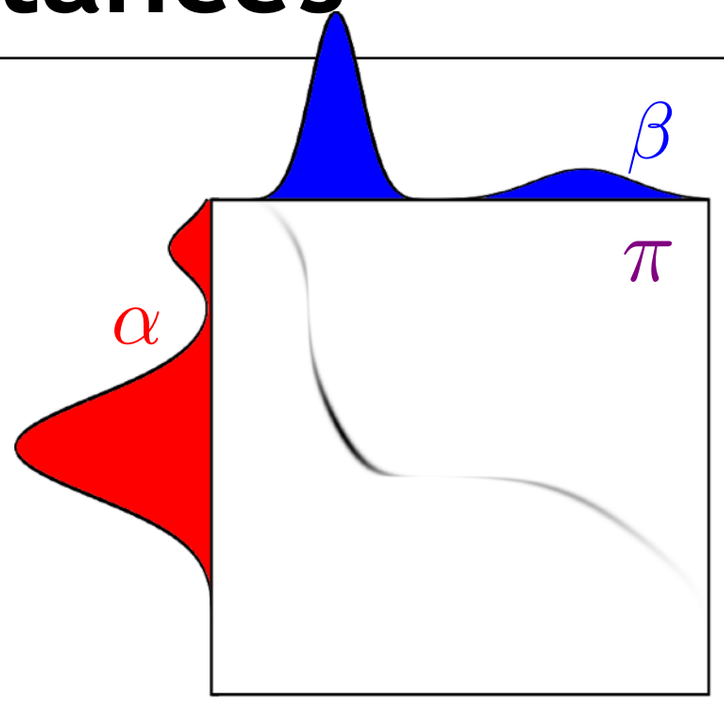

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Theorem: W_p is a distance and $\alpha_n \rightharpoonup \beta \;\Leftrightarrow\; \mathrm{W}_p(\alpha_n, \beta) \to 0$

Weak* (aka in law) convergence: $\alpha_n \rightharpoonup \beta \;\Leftrightarrow\; \begin{array}{c} \forall\, f \in \mathcal{C}(\mathcal{X}), \\ \int_{\mathcal{X}} f \mathrm{d}\alpha_n \to \int_{\mathcal{X}} f \mathrm{d}\beta \end{array}$

$$\|\delta_{x_n} - \delta_x\|_1 = 2 \quad \textbf{vs.} \quad \mathrm{W}_p(\delta_{x_n}, \delta_x) = d(x_n, x)$$

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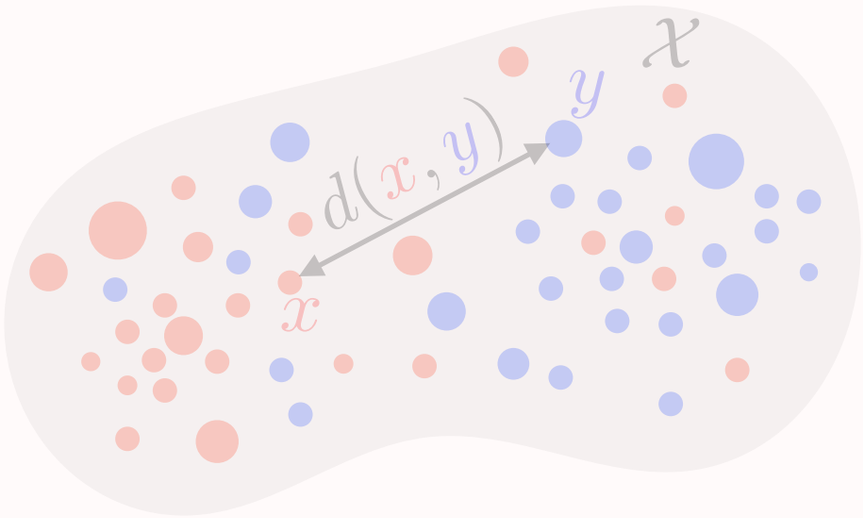

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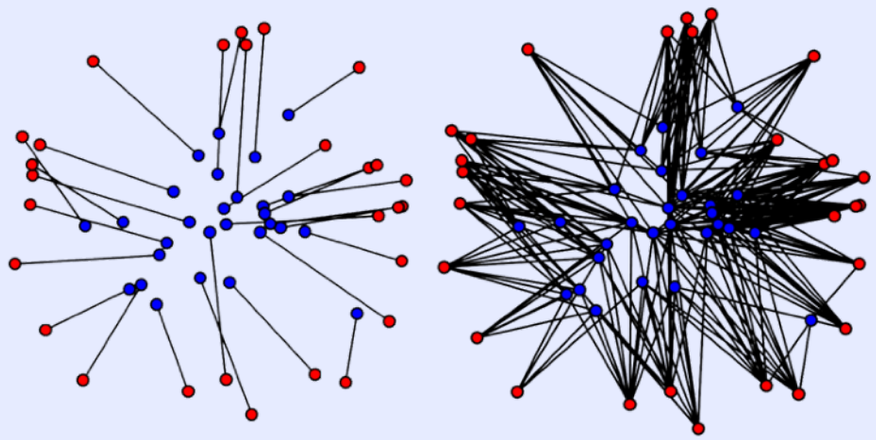

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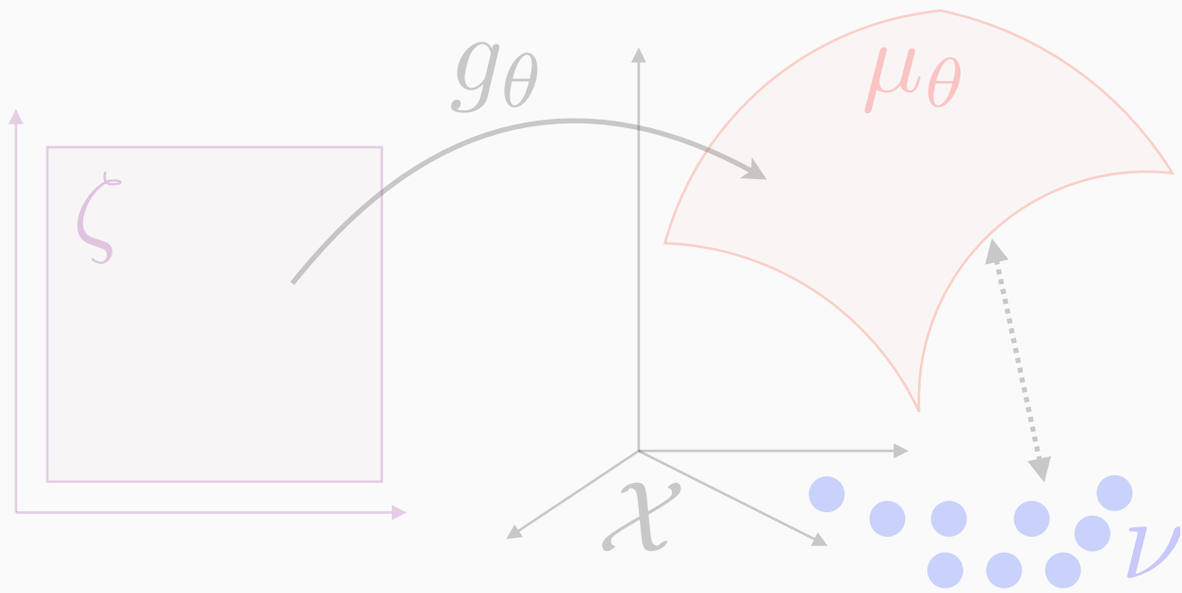
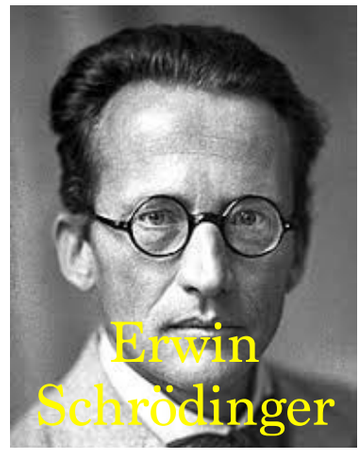


Entropic Regularization

Schrödinger's problem: [1931]

$$\min_{\mathbf{P}\in\mathbf{U}(\mathbf{a},\mathbf{b})} \sum_{i,j} d(x_i, y_j)^p \mathbf{P}_{i,j} + \varepsilon \mathbf{P}_{i,j} \log\left(\frac{\mathbf{P}_{i,j}}{\mathbf{a}_i \mathbf{b}_j}\right)$$



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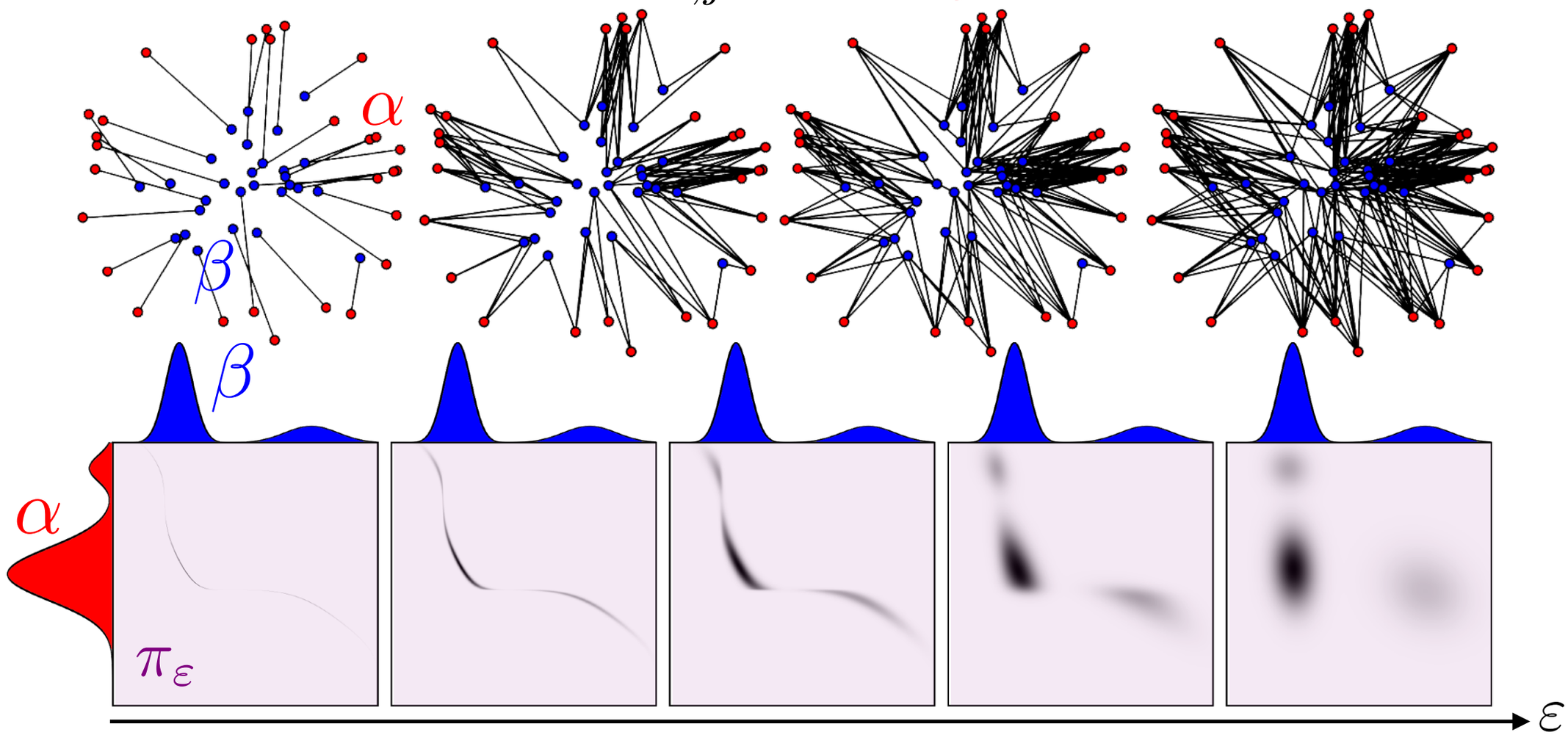

Sinkhorn's Algorithm

$$\min_{\mathbf{P} \in \mathbf{U}(\mathbf{a},\mathbf{b})} \sum_{i,j} d(x_i, y_j)^p \mathbf{P}_{i,j} + \varepsilon \mathbf{P}_{i,j} \log\left(\frac{\mathbf{P}_{i,j}}{\mathbf{a}_i \mathbf{b}_j}\right)$$

Proposition: $\quad \mathbf{P}_{i,j} = \mathbf{u}_i \, \mathbf{K}_{i,j} \, \mathbf{v}_j \qquad \mathbf{K}_{i,j} \overset{\text{def.}}{=} e^{-\frac{d(x_i,y_j)^p}{\varepsilon}}$

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Row constraint: $\mathbf{u} \odot (\mathbf{K}\mathbf{v}) = \mathbf{a}$

Col. constraint: $\mathbf{v} \odot (\mathbf{K}^\top \mathbf{u}) = \mathbf{b}$

Sinkhorn's Algorithm

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Theorem: [Sinkhorn 1964] $\quad (\mathbf{u}, \mathbf{v})$ converges.

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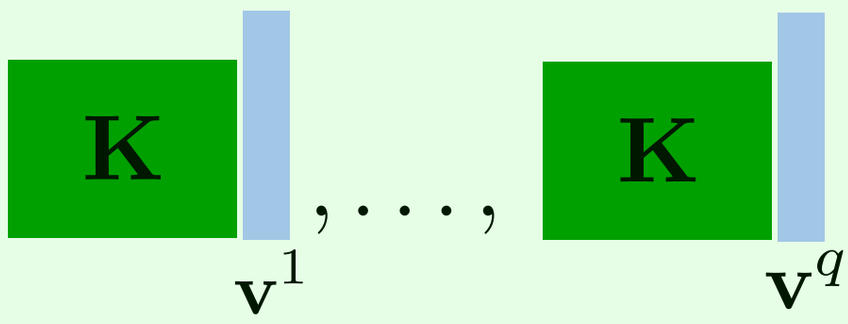
Theorem: [Sinkhorn 1964] $(\mathbf{u}, \mathbf{v})$ converges.

Only matrix/vector multiplications.

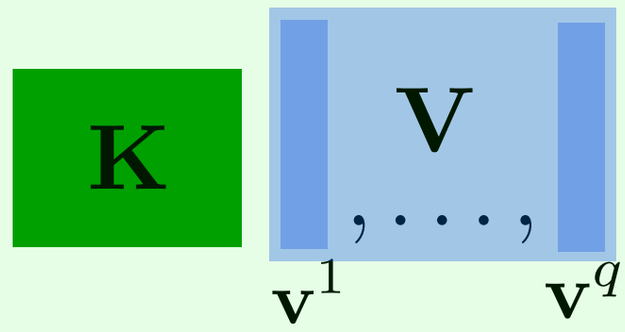
Matrix-vectors



parallelization

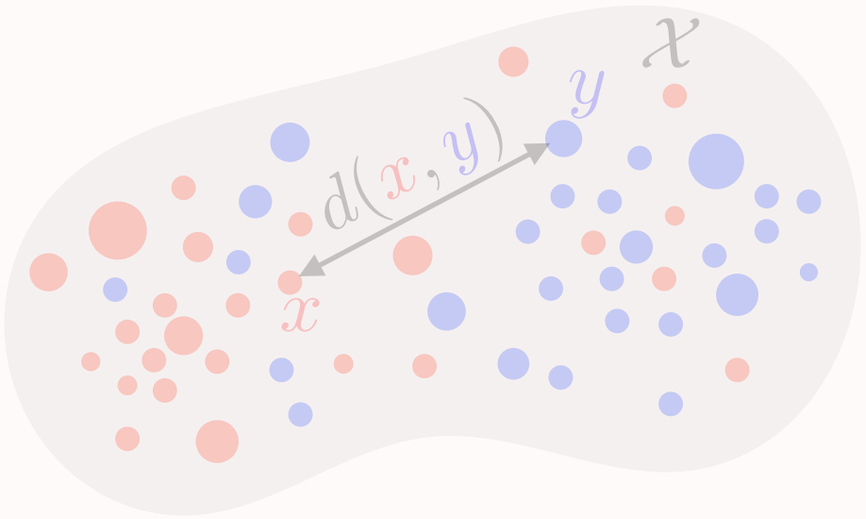
GPU

Matrix-matrix

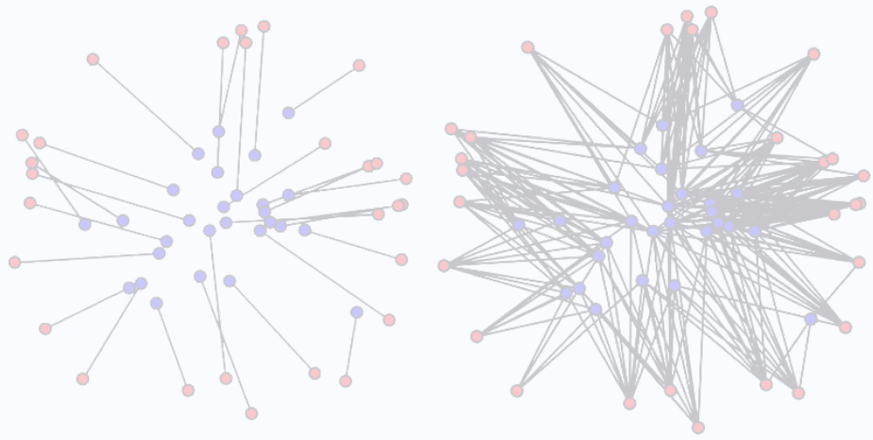


$\rightarrow$ Convolution on regular grids, separable kernels.

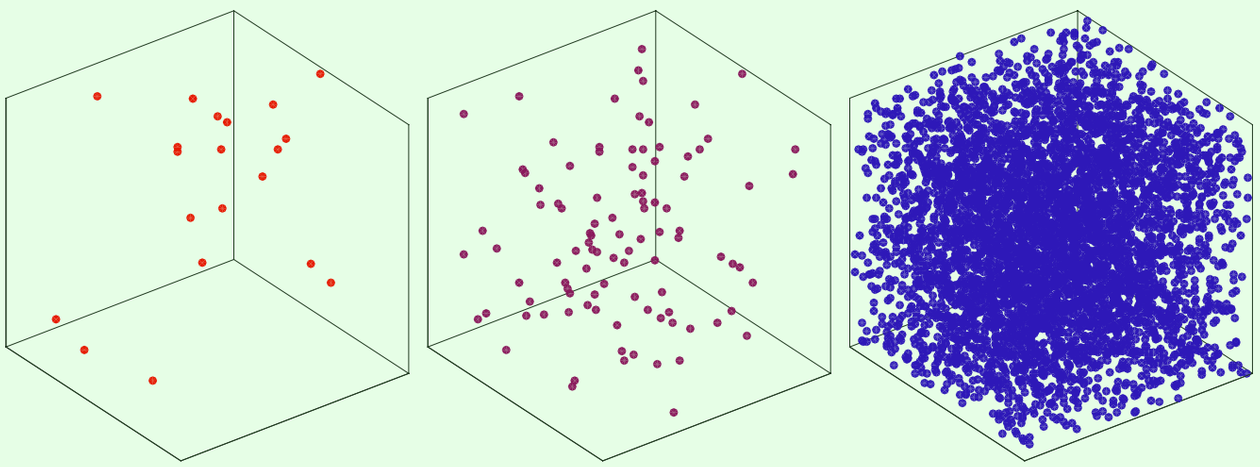
1. Optimal Transport



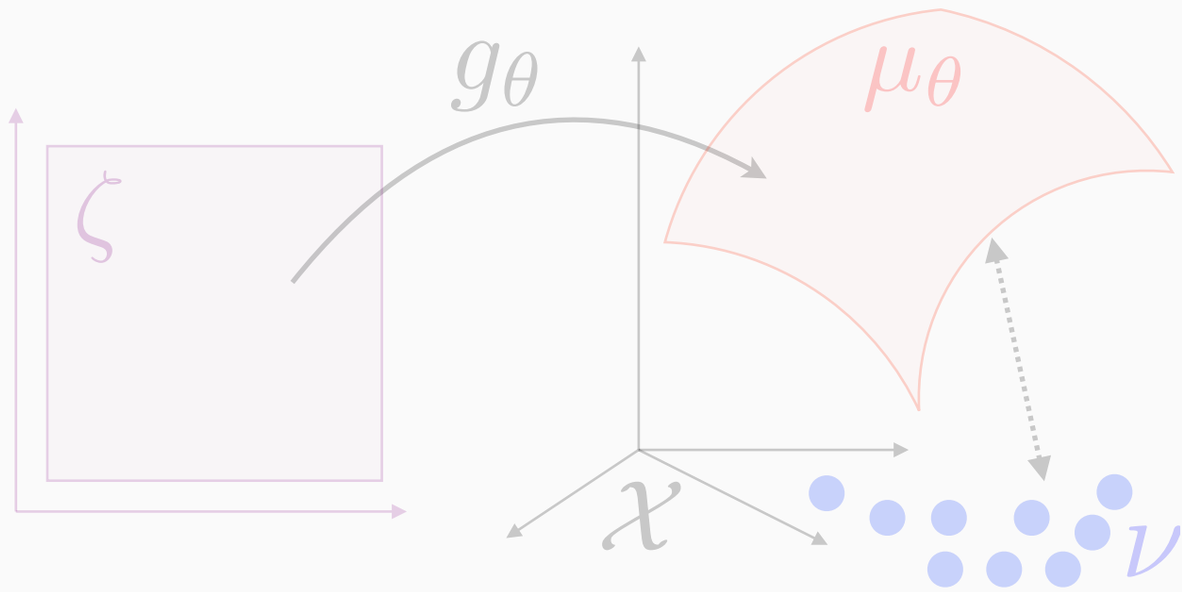
2. Entropic Regularization



3. Sinkhorn Divergences



4. Application to Generative Models

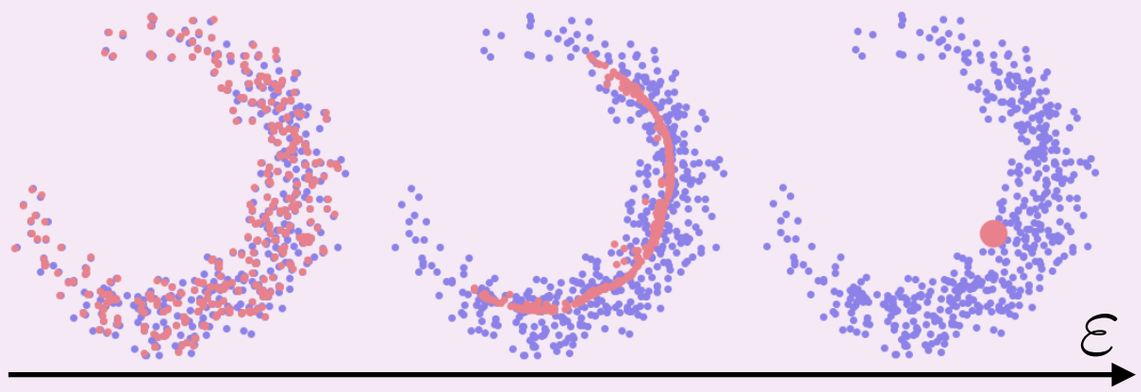


Sinkhorn Divergences

$$\mathrm{W}^p_{\varepsilon,p}(\alpha,\beta) \overset{\text{def.}}{=} \min_{\pi_1=\alpha,\pi_2=\beta} \int_{\mathcal{X}^2} d^p(x,y)\mathrm{d}\pi(x,y) + \varepsilon \mathrm{KL}(\pi|\xi)$$

Problem: $\mathrm{W}_\varepsilon(\alpha,\alpha) \neq 0$

$$\min_{\alpha} \mathrm{W}^p_{\varepsilon,p}(\alpha,\beta)$$



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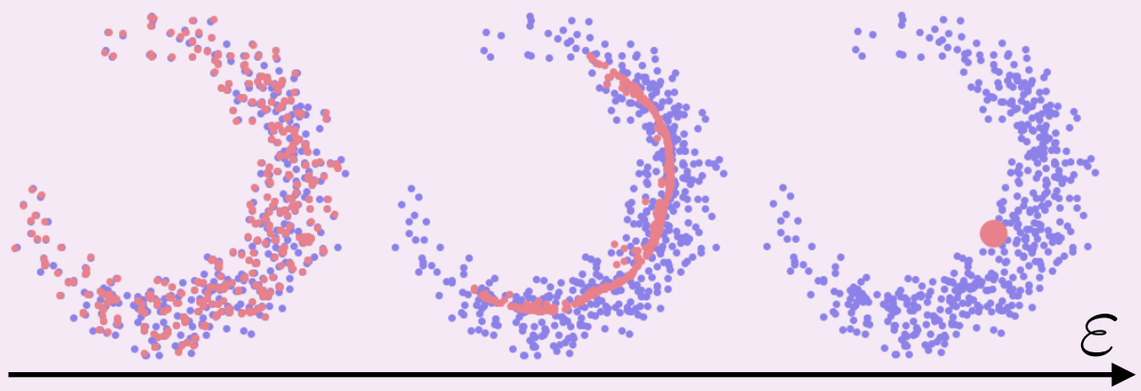

$$\overline{\mathrm{W}}^p_{p,\varepsilon}(\alpha,\beta) \stackrel{\text{def.}}{=} \mathrm{W}^p_{p,\varepsilon}(\alpha,\beta) - \tfrac{1}{2}\mathrm{W}^p_{p,\varepsilon}(\alpha,\alpha) - \tfrac{1}{2}\mathrm{W}^p_{p,\varepsilon}(\beta,\beta)$$

[Ramdas, García Trillos, Cuturi, 2017]

Sinkhorn Divergences

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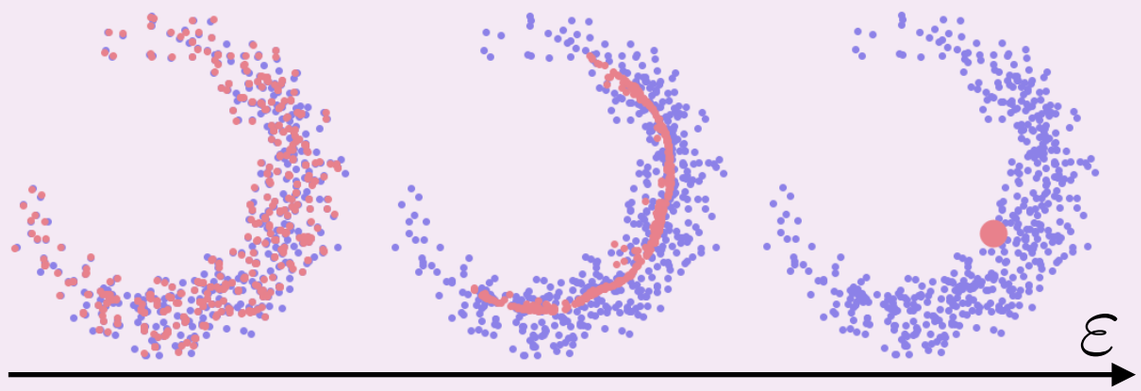

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[Ramdas, García Trillos, Cuturi, 2017]

Theorem: $\mathrm{W}^p_p(\alpha,\beta) \xleftarrow{\varepsilon \to 0} \overline{\mathrm{W}}^p_{\varepsilon,p}(\alpha,\beta) \xrightarrow{\varepsilon \to +\infty} \|\alpha-\beta\|^2_{-d^p}$

[Léonard 2012] [Carlier et al 2017]

[Ramdas, García Trillos, Cuturi, 2017]

Kernel norms (MMD): $\|\xi\|^2_{-d^p} \stackrel{\text{def.}}{=} -\int_{\mathcal{X}^2} d(x,y)^p \mathrm{d}\xi(x)\mathrm{d}\xi(y)$

Proposition: $\|\cdot\|_{-\|\cdot\|^p}$ is a norm for $0 < p < 2$.

Sinkhorn Divergences

$$\overline{\mathrm{W}}^p_{p,\varepsilon}(\alpha,\beta) \overset{\text{def.}}{=} \mathrm{W}^p_{p,\varepsilon}(\alpha,\beta) - \tfrac{1}{2}\mathrm{W}^p_{p,\varepsilon}(\alpha,\alpha) - \tfrac{1}{2}\mathrm{W}^p_{p,\varepsilon}(\beta,\beta)$$

concave (under $\mathrm{W}^p_{p,\varepsilon}(\alpha,\alpha)$) concave (under $\mathrm{W}^p_{p,\varepsilon}(\beta,\beta)$)

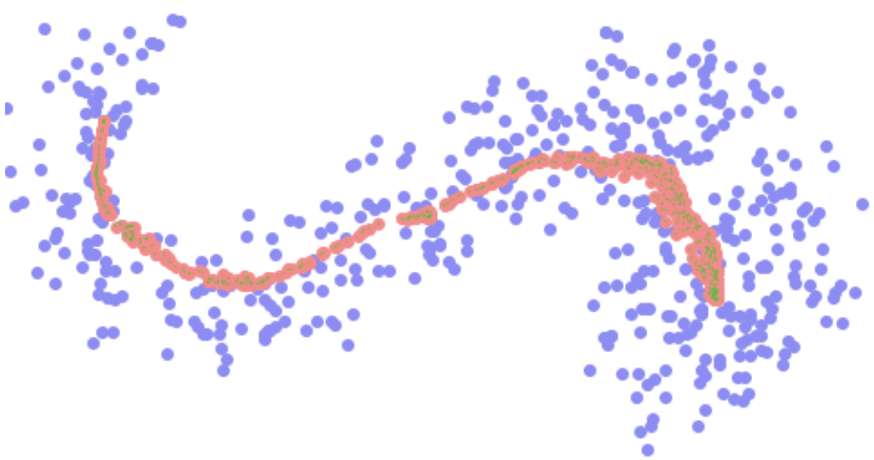
Theorem: [Feydy, Séjourné, P, Vialard, Trouvé, Amari 2018]

If $e^{-\frac{d^p}{\varepsilon}}$ is positive:

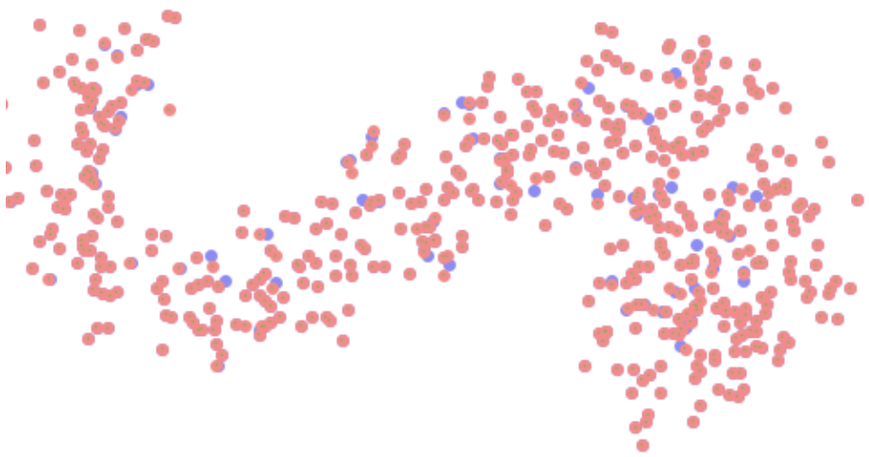
$$\overline{\mathrm{W}}_{\varepsilon,p} \geqslant 0 \text{ and } \overline{\mathrm{W}}^p_{\varepsilon,p}(\cdot,\beta) \text{ is convex.}$$

$$\overline{\mathrm{W}}_{\varepsilon,p}(\alpha_n,\beta) \to 0 \iff \alpha_n \overset{\text{weak}*}{\rightharpoonup} \beta$$

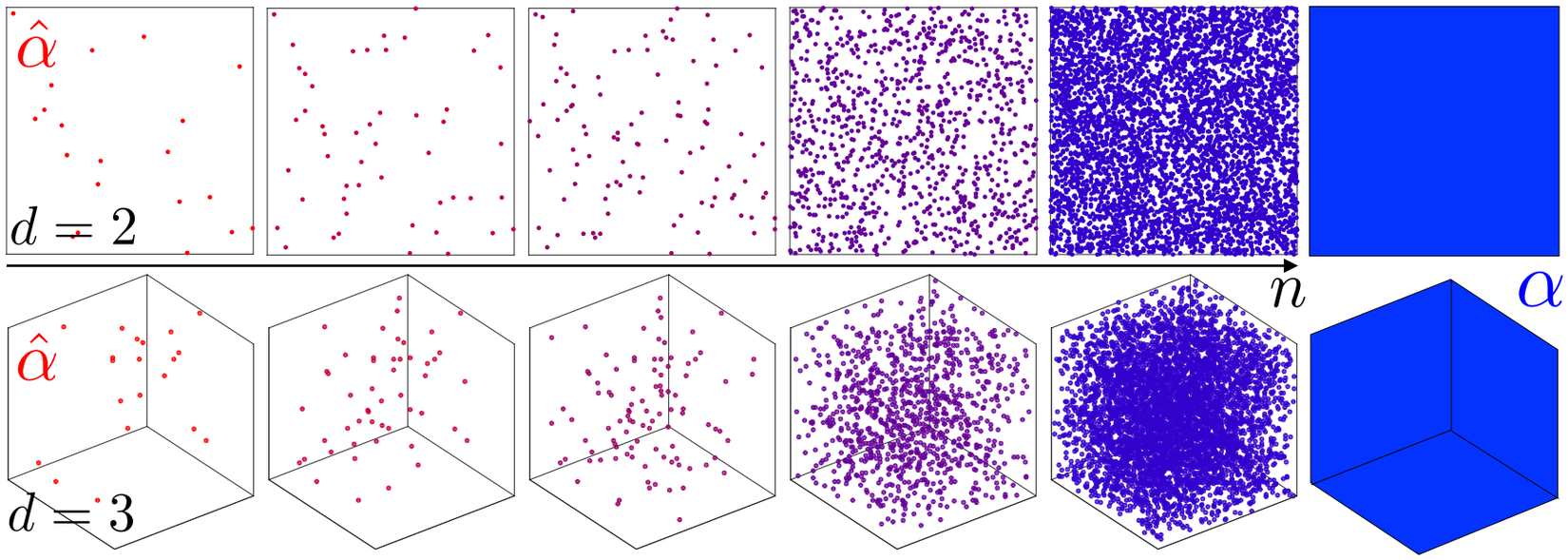
$\min_\alpha \mathrm{W}^p_{\varepsilon,p}(\alpha,\beta)$

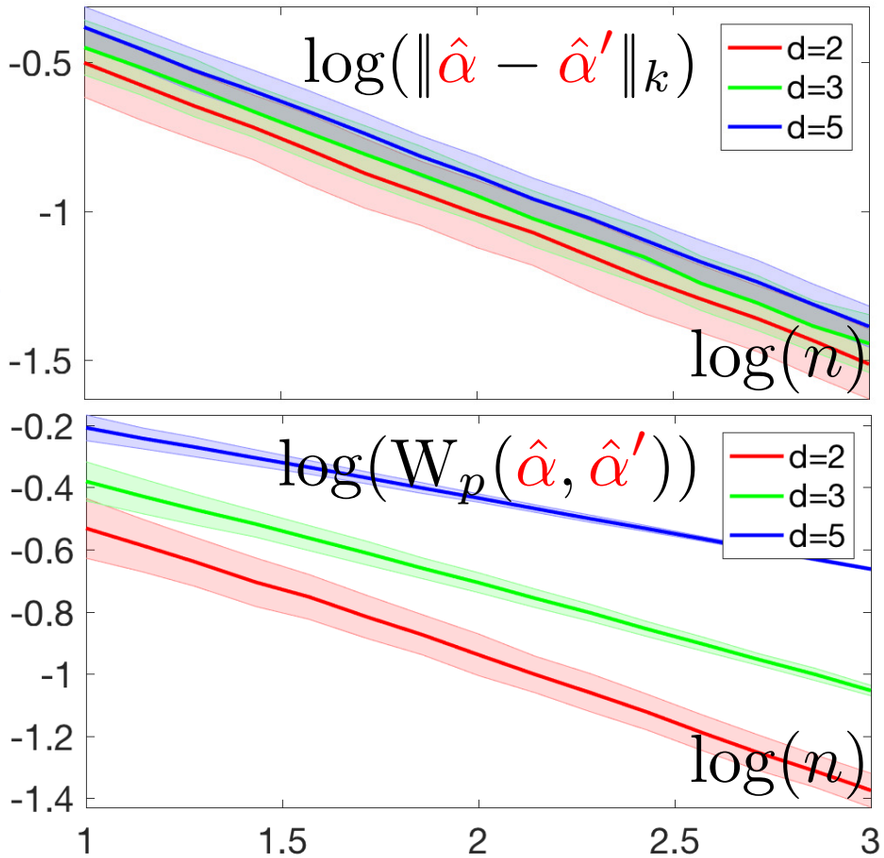


$\min_\alpha \overline{\mathrm{W}}^p_{\varepsilon,p}(\alpha,\beta)$



Sample Complexity





Theorem:

$$\mathbb{E}(|\mathrm{W}_p(\hat{\alpha}, \hat{\beta}) - \mathrm{W}_p(\alpha, \beta)|) = O(n^{-\frac{1}{d}})$$

$$\mathbb{E}(|\|\hat{\alpha} - \hat{\beta}\|_k - \|\alpha - \beta\|_k|) = O(n^{-\frac{1}{2}})$$

Optimal transport: suffers from curse of dimensionality.

$\rightarrow$ Adapt to support dimensionality [Weed, Bach 2017]

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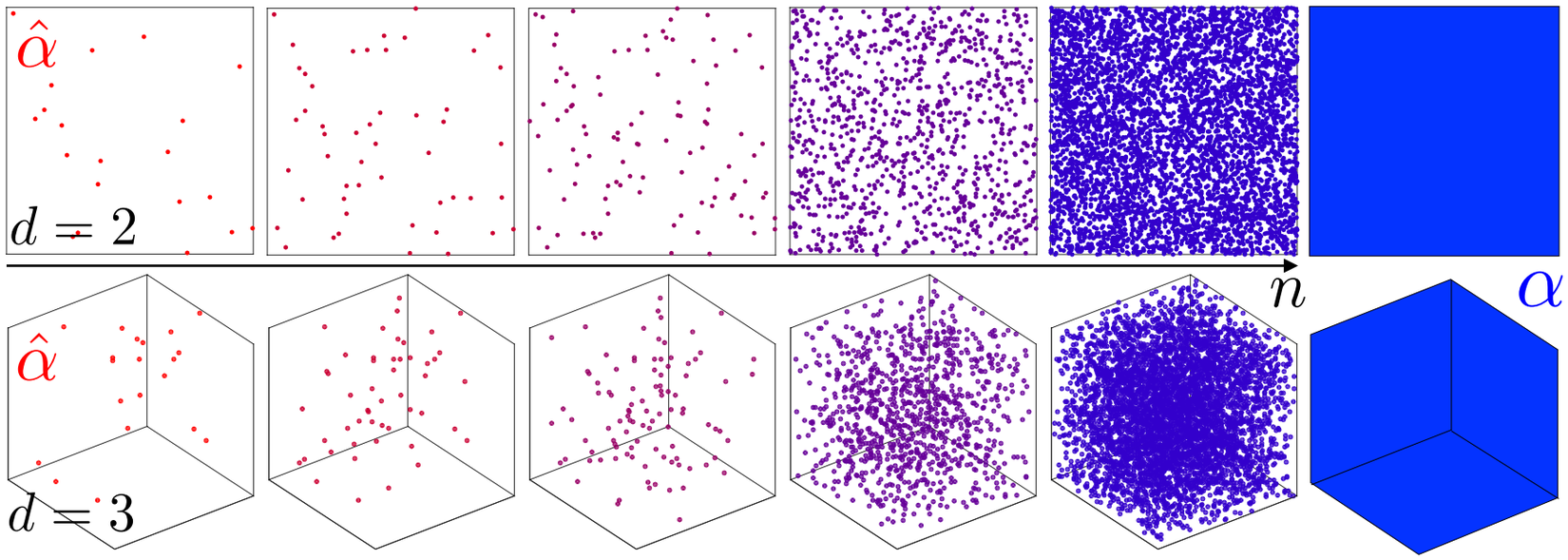

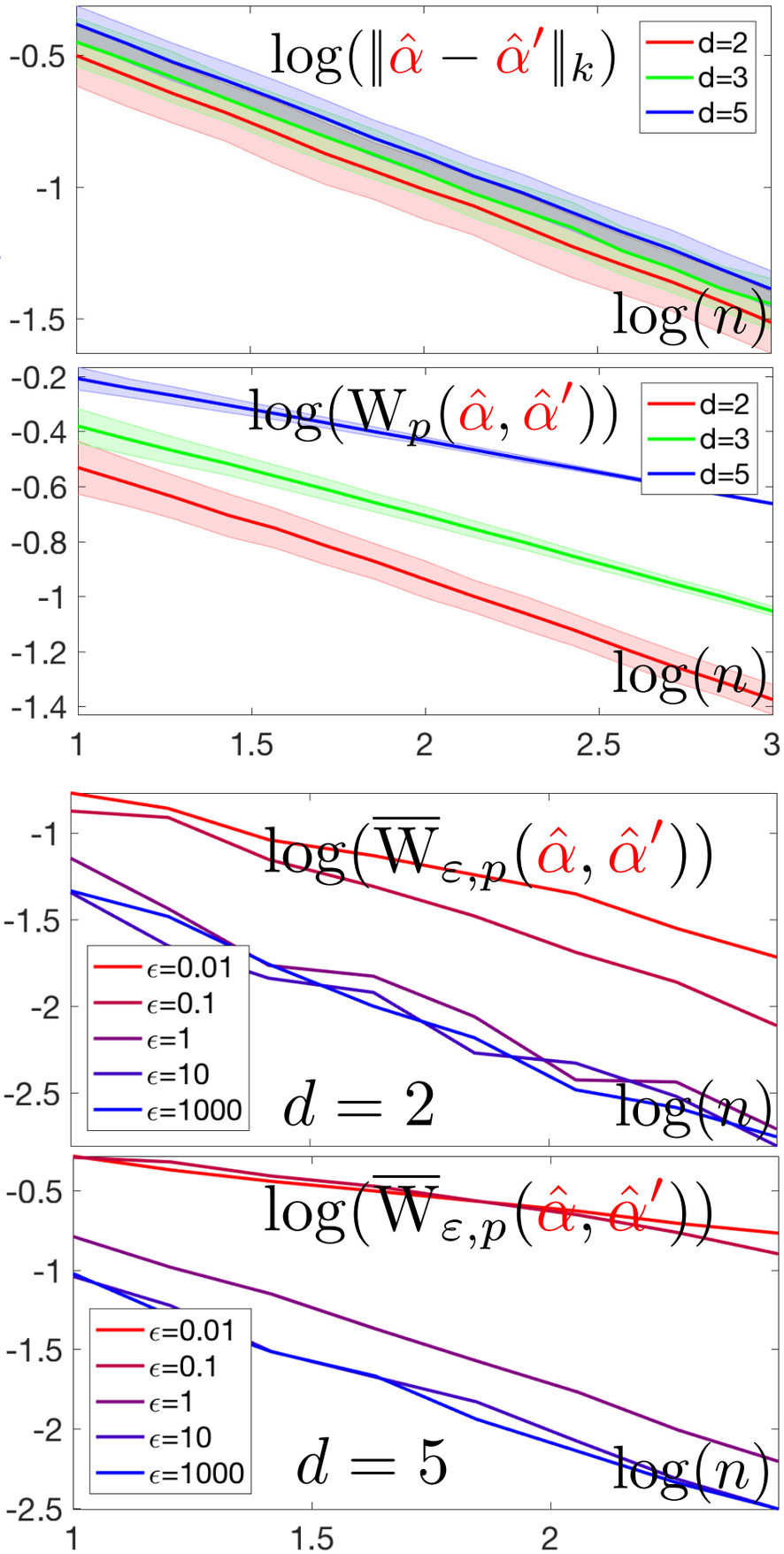

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Theorem: [Genevay, Bach, P, Cuturi]

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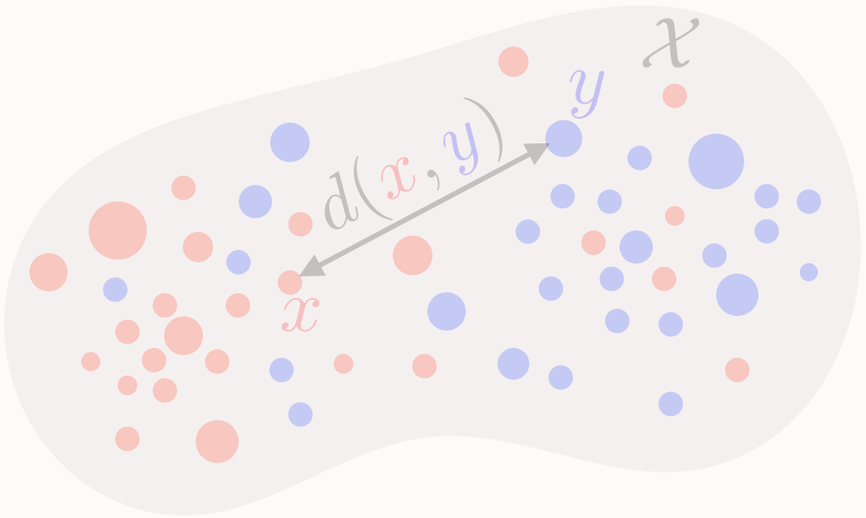

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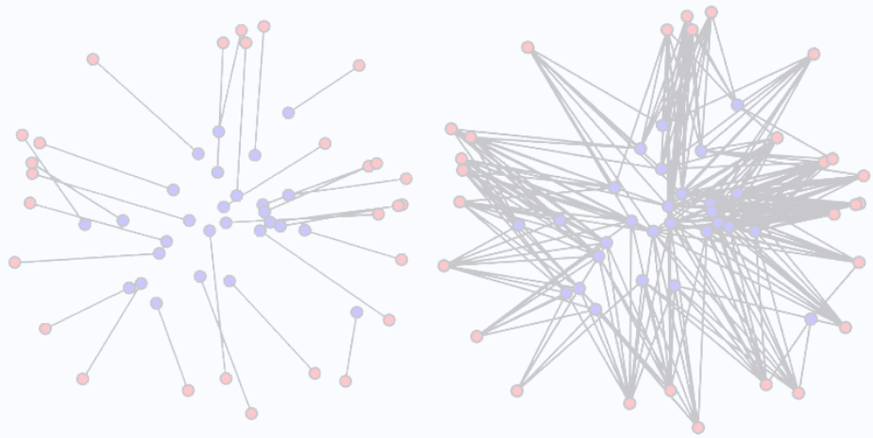

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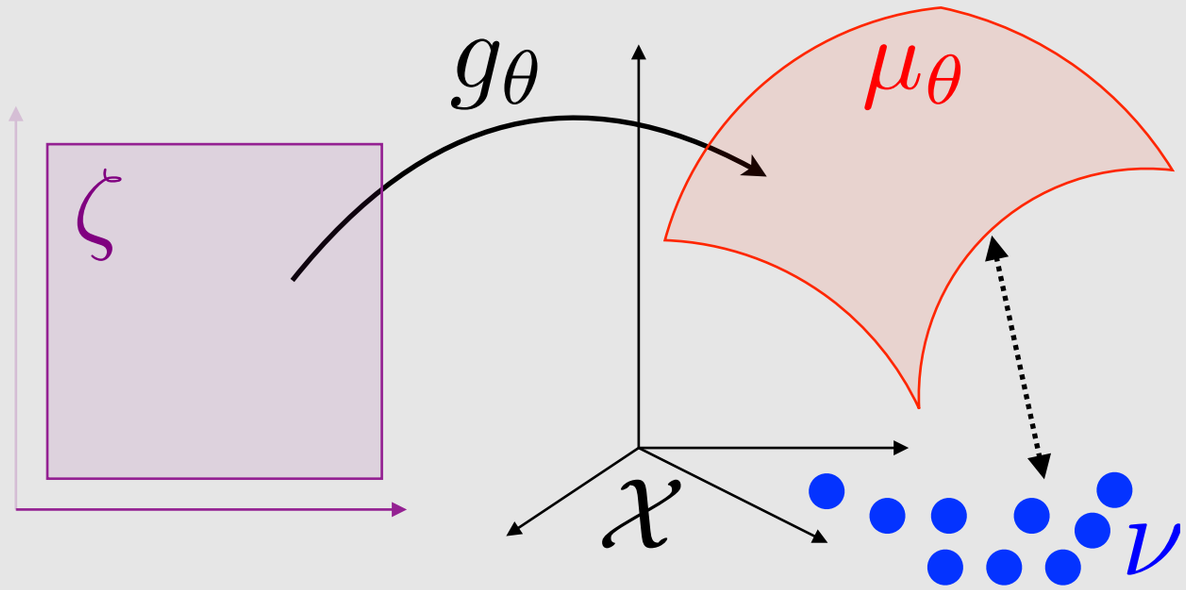
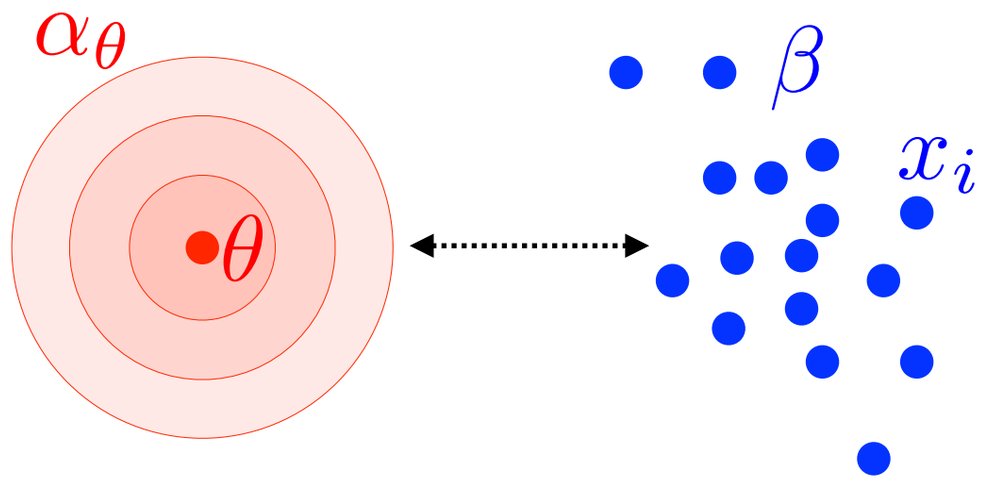


Density Fitting and Generative Models

$$\textit{Observations: } \beta \overset{\text{def.}}{=} \frac{1}{n}\sum_{i=1}^{n} \delta_{x_i}$$

$$\textit{Parametric model: } \theta \mapsto \alpha_\theta$$



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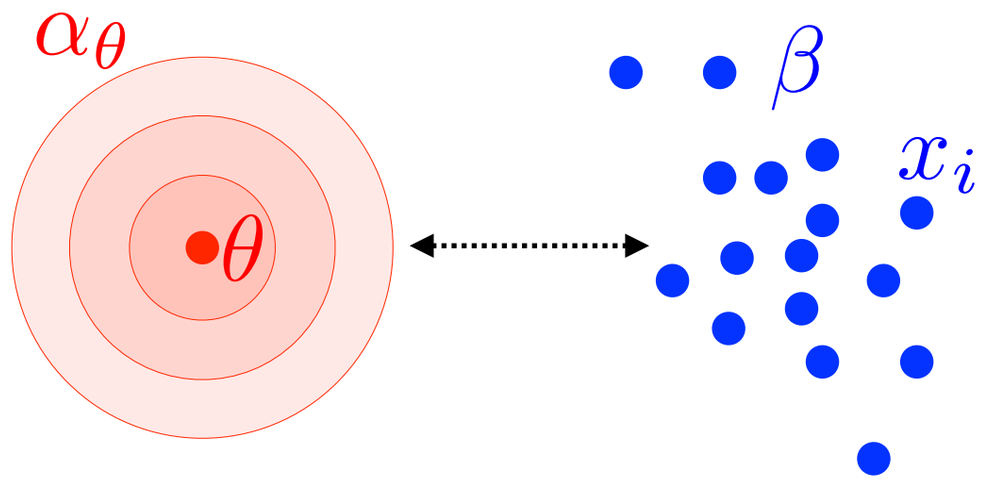

Density fitting: $\mathrm{d}\alpha_\theta(x) = \rho_\theta(x)\mathrm{d}x$

$$\min_\theta \widehat{\mathrm{KL}}(\alpha_\theta|\beta) \overset{\text{def.}}{=} -\sum_i \log(\rho_\theta(x_i))$$

Maximum likelihood (MLE)

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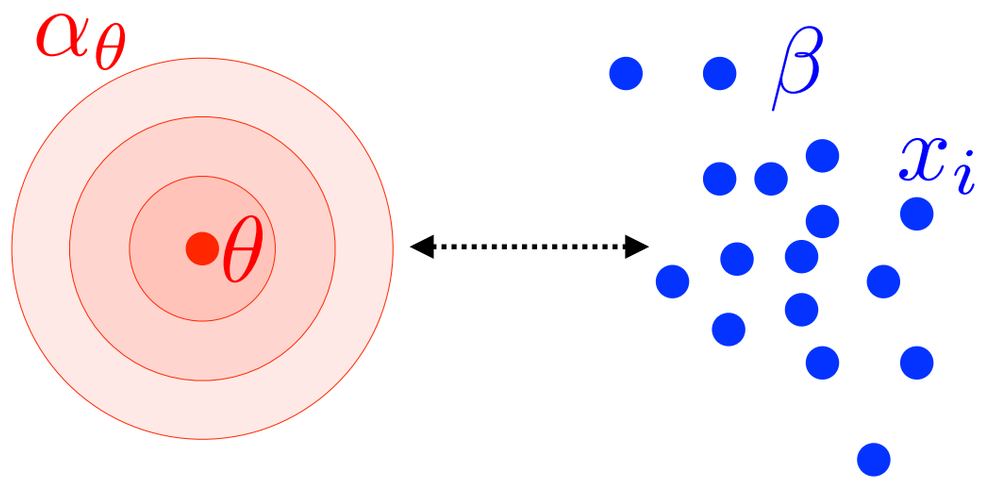

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Maximum likelihood (MLE)

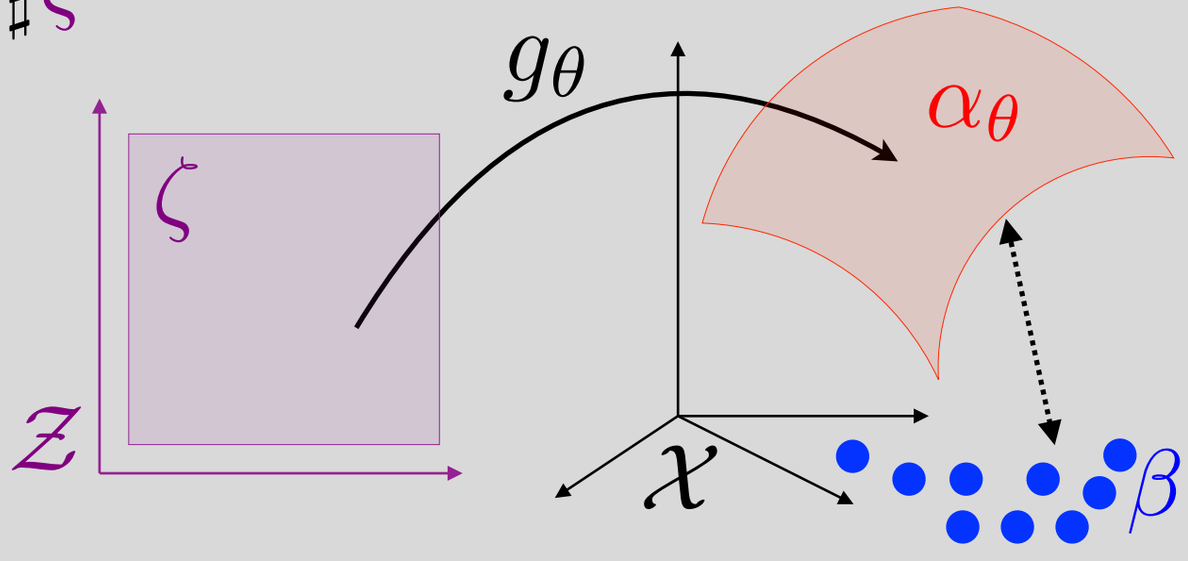
Generative model fit: $\alpha_\theta = g_{\theta,\sharp}\zeta$

$$\widehat{\mathrm{KL}}(\alpha_\theta|\beta) = +\infty$$

$\rightarrow$ MLE undefined.

$\rightarrow$ Need a weaker metric.

$$\min_\theta \overline{\mathrm{W}}^p_{\varepsilon,p}(\alpha_\theta, \beta)$$

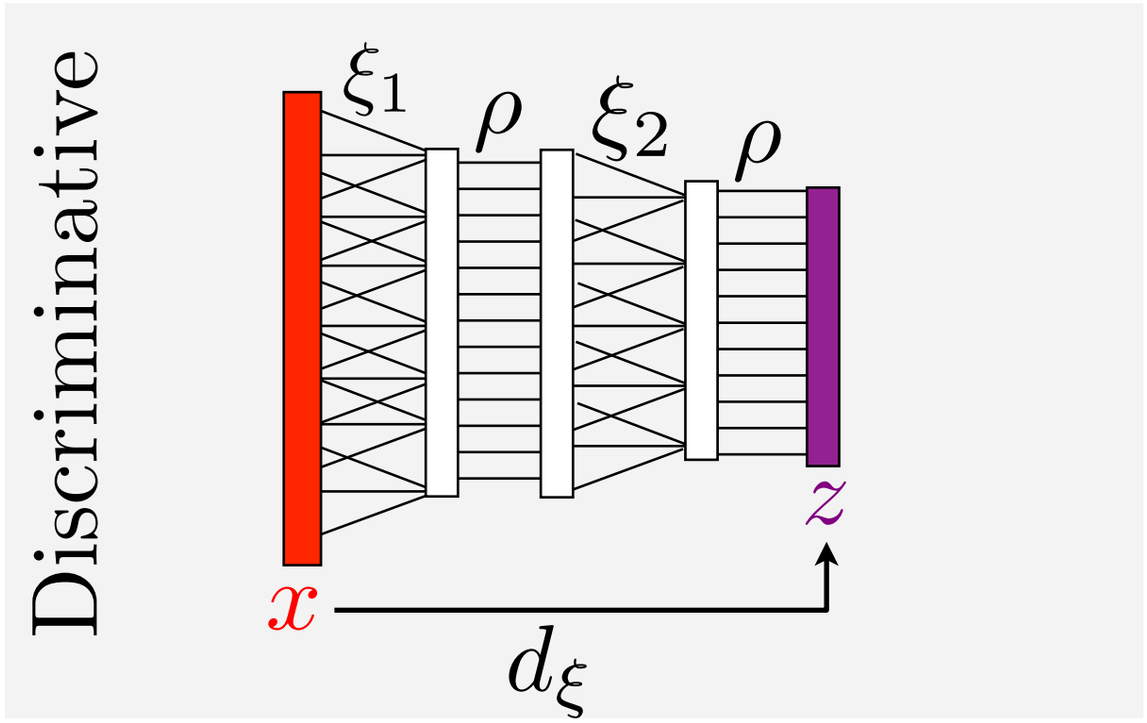


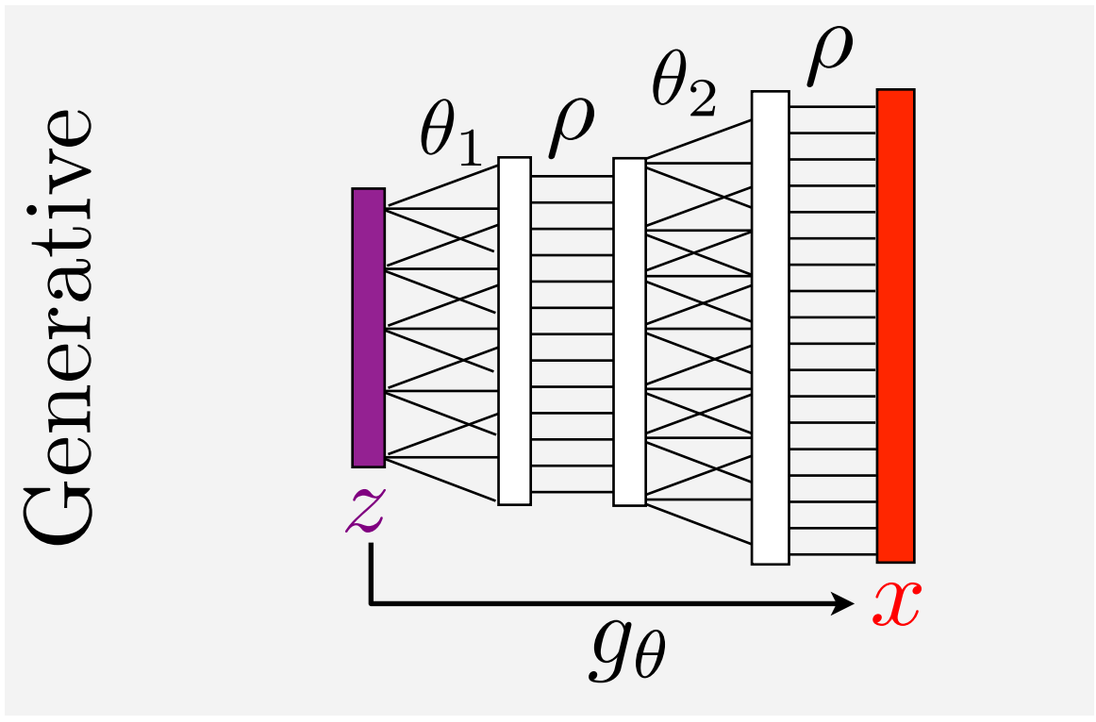
Deep Discriminative vs Generative Models

Deep networks:

$$d_\xi(x) = \rho(\xi_K(\dots\rho(\xi_2(\rho(\xi_1(x)\dots)$$

$$g_\theta(z) = \rho(\theta_K(\dots\rho(\theta_2(\rho(\theta_1(z)\dots)$$





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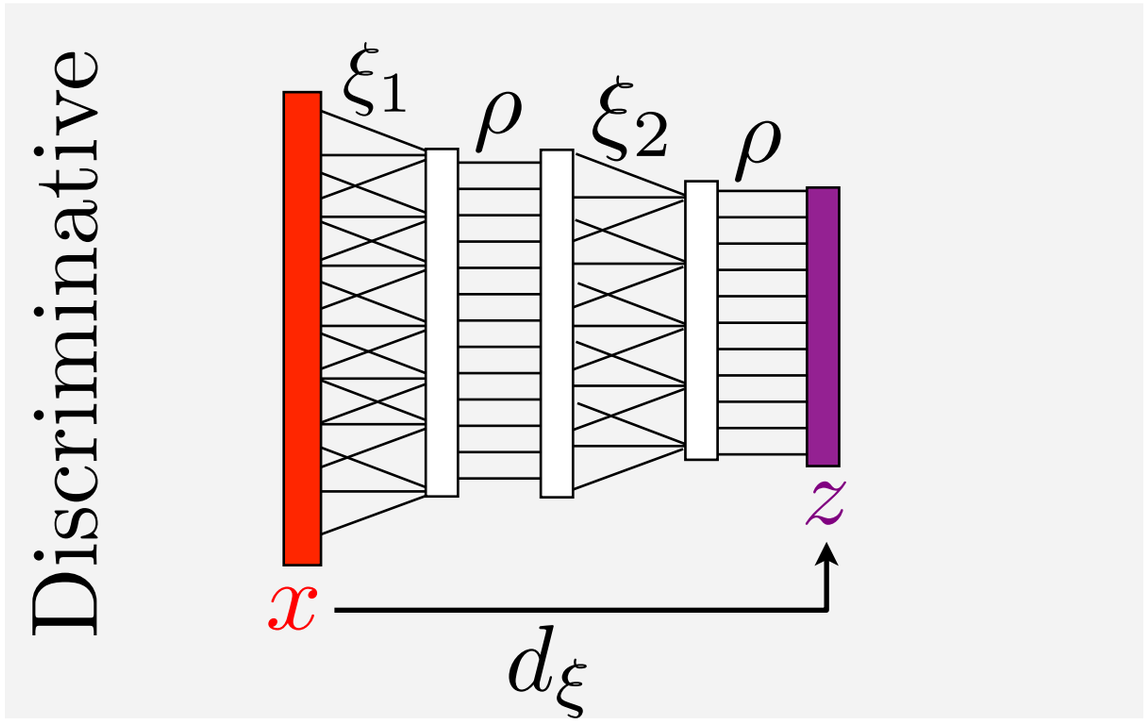
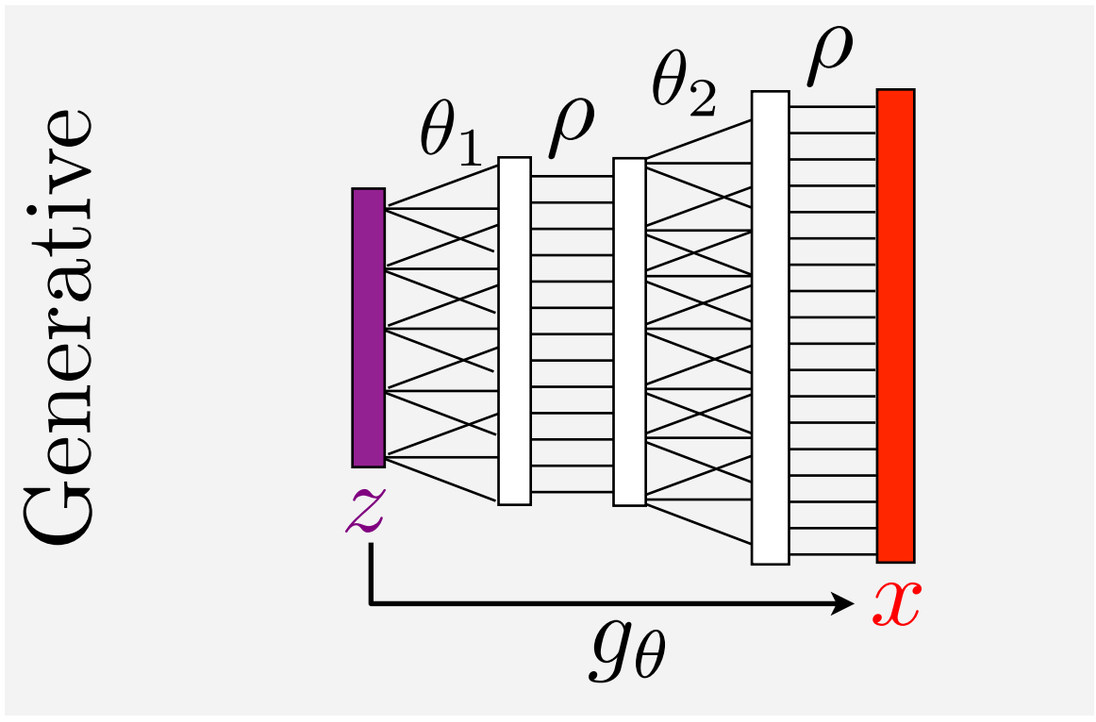
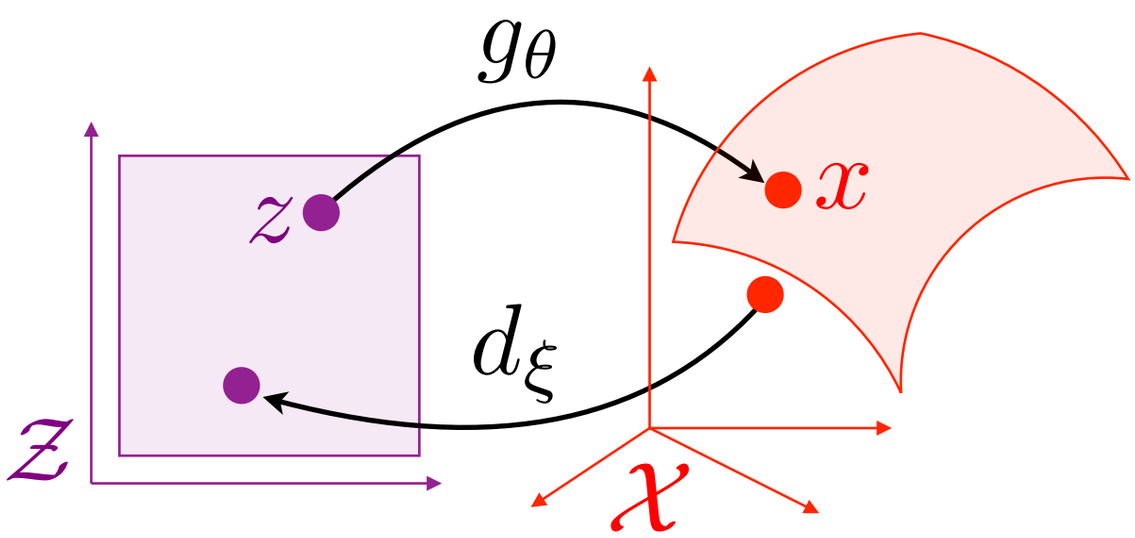
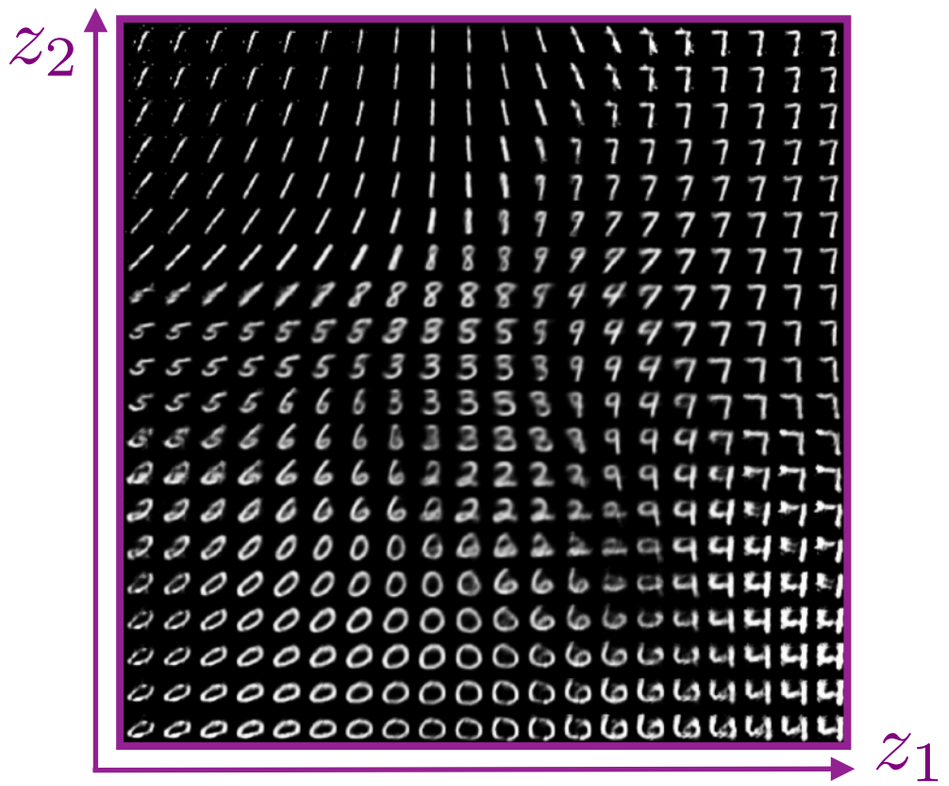
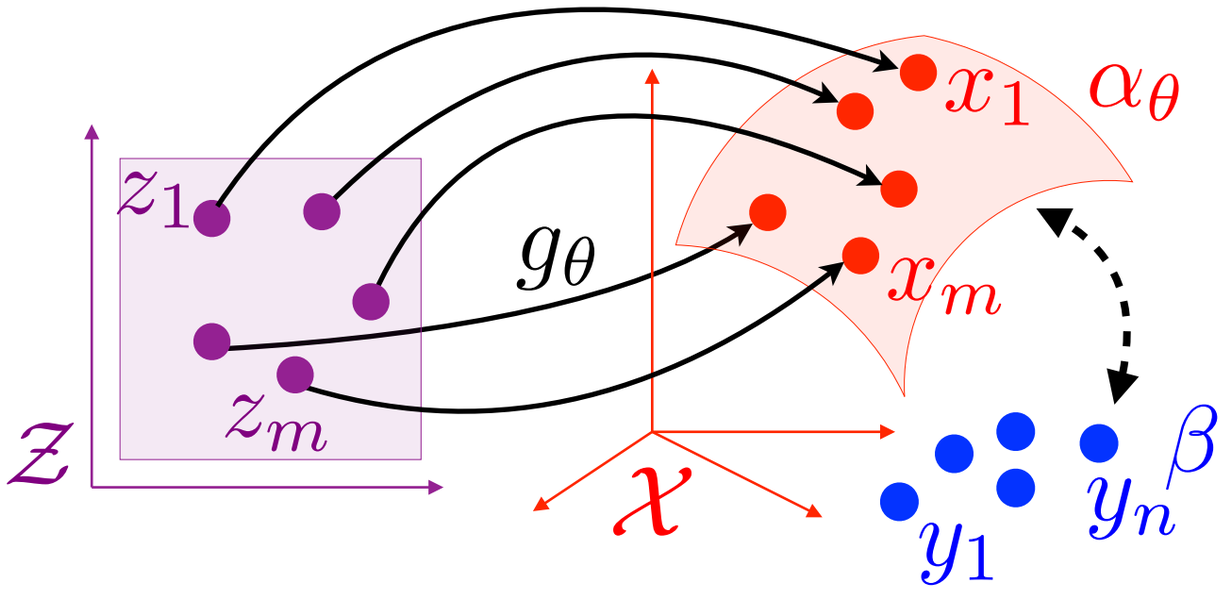








Training Architecture



$$\min_\theta \mathcal{E}(\theta) \overset{\text{def.}}{=} \overline{\mathrm{W}}^p_{\varepsilon,p}(\alpha_\theta, \beta)$$

Stochastic gradient descent

$$\theta \leftarrow \theta - \tau \nabla \hat{\mathcal{E}}(\theta)$$

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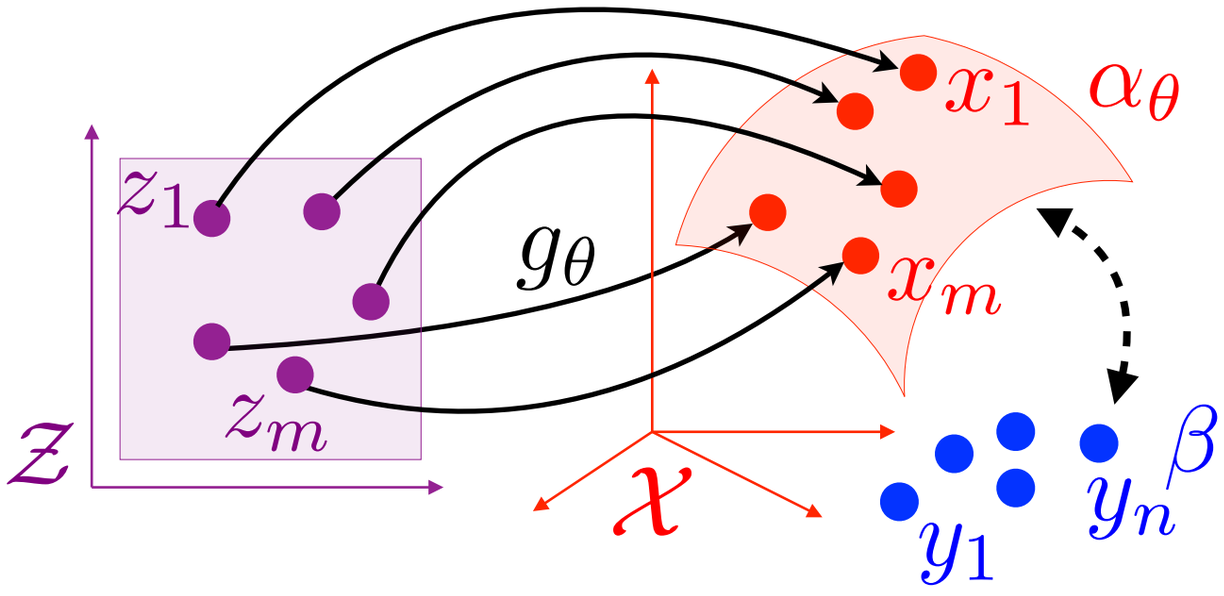

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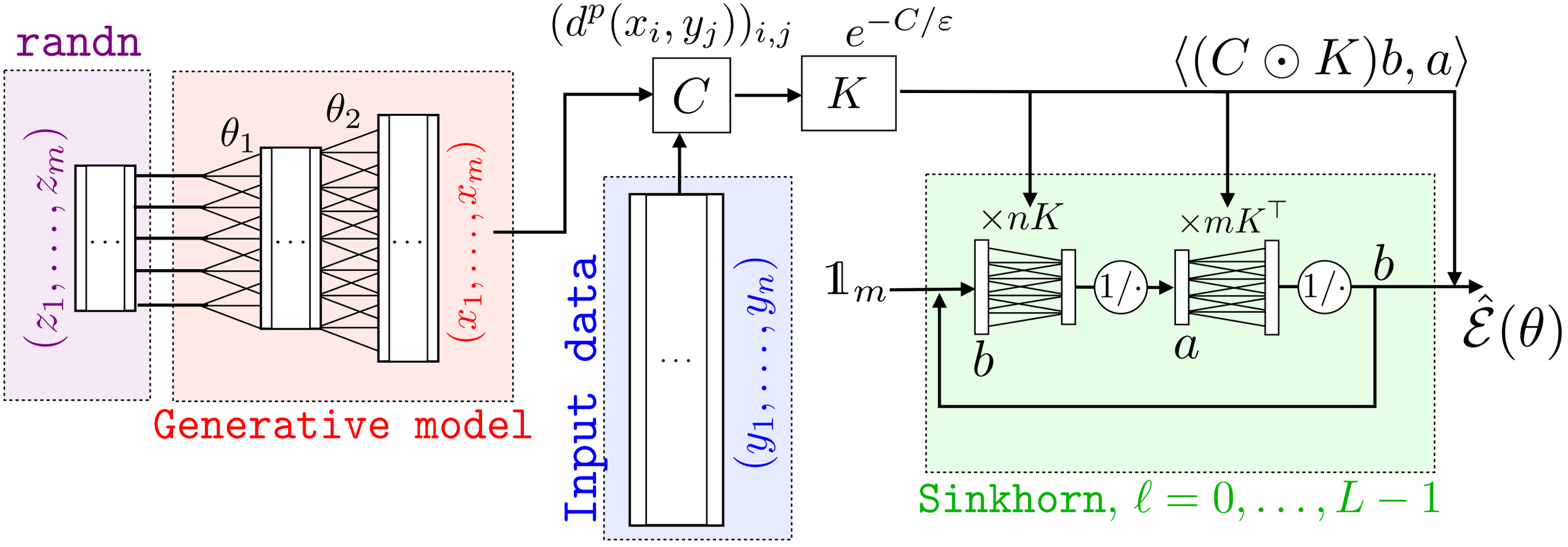
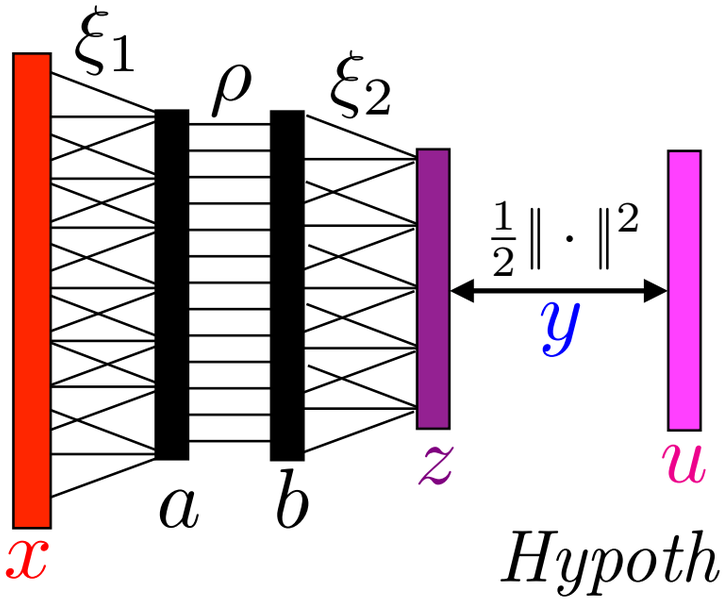


Automatic Differentiation

Setup: $\mathcal{E} : \mathbb{R}^n \to \mathbb{R}$ computable in K operations.




```
function y = E(x)
 a = xi1*x
 b = rho(a)
 z = xi2*b
 y = 1/2*norm(z-u)^2
```

Hypothesis: elementary operations $(a \times b, \log(a), \sqrt{a} \ldots)$ and their derivatives cost $O(1)$.

Question: What is the complexity of computing $\nabla\mathcal{E} : \mathbb{R}^n \to \mathbb{R}^n$?

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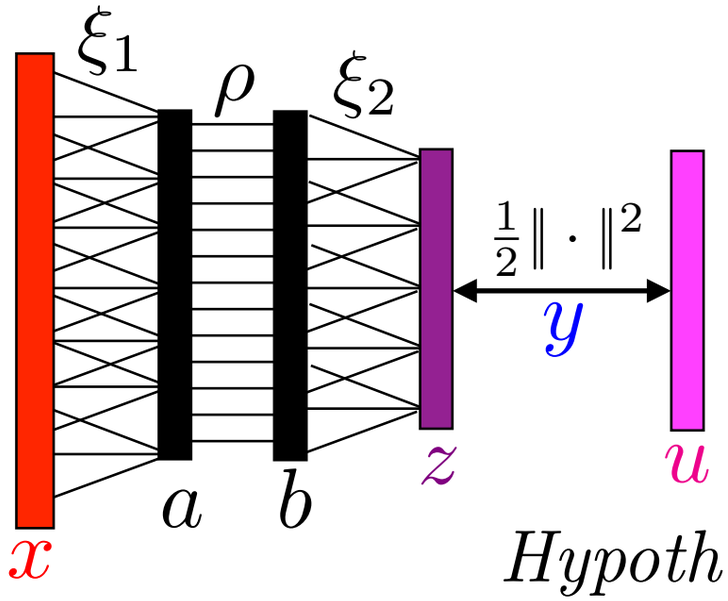


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Finite differences: $\nabla\mathcal{E}(\theta) \approx \frac{1}{\varepsilon}(\mathcal{E}(\theta + \varepsilon\delta_1) - \mathcal{E}(\theta), \ldots \mathcal{E}(\theta + \varepsilon\delta_n) - \mathcal{E}(\theta))$

$K(n+1)$ operations, intractable for large n.

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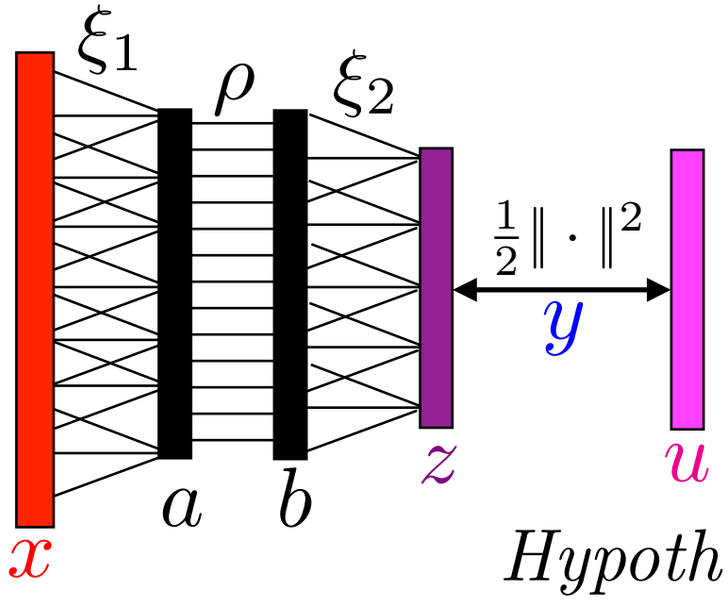


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```

```
function dx = nablaE(x)
 dz = z-u
 db = xi2'*dz
 da = diag(dphi(a)) * db
 dx = xi1'*da
```

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$K(n+1)$ operations, intractable for large n.

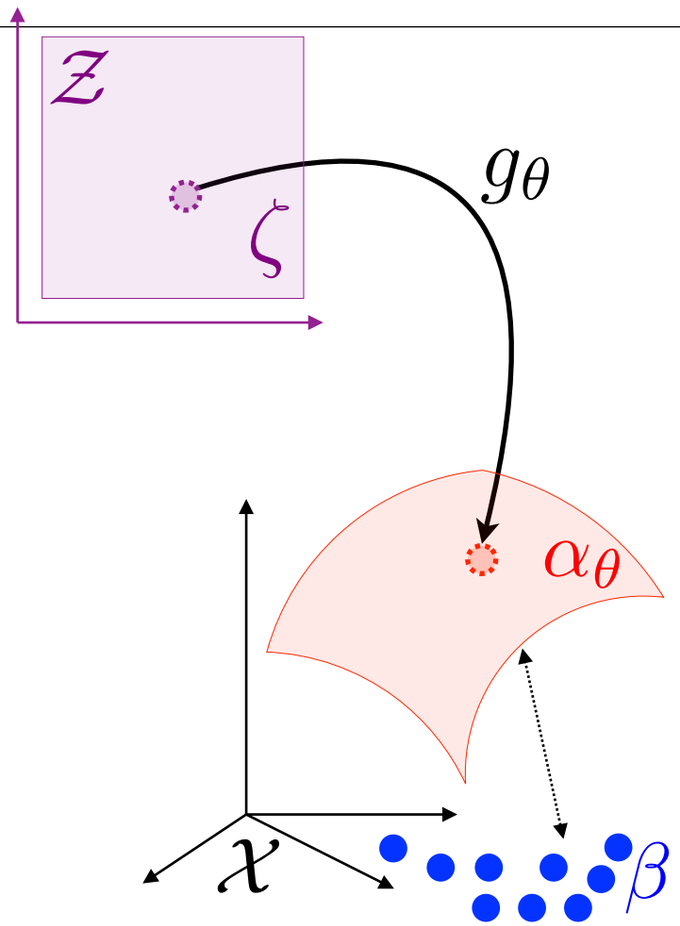
Theorem: there is an algorithm to compute $\nabla\mathcal{E}$ in $O(K)$ operations. [Seppo Linnainmaa, 1970]

This algorithm is reverse mode automatic differentiation

Examples of Images Generation

Inputs β

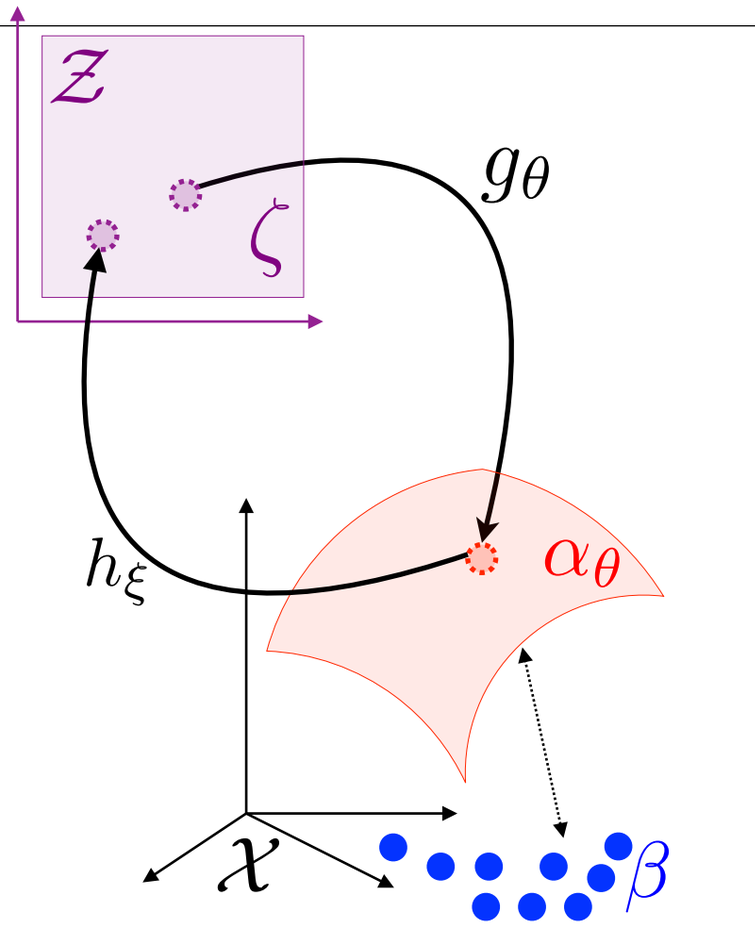
Generated α_θ

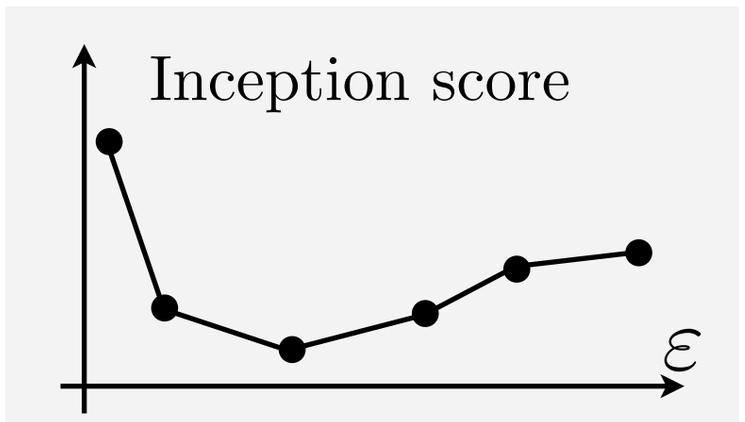


Examples of Images Generation

Inputs β

Generated α_θ



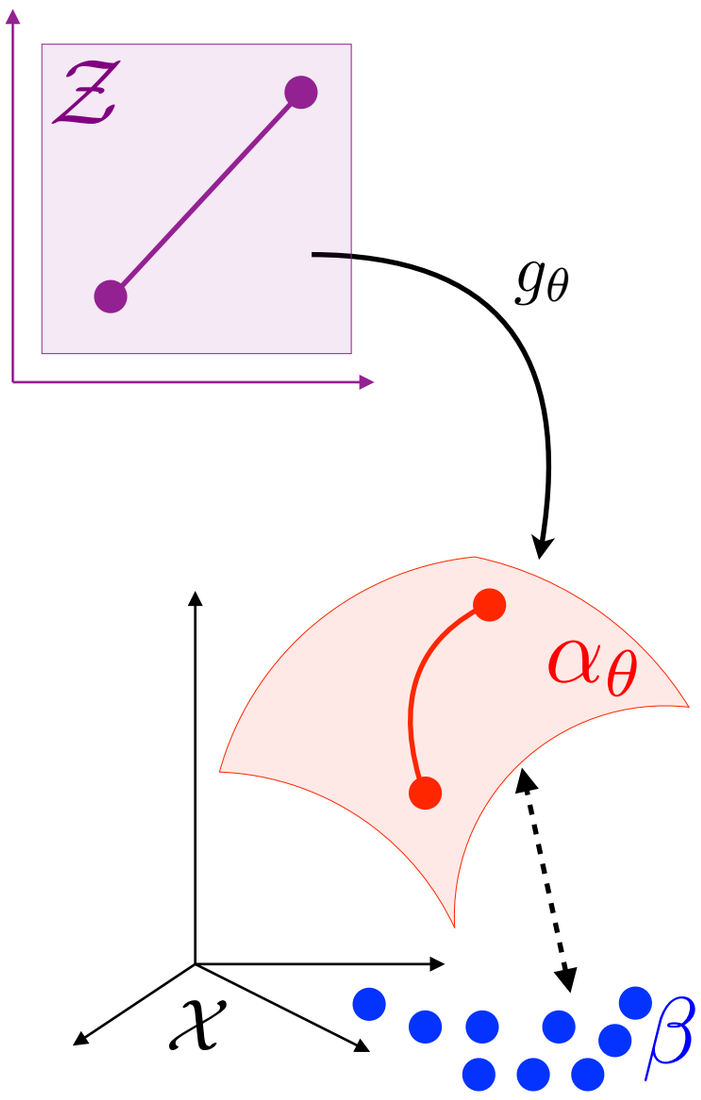


$\rightarrow$ Need to learn the metric $d(x, y) = \|h_\xi(x) - h_\xi(y)\|$ (GANs)

$\rightarrow$ Influence of ε?

$\rightarrow$ Performance evaluation of generative models is an open problem.

Generative Adversarial Networks



Progressive Growing of GANs for Improved Quality, Stability, and Variation
Tero Karras, Timo Aila, Samuli Laine, Jaakko Lehtinen, ICLR 2018

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Open Problems

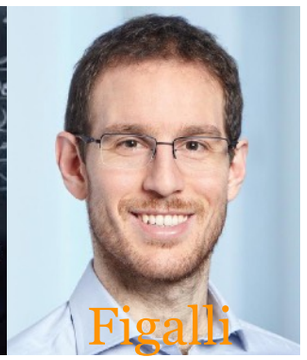

Monge

Kantorovic


Dantzig


Brenier


Villani

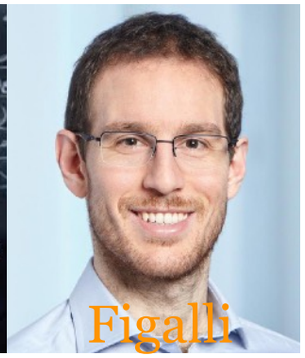

Figalli

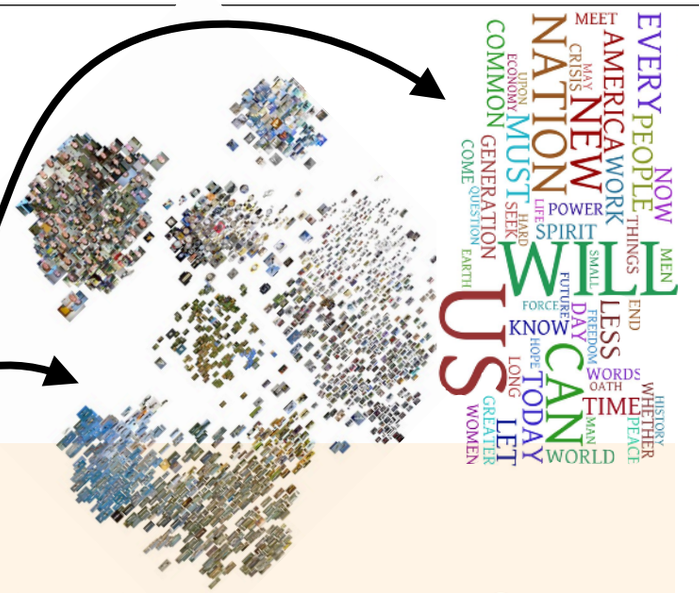
Toward high-dimensional OT:

$\rightarrow$ Scalable geometrical loss functions in high dimension?

$\rightarrow$ Performance quality measures for unsupervised learning?

Open Problems





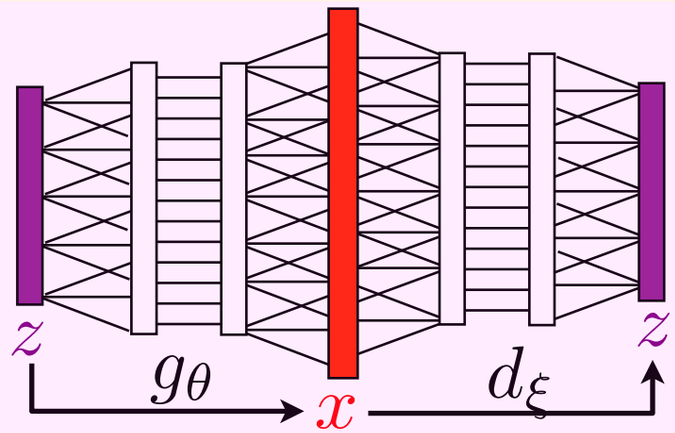
Toward high-dimensional OT:

$\rightarrow$ Scalable geometrical loss functions in high dimension?

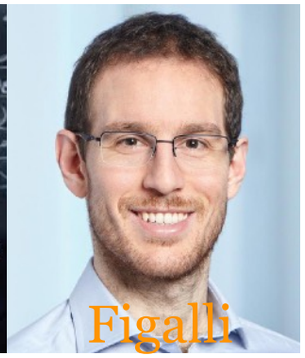
$\rightarrow$ Performance quality measures for unsupervised learning?

Metric learning for OT:

$\rightarrow$ Adversarial training to leverage multi scale priors?



Open Problems



Toward high-dimensional OT:

→ Scalable geometrical loss functions in high dimension?

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Metric learning for OT:

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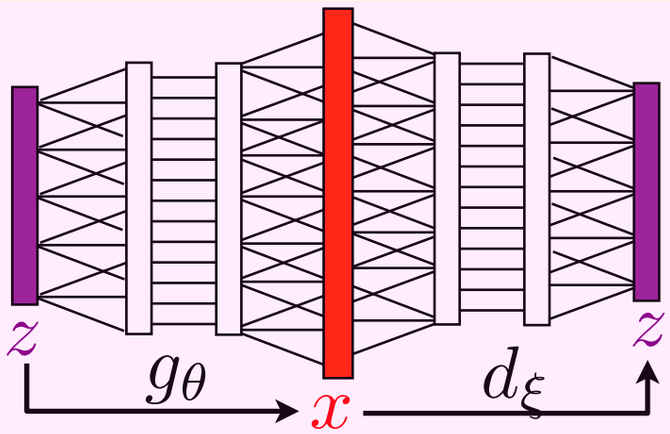

Beyond comparing measures:

→ Learning for surfaces, graphs, metric spaces?

→ Using Gromov-Wasserstein geometry?