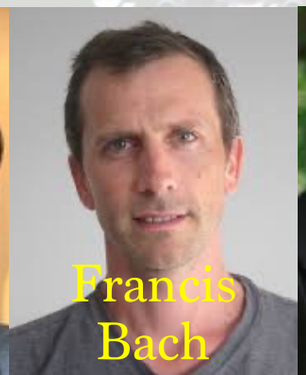
Scaling Optimal Transport to High Dimensional Learning

Gabriel Peyré

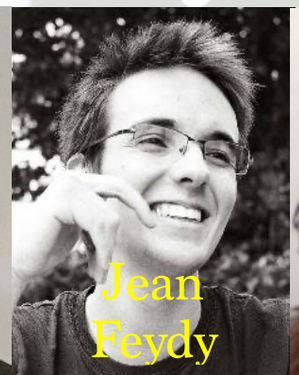
Joint work with:


Shun'ichi Amari

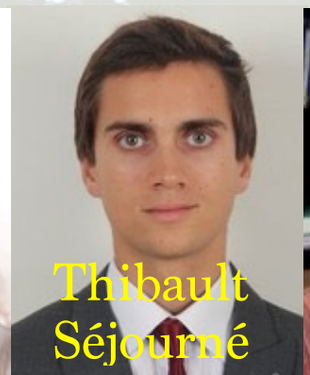

Francis Bach


Lénaic Chizat


Marco Cuturi


Jean Feydy

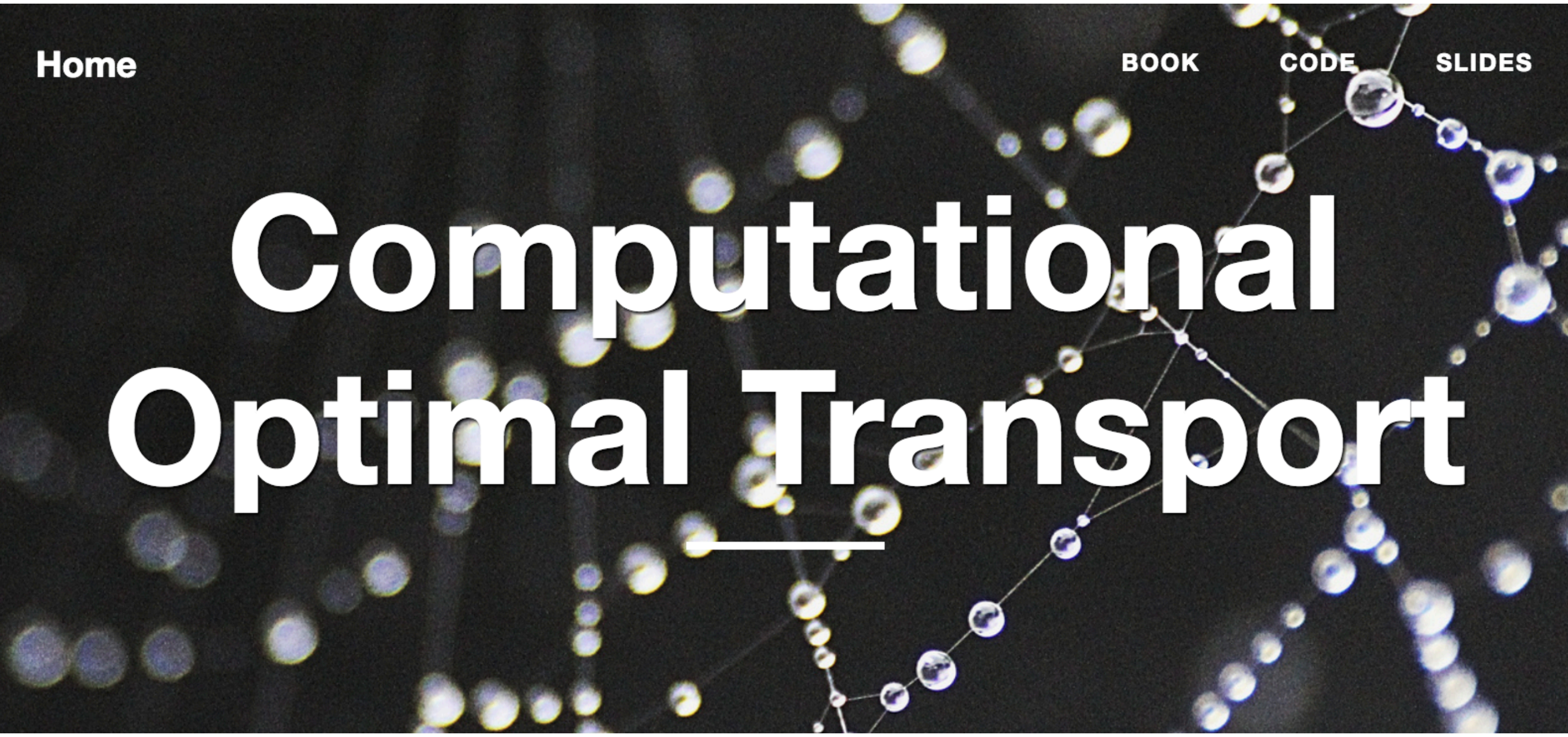

Aude Genevay


Thibault Séjourné


Alain Trouvé


François-Xavier Vialard

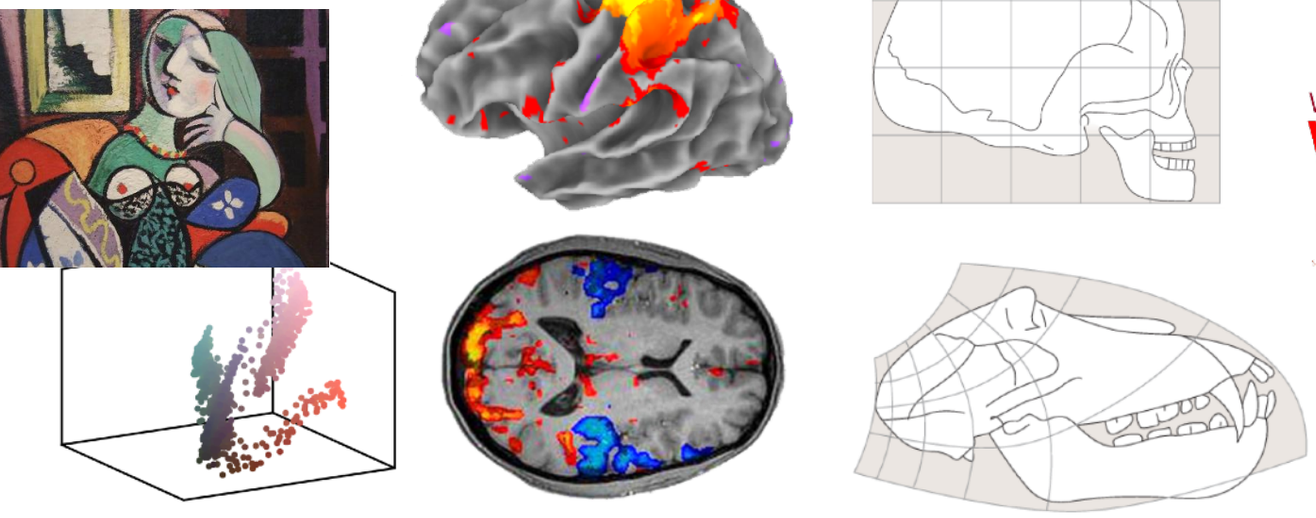
https://optimaltransport.github.io



Probability Distributions in Data Sciences

Probability distributions and histograms

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



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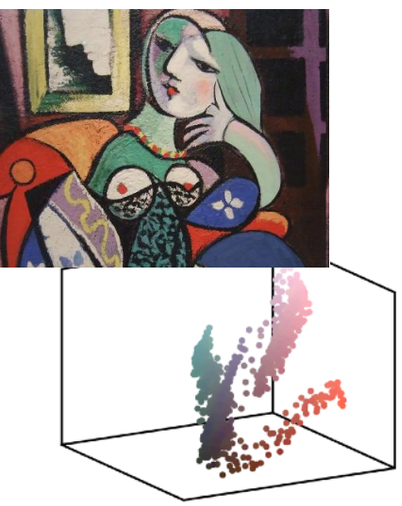
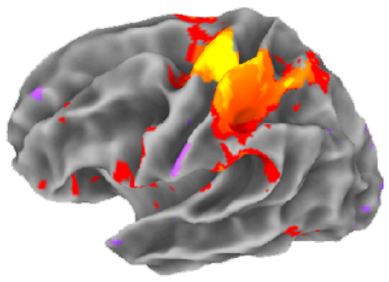
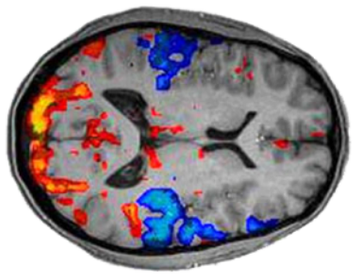
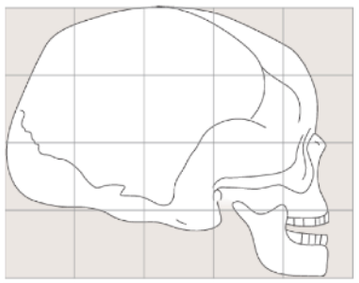
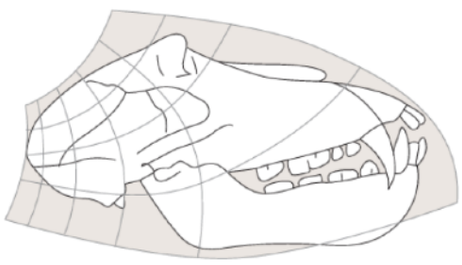
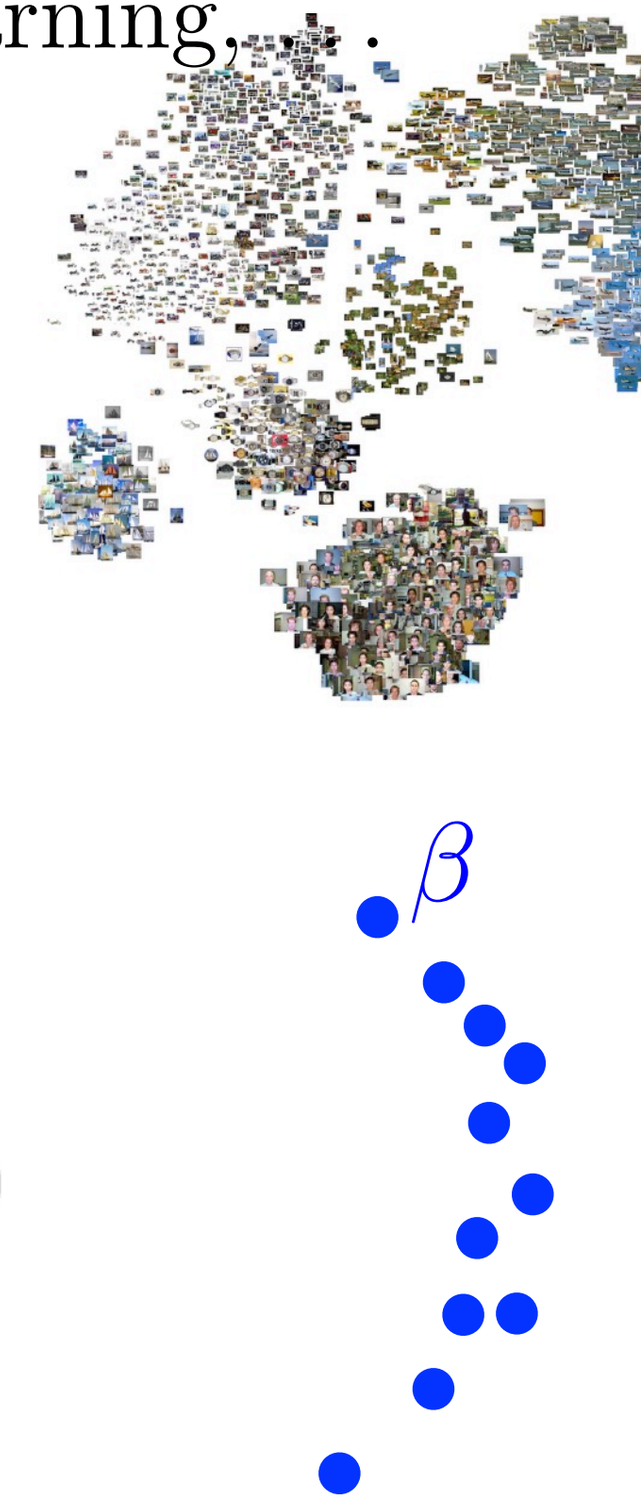








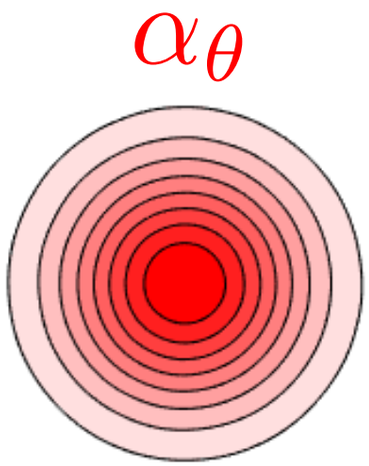




Unsupervised learning

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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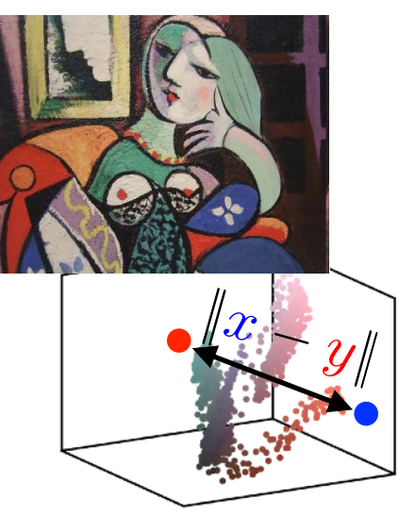

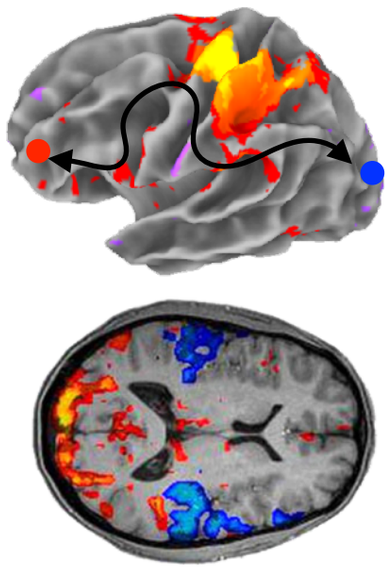

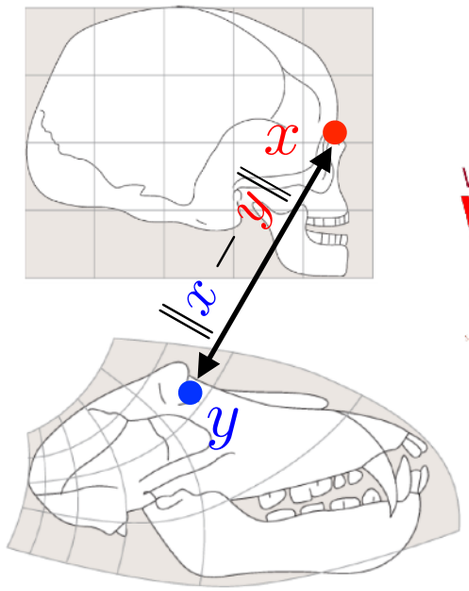

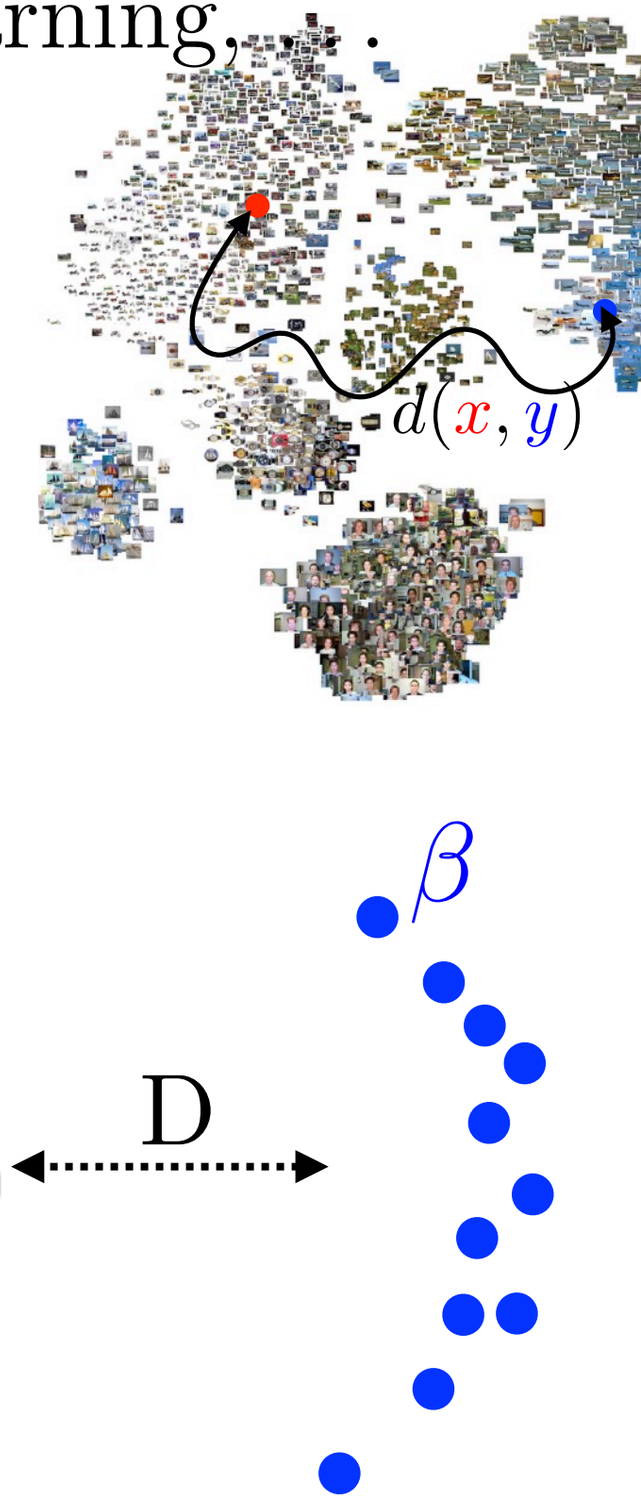

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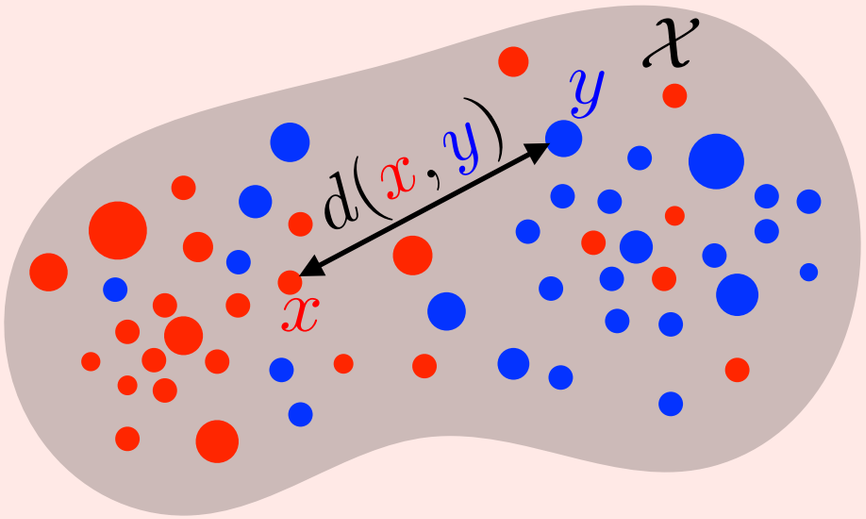
Observations: $\beta \stackrel{\text{def.}}{=} \frac{1}{n} \sum_{i=1}^{n} \delta_{x_i}$

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

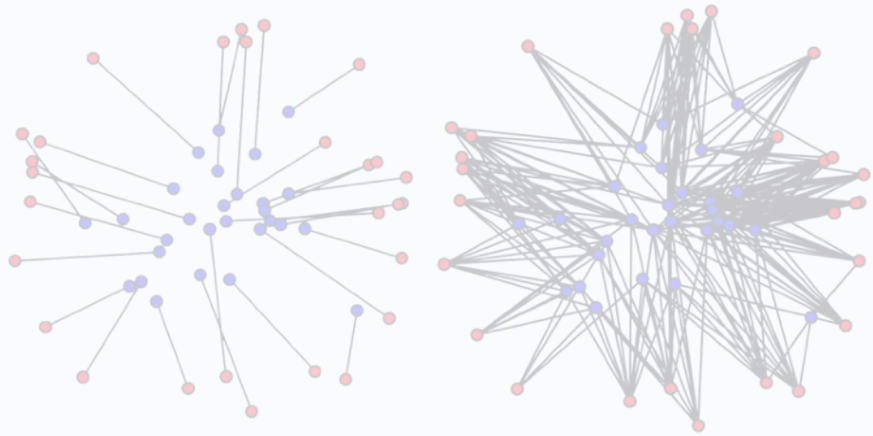
Density fitting: $\min_\theta \mathrm{D}(\alpha_\theta, \beta)$

$\rightarrow$ takes into account a metric d.

1. Optimal Transport

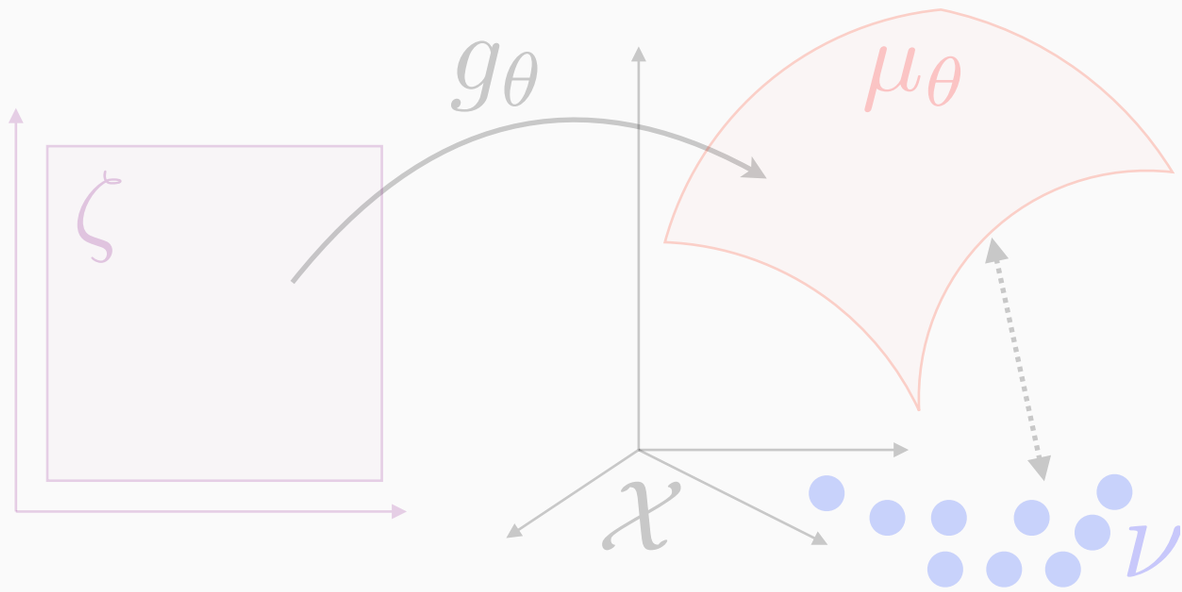


2. Entropic Regularization



3. Sinkhorn Divergences

4. Application to Generative Models

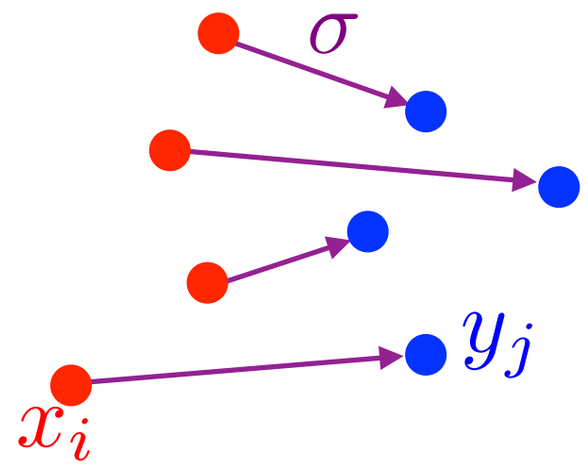


Monge's Problem

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

Permutation:

$$\sigma : \{1, \ldots, n\} \to \{1, \ldots, n\}$$



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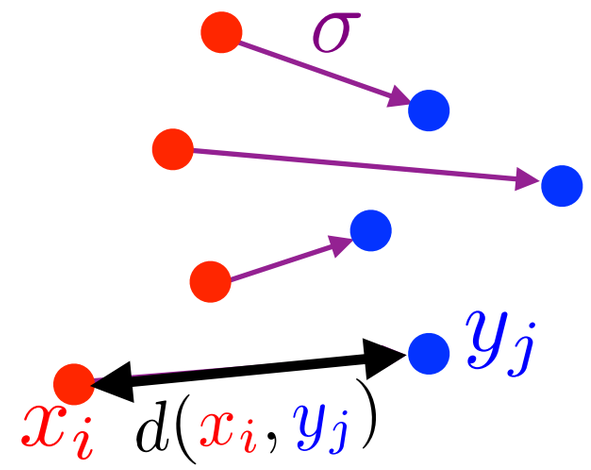

Monge optimal matching: $\min_{\sigma} \sum_{i=1}^{n} d(x_i, y_{\sigma(i)})$

[Monge 1784]

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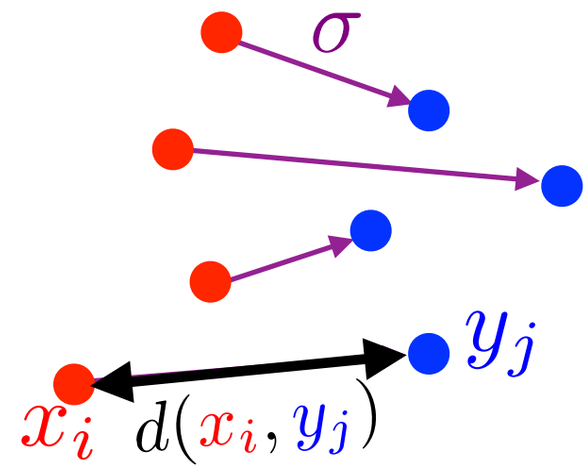

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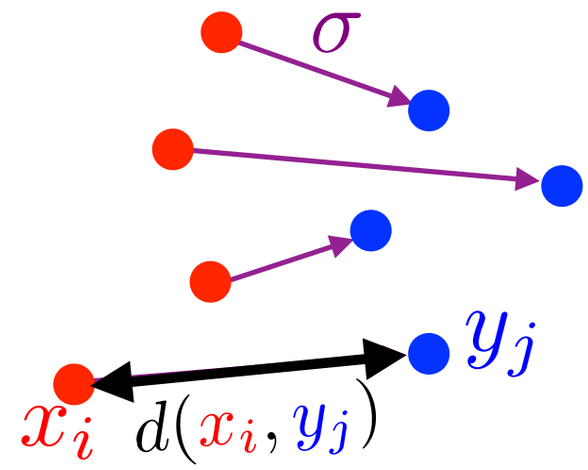

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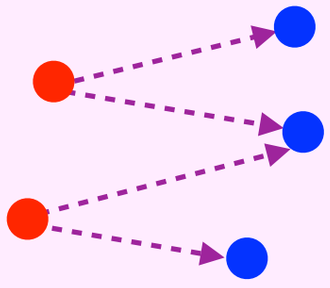
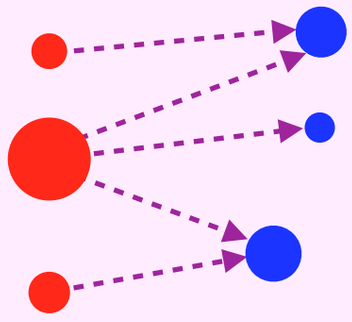


Different # points?



Weights?

Monge's Problem

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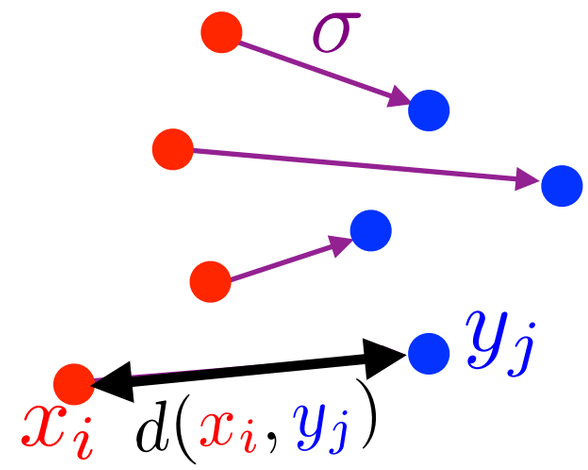

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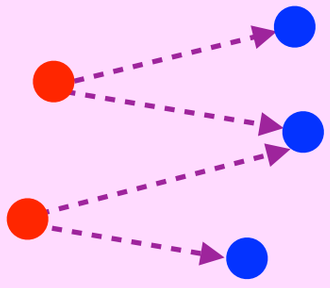

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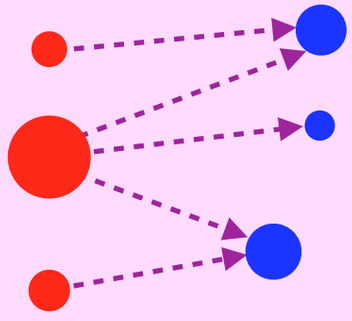


Weights?

$\Longrightarrow$

"Relax"

points $\to$ mass

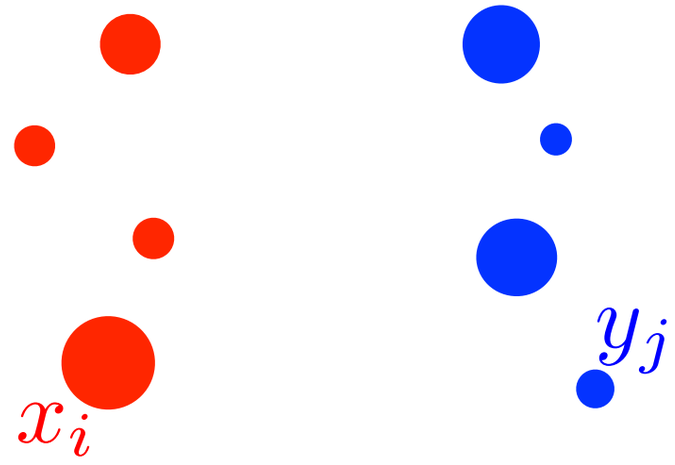
permutation $\to$ coupling

Kantorovitch's Formulation

Discrete distributions:

$$\alpha = \sum_{i=1}^{n} \mathbf{a}_i \delta_{x_i}$$

$$\beta = \sum_{j=1}^{m} \mathbf{b}_j \delta_{y_j}$$



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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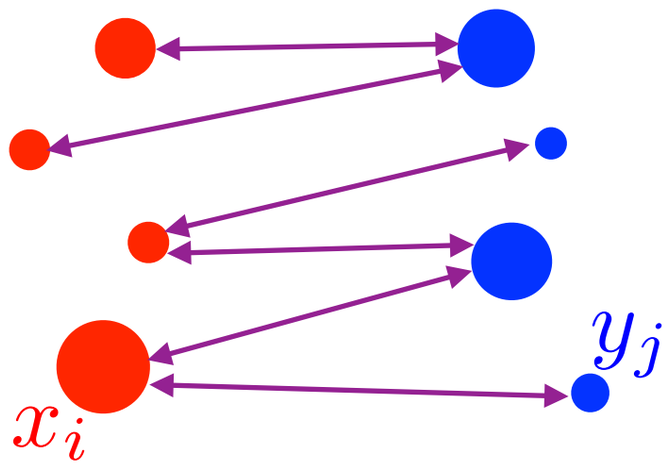

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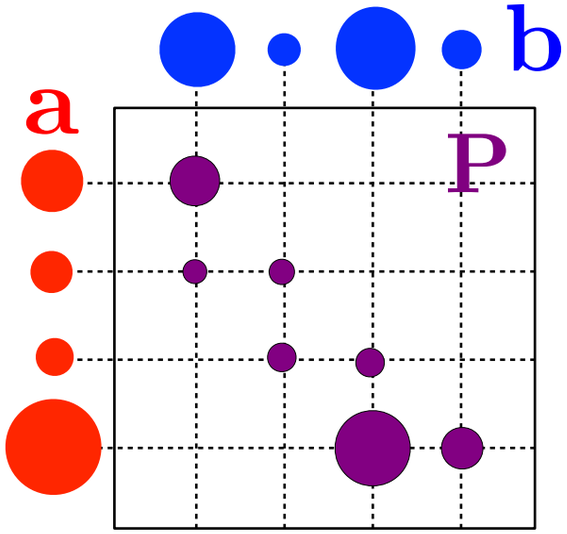

Couplings: $\sum_j \mathbf{P}_{i,j} = \mathbf{a}_i$ $\sum_i \mathbf{P}_{i,j} = \mathbf{b}_j$

$\mathbf{P} \geqslant 0$, $\mathbf{P}\mathbb{1}_m = \mathbf{a}$, $\mathbf{P}^\top \mathbb{1}_n = \mathbf{b}$

Kantorovitch's Formulation

Discrete distributions: $\alpha = \sum_{i=1}^{n} \mathbf{a}_i \delta_{x_i}$

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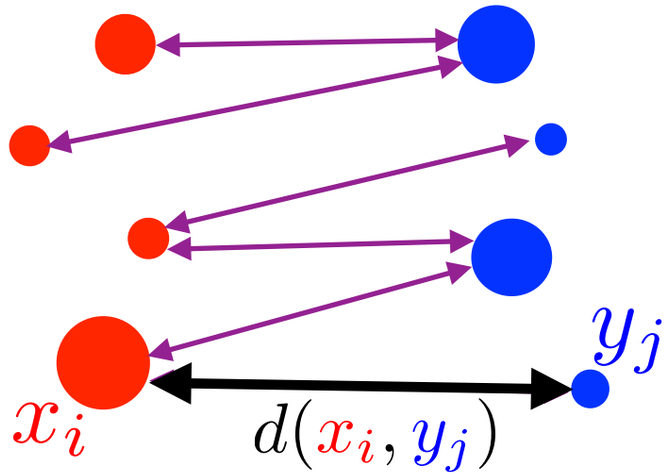

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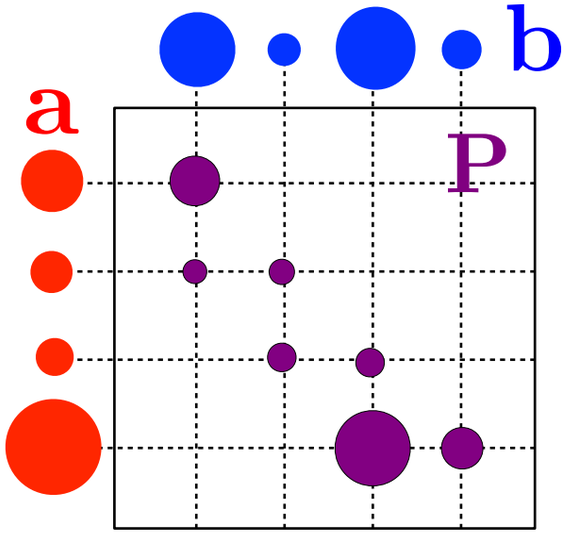


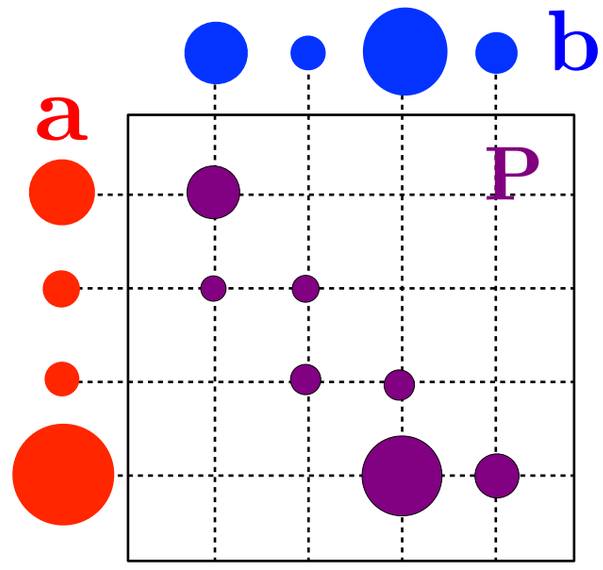
Couplings: $\sum_j \mathbf{P}_{i,j} = \mathbf{a}_i$ $\sum_i \mathbf{P}_{i,j} = \mathbf{b}_j$

[Kantorovich 1942]

$$\min_{\mathbf{P}} \left\{ \sum_{i,j} d(x_i, y_j)^p \mathbf{P}_{i,j} \;;\; \mathbf{P} \geqslant 0, \mathbf{P}\mathbb{1}_m = \mathbf{a}, \mathbf{P}^\top \mathbb{1}_n = \mathbf{b} \right\}$$

Optimal Transport Distances

$$\mathrm{W}_p(\alpha,\beta) \overset{\text{def.}}{=} \left(\min_{\mathbf{P}\mathbb{1}=\mathbf{a},\mathbf{P}^\top\mathbb{1}=\mathbf{b}} \sum_{i,j} d(x_i,y_j)^p \mathbf{P}_{i,j} \right)^{\frac{1}{p}}$$



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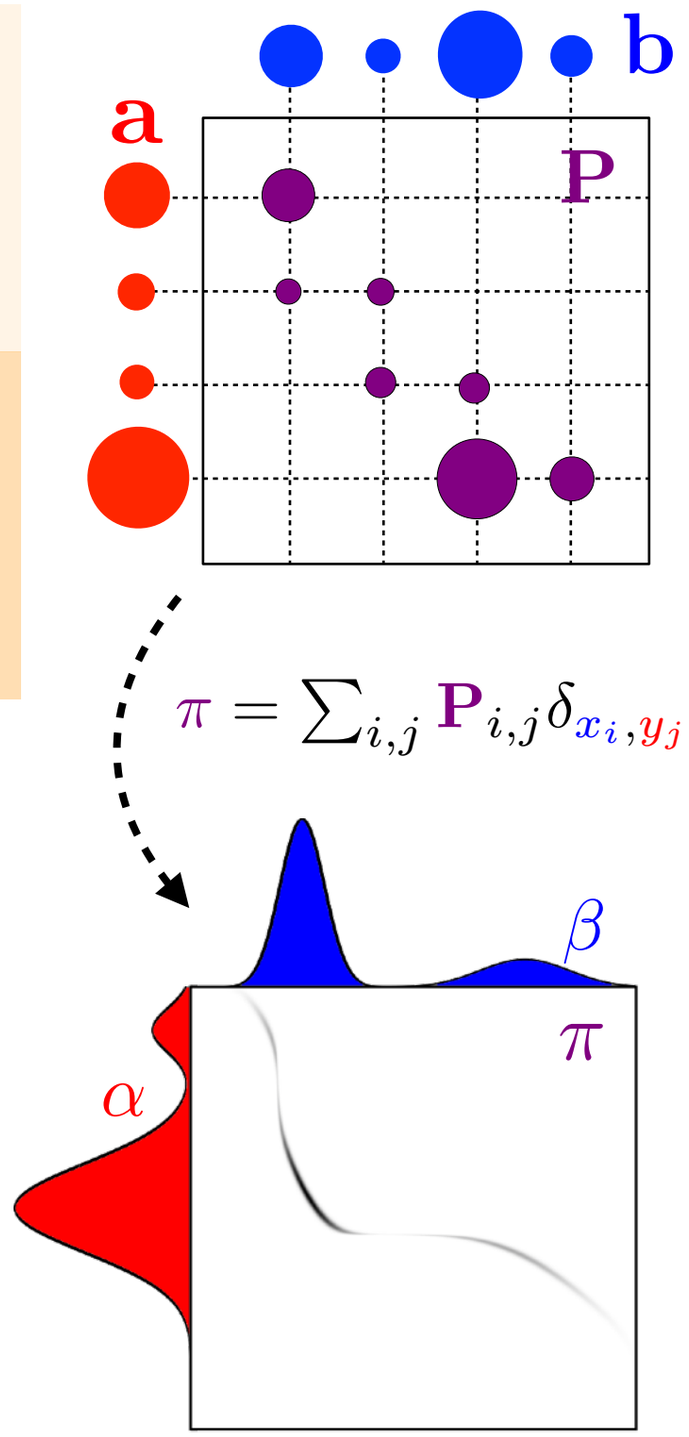
$$\min_{\pi\in\mathcal{M}_+^1(\mathcal{X}^2)} \left\{ \int_{\mathcal{X}^2} d(x,y)^p \mathrm{d}\pi(x,y) \;;\; \pi_1=\alpha, \pi_2=\beta \right\}$$



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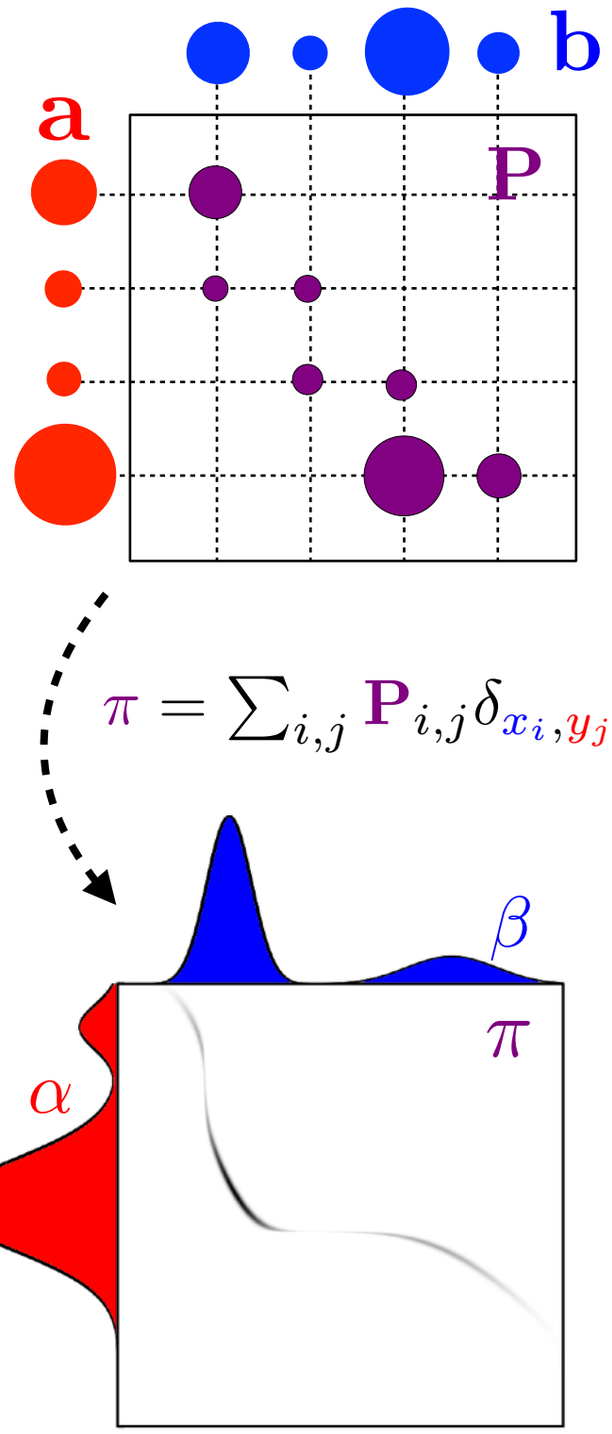

Convergence in law: $\alpha_n \rightharpoonup \beta$

$\Leftrightarrow \quad \forall f \in \mathcal{C}(\mathcal{X}),\ \int_{\mathcal{X}} f \mathrm{d}\alpha_n \to \int_{\mathcal{X}} f \mathrm{d}\beta$

$\delta_{x_1} \quad \delta_{x_2} \quad \delta_{x_3} \quad \dots \quad \delta_x$

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

Optimal Transport Distances

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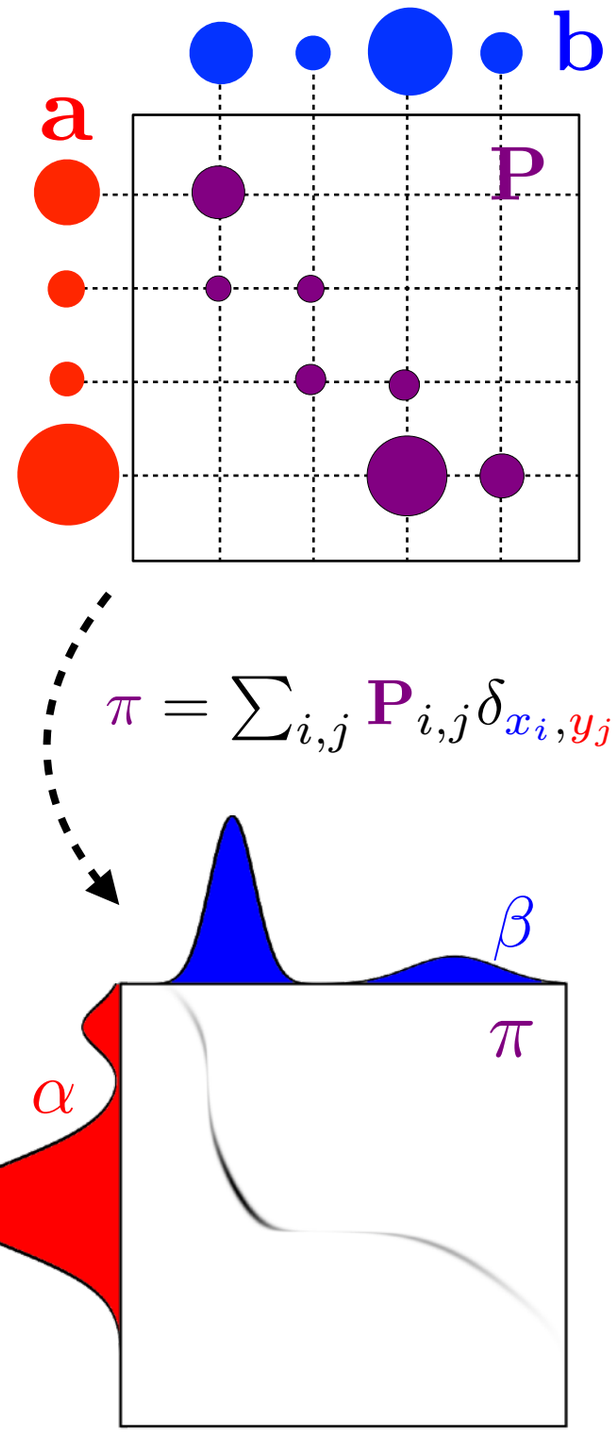

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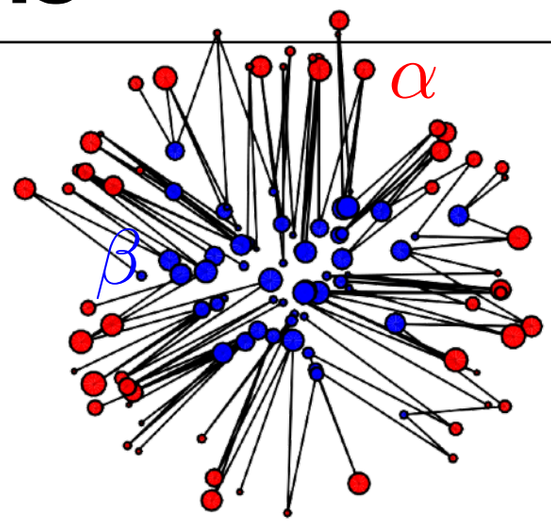
$\delta_{x_1} \quad \delta_{x_2} \quad \delta_{x_3} \quad \dots \quad \delta_x$

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

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

Algorithms

Linear programming: $O(n^3 \log(n)^2)$



Algorithms

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Hungarian/Auction: $O(n^3)$

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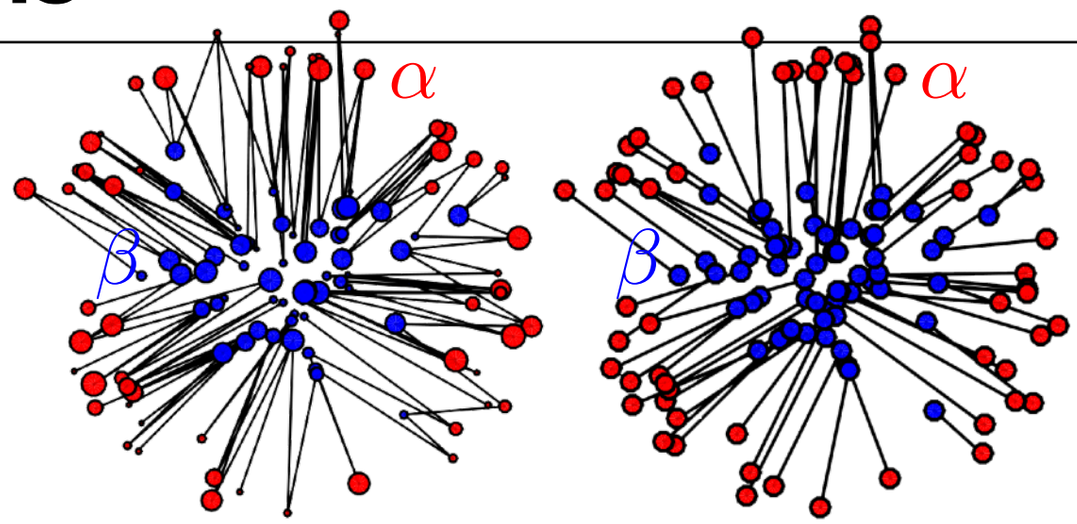

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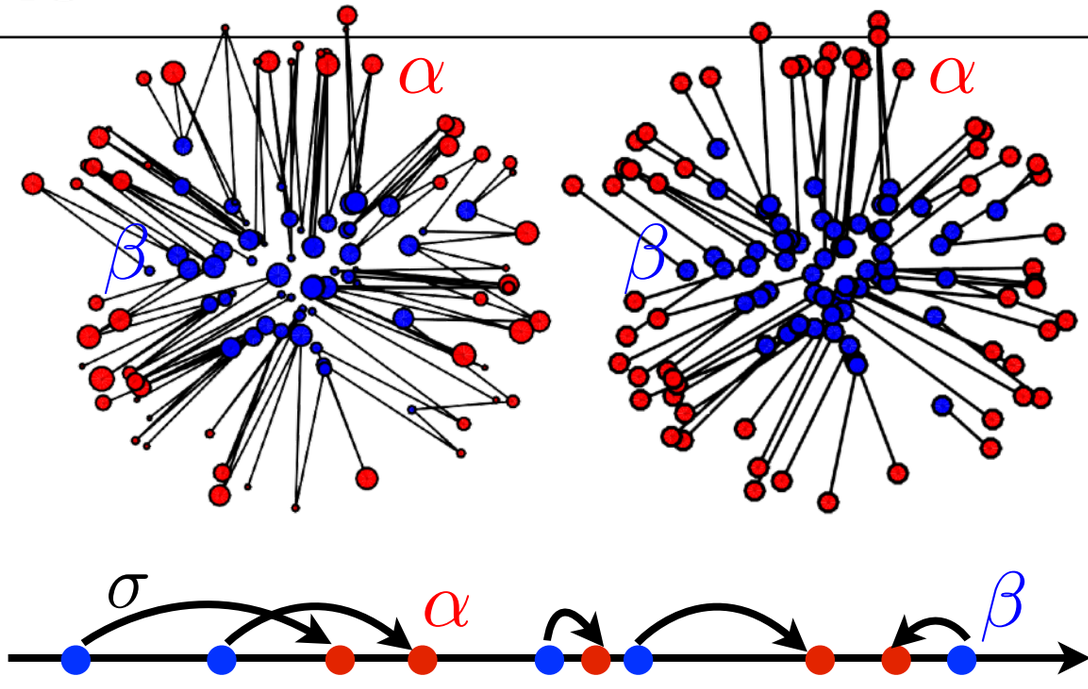
1-D case: sorting $O(n \log(n))$.



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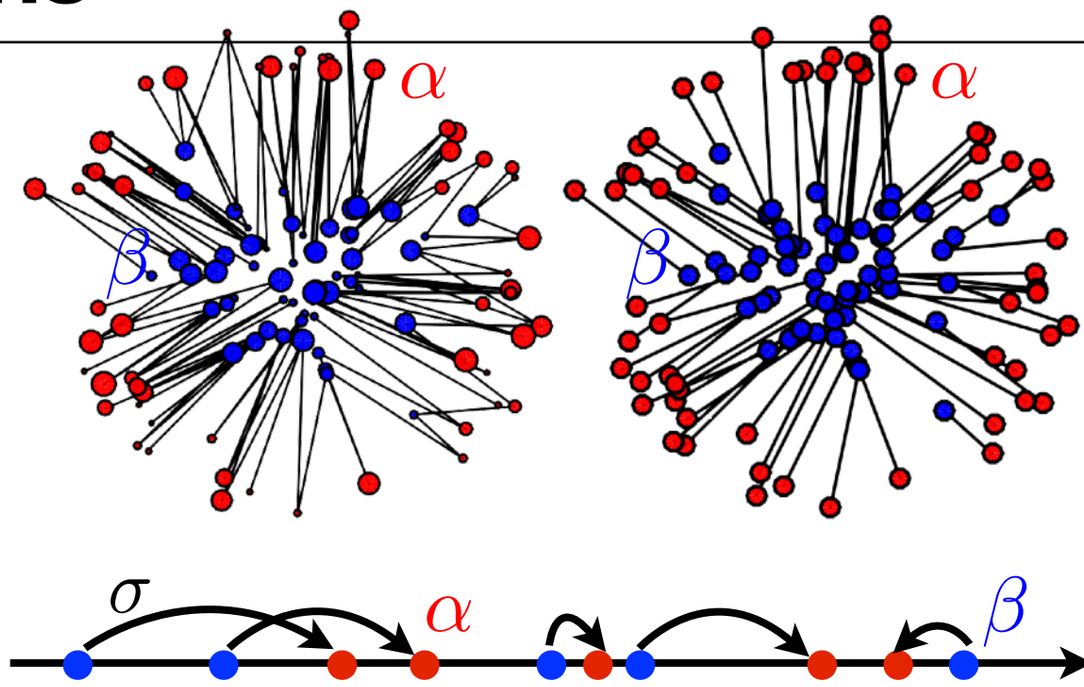

1-D case: sorting $O(n \log(n))$.

$p = 1$
$d = \|\cdot\|$

$$W_1(\alpha, \beta) = \min_{\mathrm{div}(u)=\alpha-\beta} \int \|u(x)\| \mathrm{d}x$$

$\rightarrow$ min-cost flow, on graphs $O(n^2 \log(n))$.

Algorithms

Linear programming: $O(n^3 \log(n)^2)$

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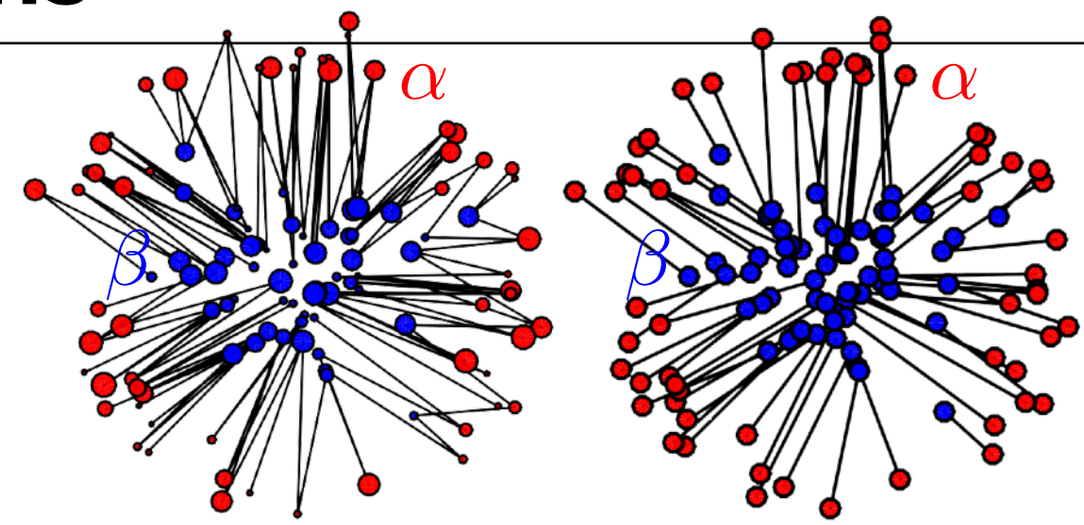

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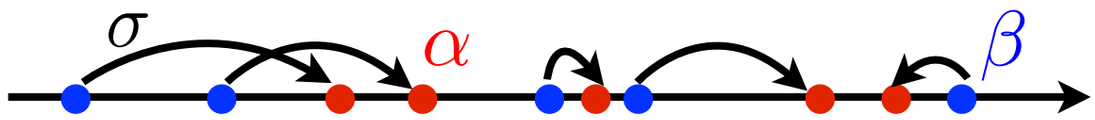

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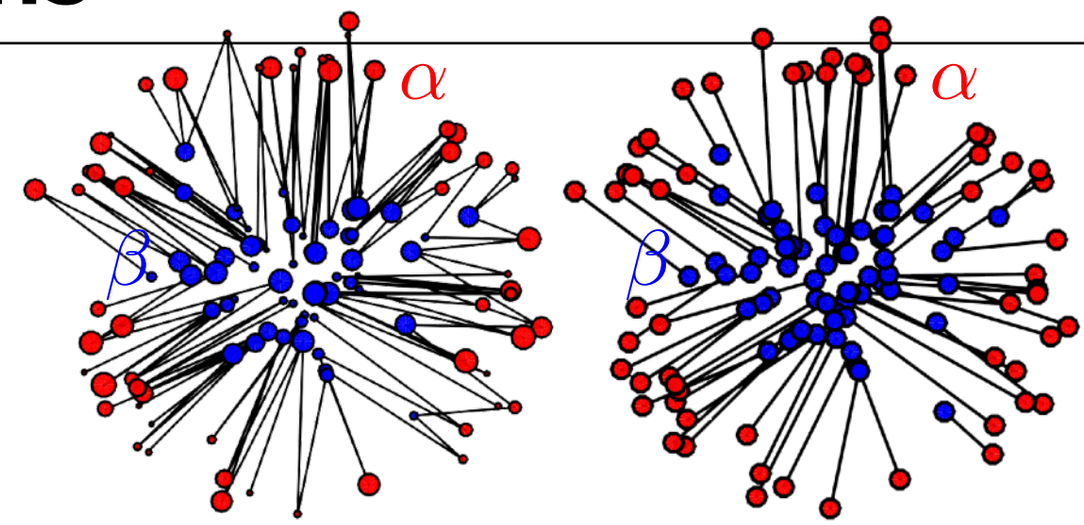

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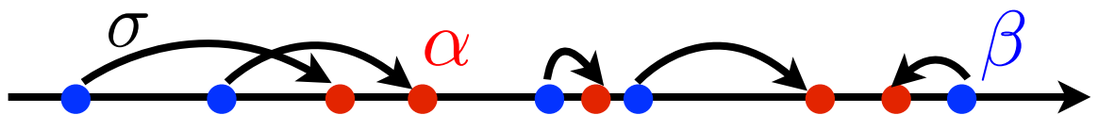

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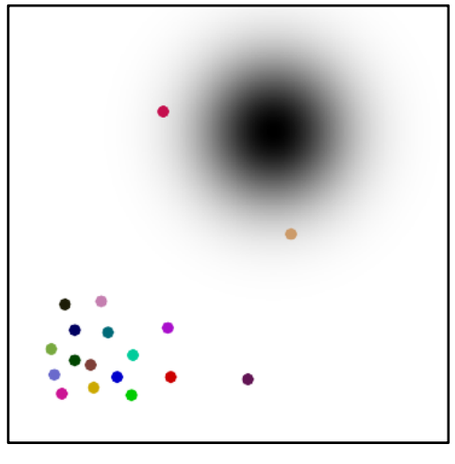
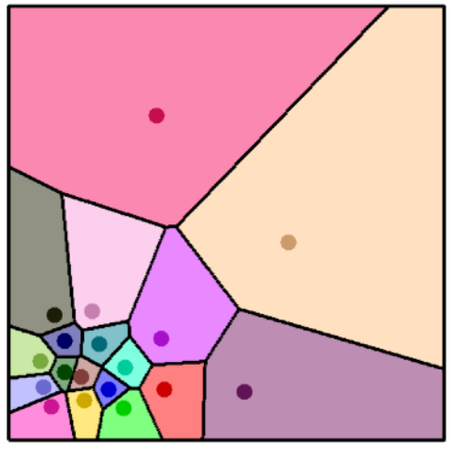


Semi-discrete: Laguerre cells, $d = \|\cdot\|_2^2$.
[Merigot 2013]



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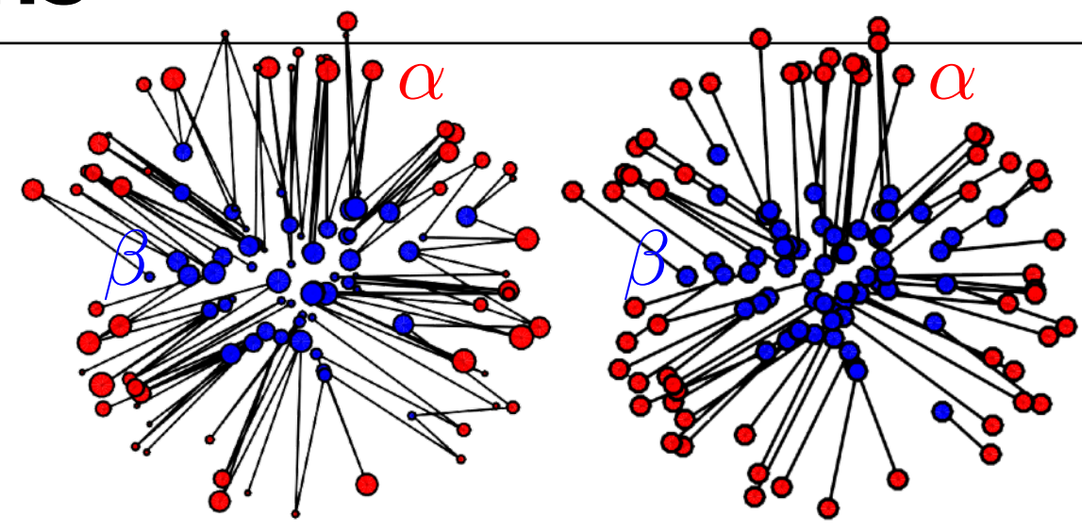

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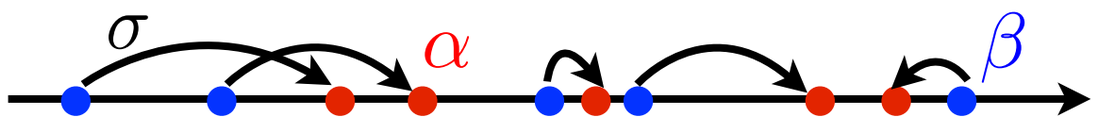

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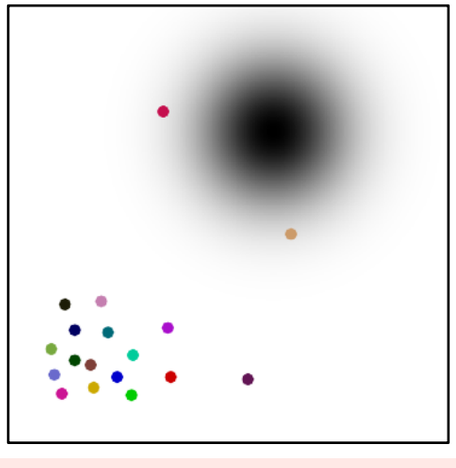

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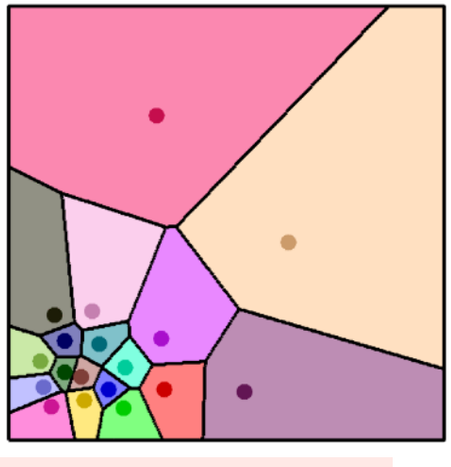

Need for fast approximate algorithms for generic $d(x,y)$.

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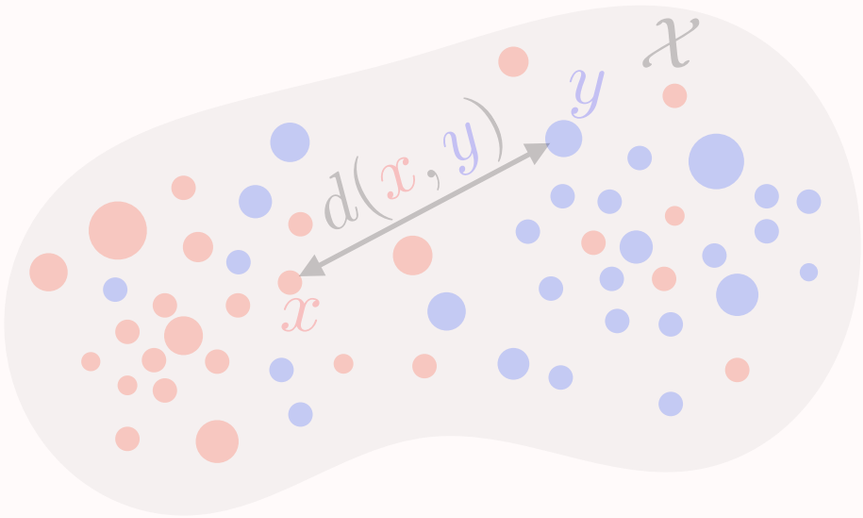

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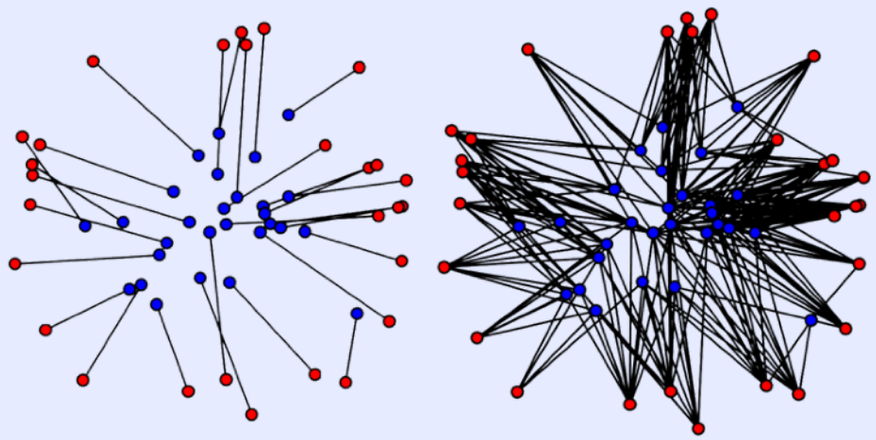

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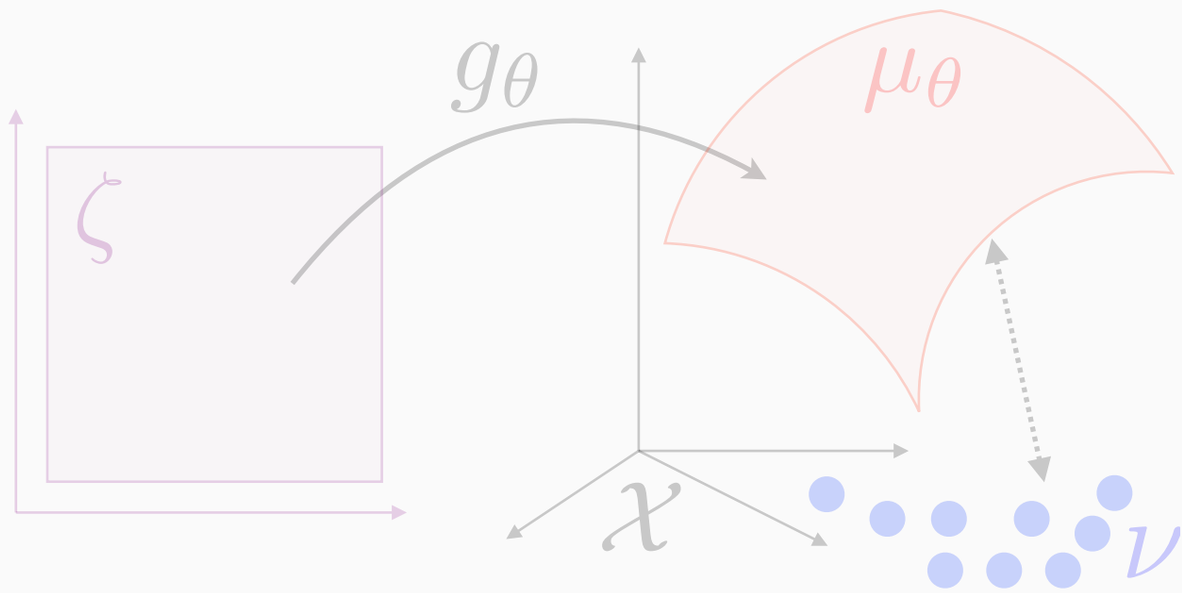
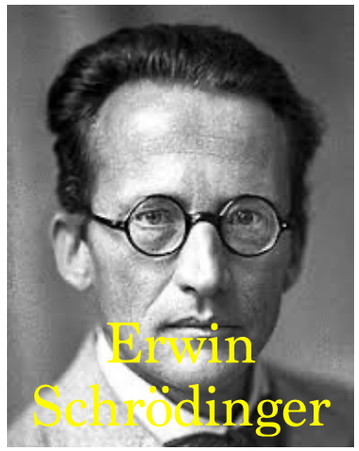
4. Application to Generative Models



Entropic Regularization

Schrödinger's problem: [1931]

$$\min_{\mathbf{P}\mathbb{1}=\mathbf{a},\mathbf{P}^\top\mathbb{1}=\mathbf{b}} \sum_{i,j} d(x_i, y_j)^p \mathbf{P}_{i,j} + \varepsilon \mathbf{P}_{i,j} \log(\mathbf{P}_{i,j})$$



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

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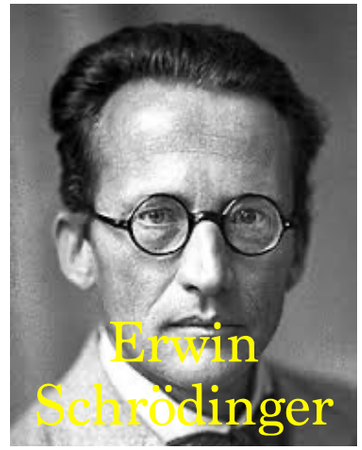

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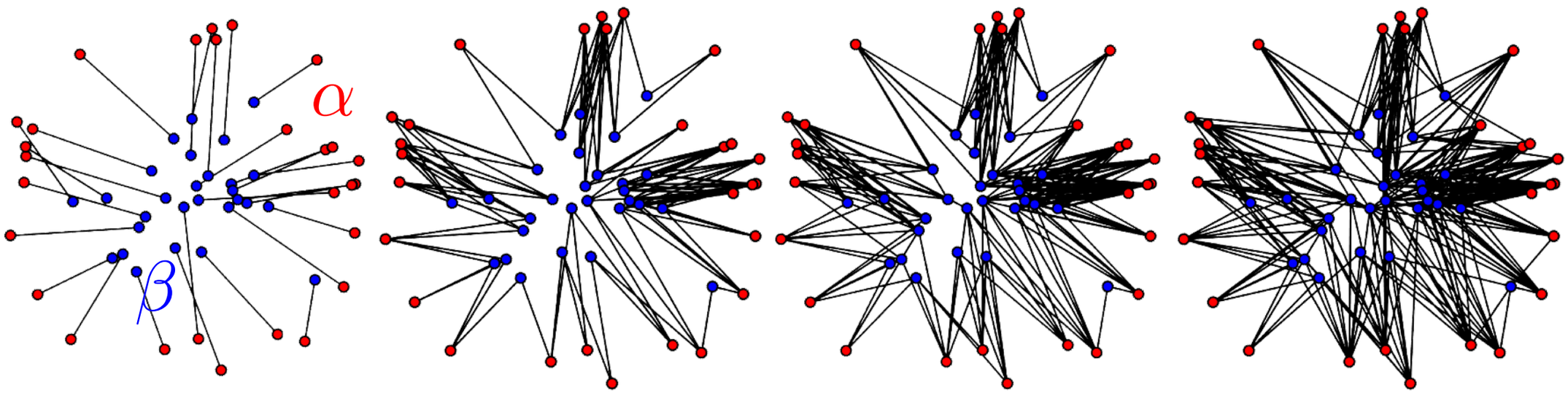

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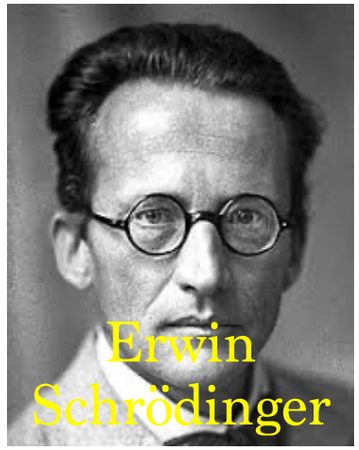

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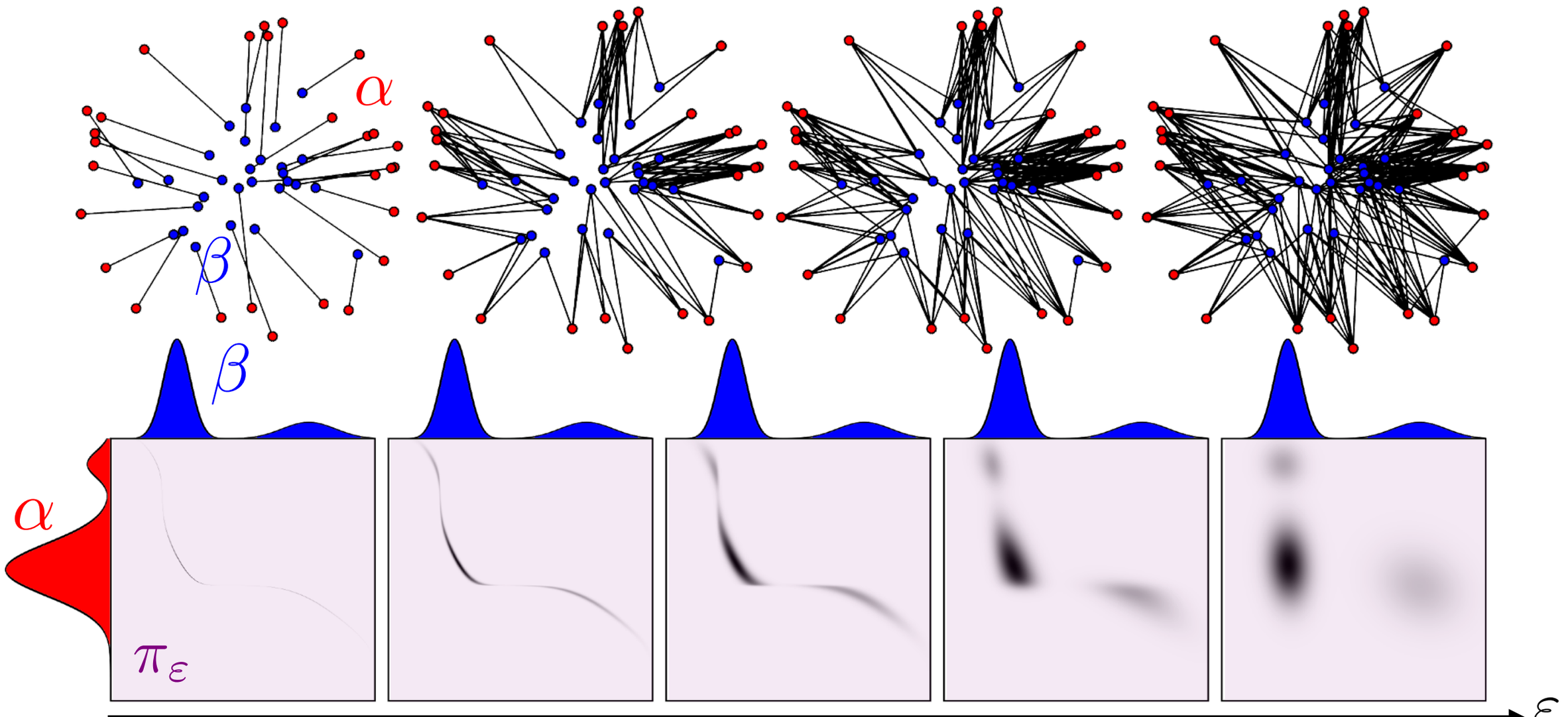

Sinkhorn's Algorithm

$$\min_{\mathbf{P}} \left\{ \sum_{i,j} d(x_i, y_j)^p \mathbf{P}_{i,j} + \varepsilon \mathbf{P}_{i,j} \log(\mathbf{P}_{i,j}) \; ; \; \mathbf{P}\mathbb{1} = \mathbf{a}, \mathbf{P}^\top \mathbb{1} = \mathbf{b} \right\}$$

Proposition:

$$\mathbf{P} \text{ solution} \Leftrightarrow \begin{cases} \mathbf{P}\mathbb{1} = \mathbf{a}, \mathbf{P}^\top \mathbb{1} = \mathbf{b} \text{ and} \\ \exists \mathbf{u}, \mathbf{v}, \;\; \mathbf{P}_{i,j} = \mathbf{u}_i \, \mathbf{K}_{i,j} \, \mathbf{v}_j \end{cases}$$

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$$\mathbf{u} \leftarrow \frac{\mathbf{a}}{\mathbf{K}\mathbf{v}} \qquad \mathbf{v} \leftarrow \frac{\mathbf{b}}{\mathbf{K}^\top \mathbf{u}}$$

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

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Matrix/vector multiplications: $\rightarrow O(n^2/\varepsilon^2)$ complexity.

$\rightarrow$ Parallelizable on GPUs.

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

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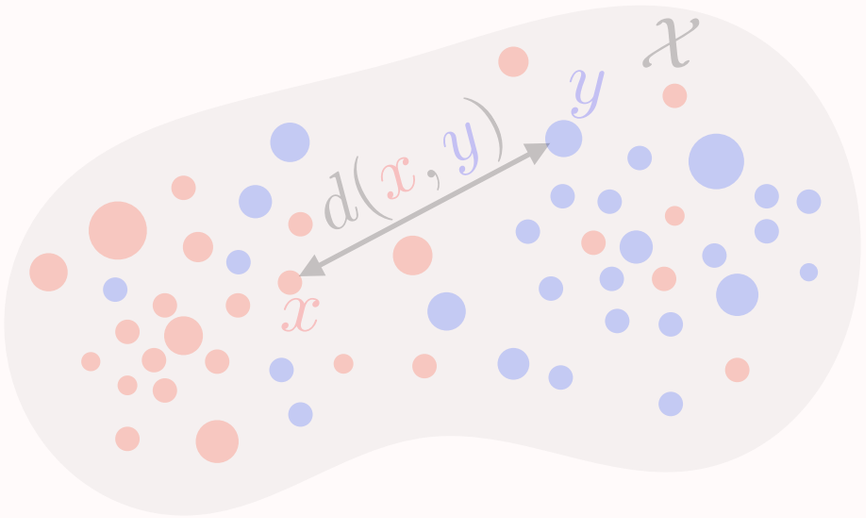

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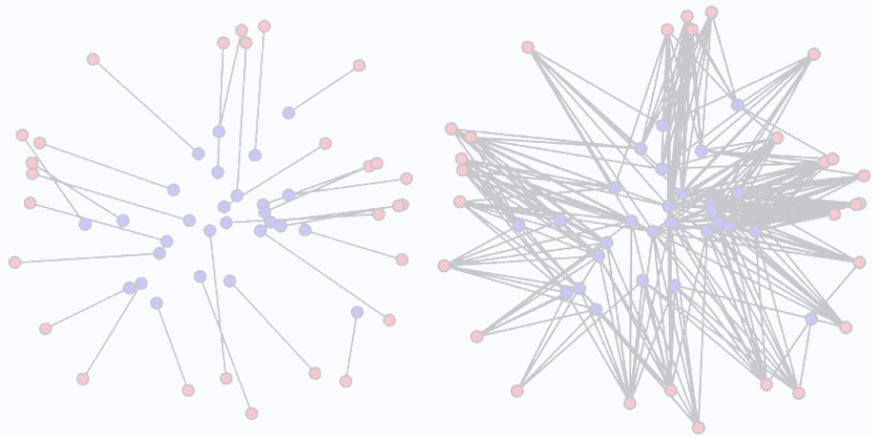

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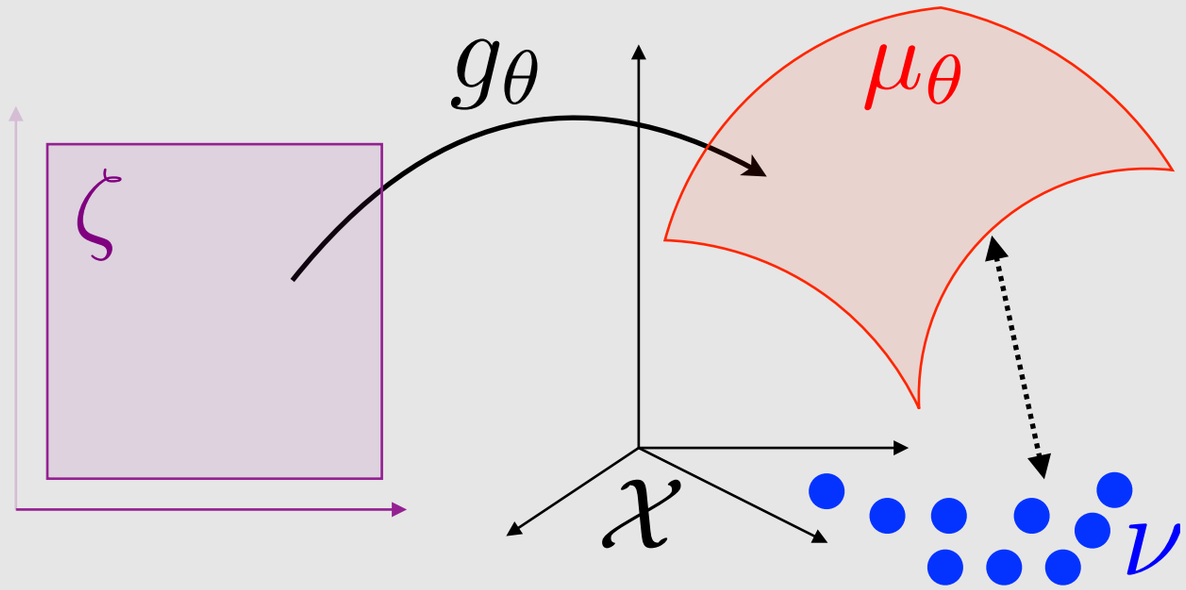
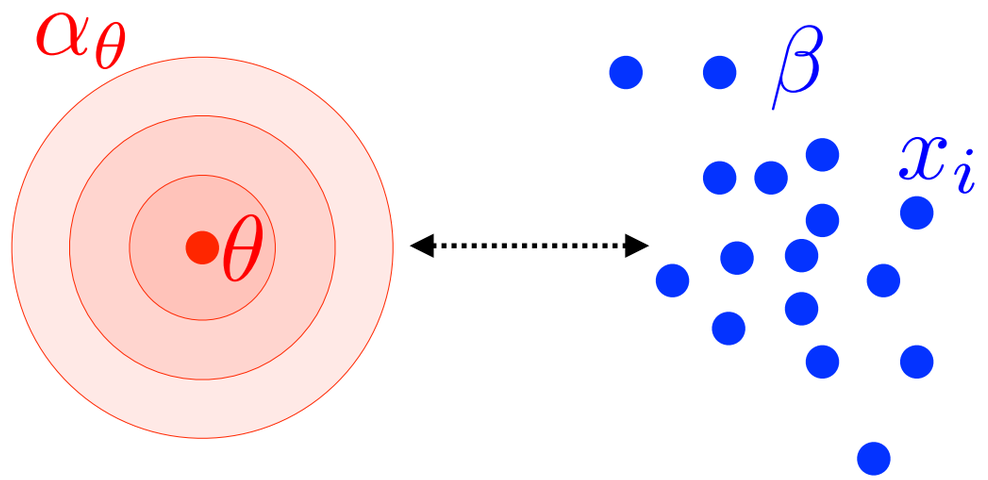


Density Fitting and Generative Models

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

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



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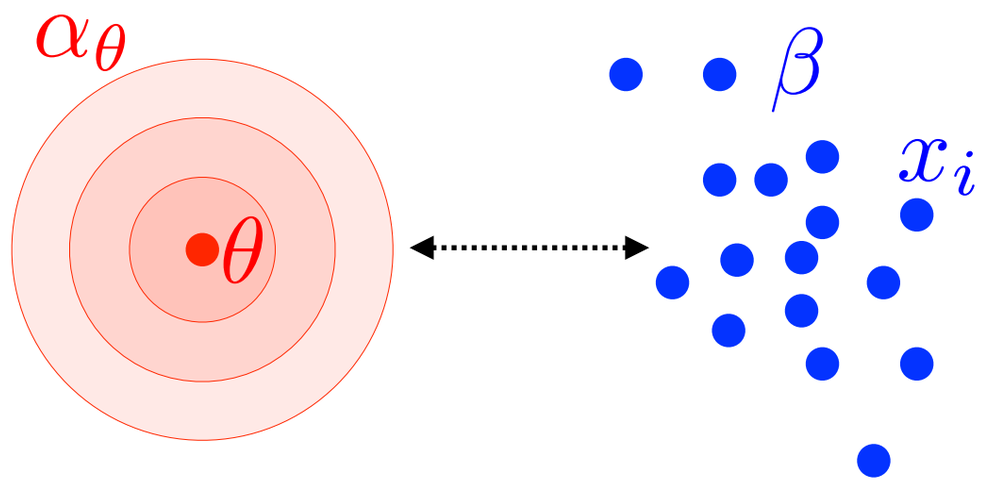

Density fitting: $\mathrm{d}\alpha_\theta(x) = \rho_\theta(x)\mathrm{d}x$

$$\min_\theta \; -\sum_i \log(\rho_\theta(x_i)) \overset{n\to+\infty}{\longrightarrow} \mathrm{KL}(\beta|\alpha_\theta)$$

Maximum likelihood (MLE)

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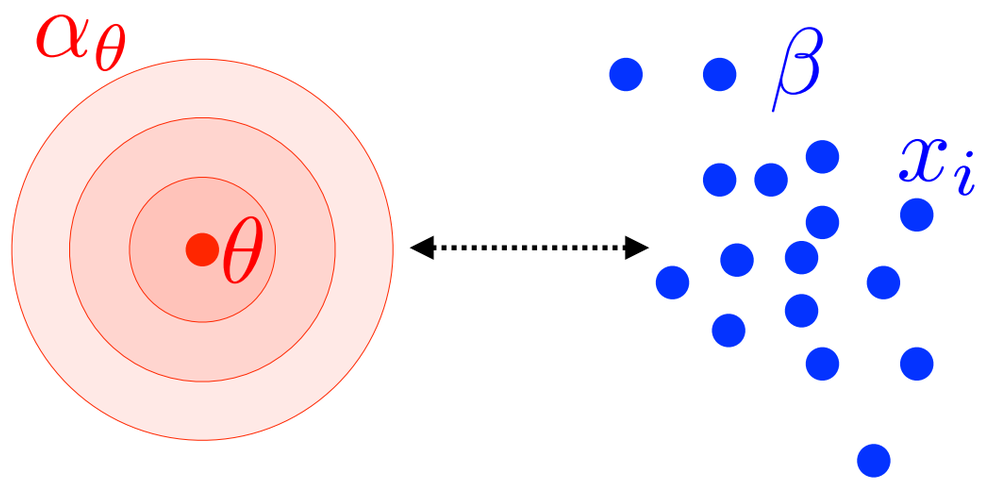

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Maximum likelihood (MLE)

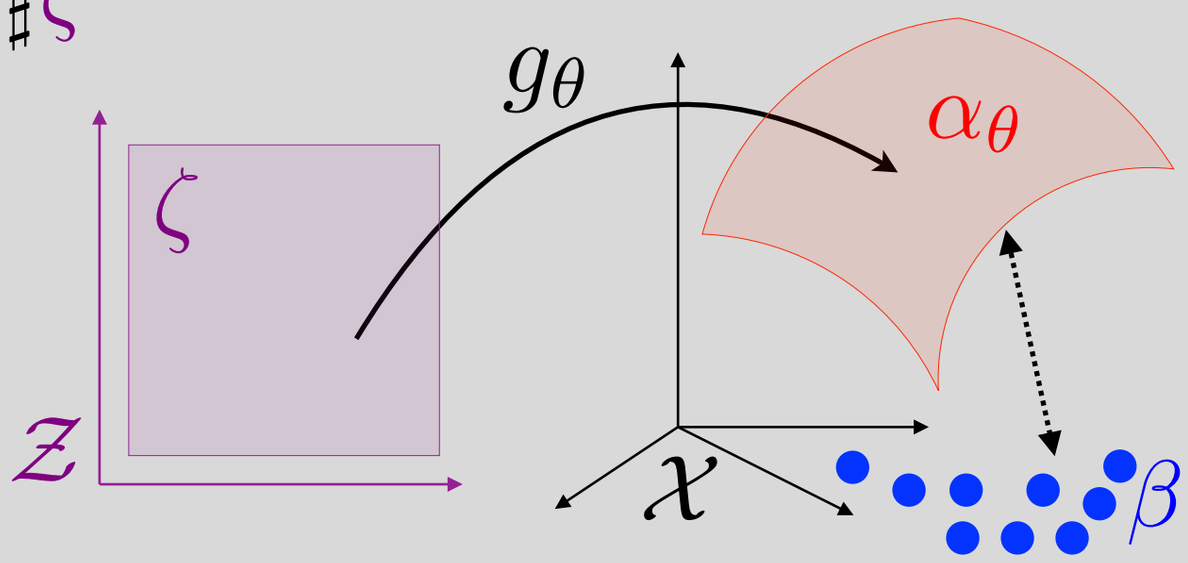
Generative model fit: $\alpha_\theta = g_{\theta,\sharp}\zeta$

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

$\to$ MLE undefined.

$\to$ Need a weaker metric.

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



Deep Discriminative vs Generative Models

Deep networks:

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

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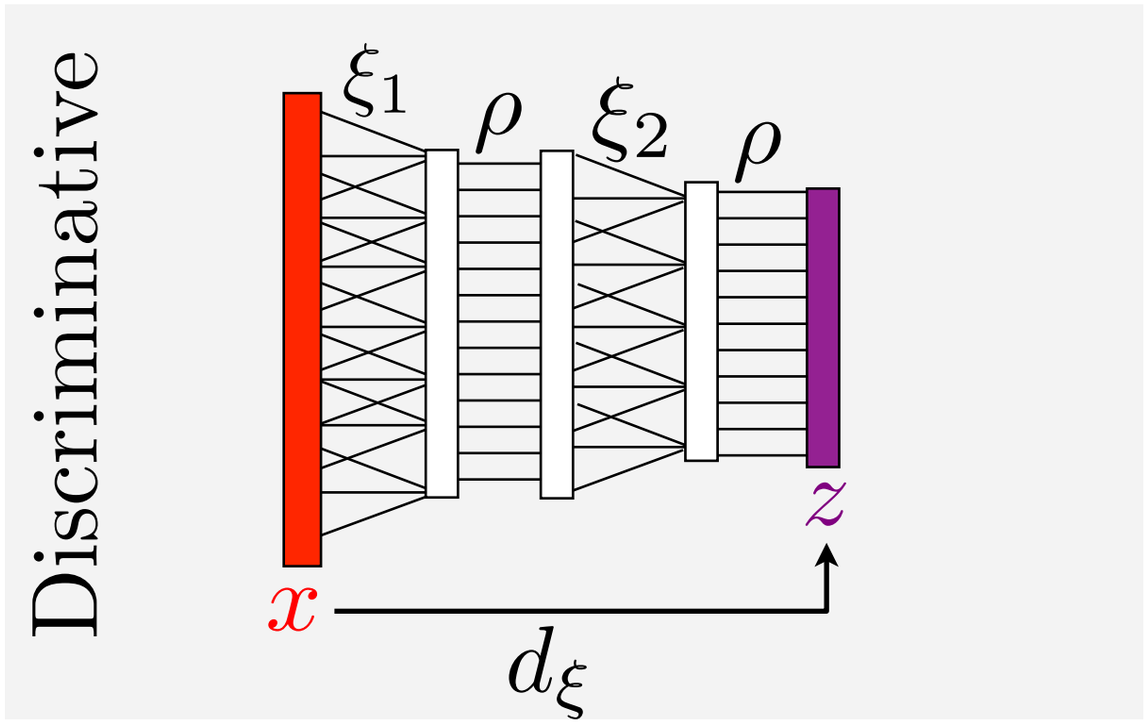

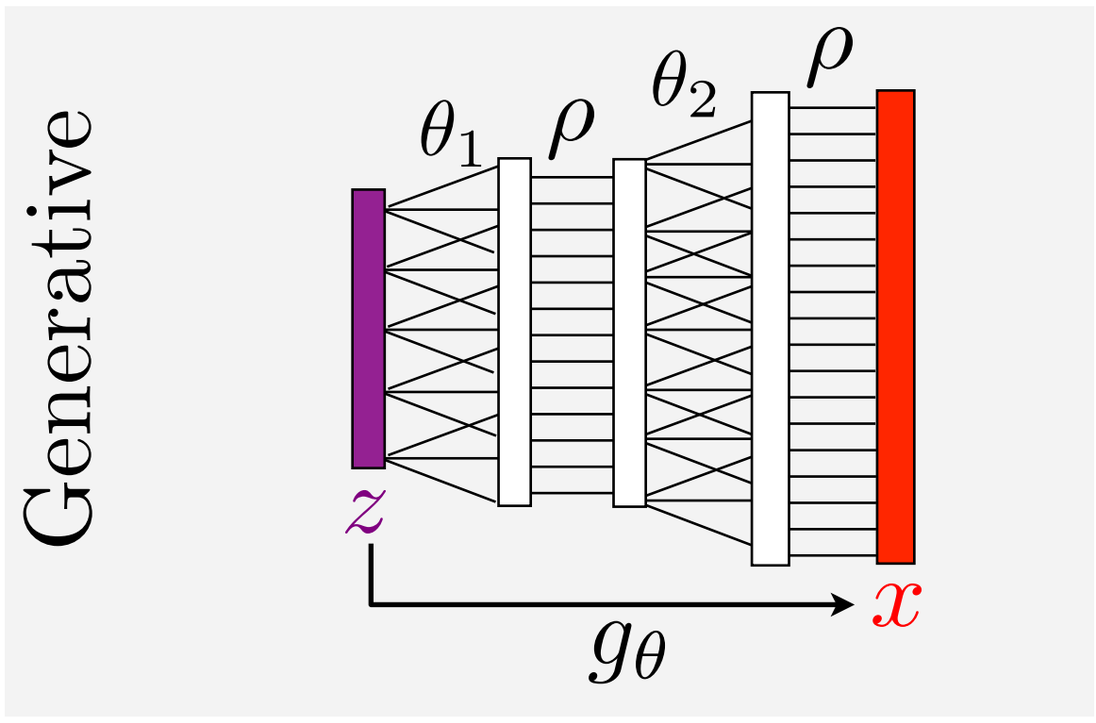

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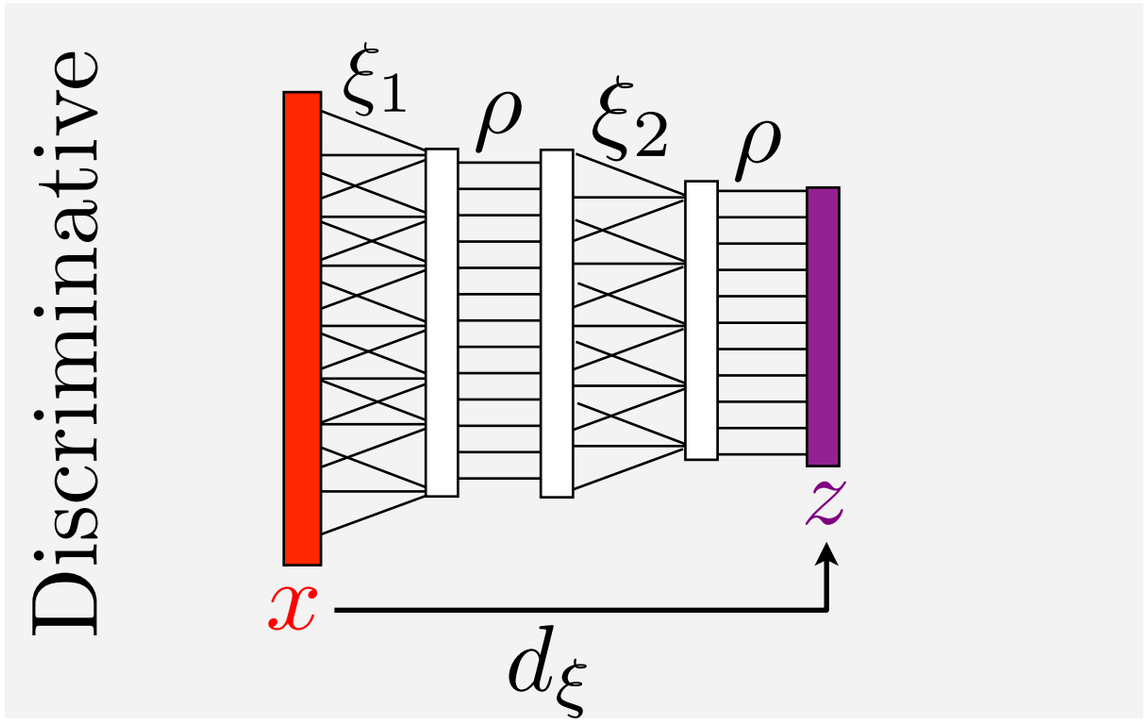
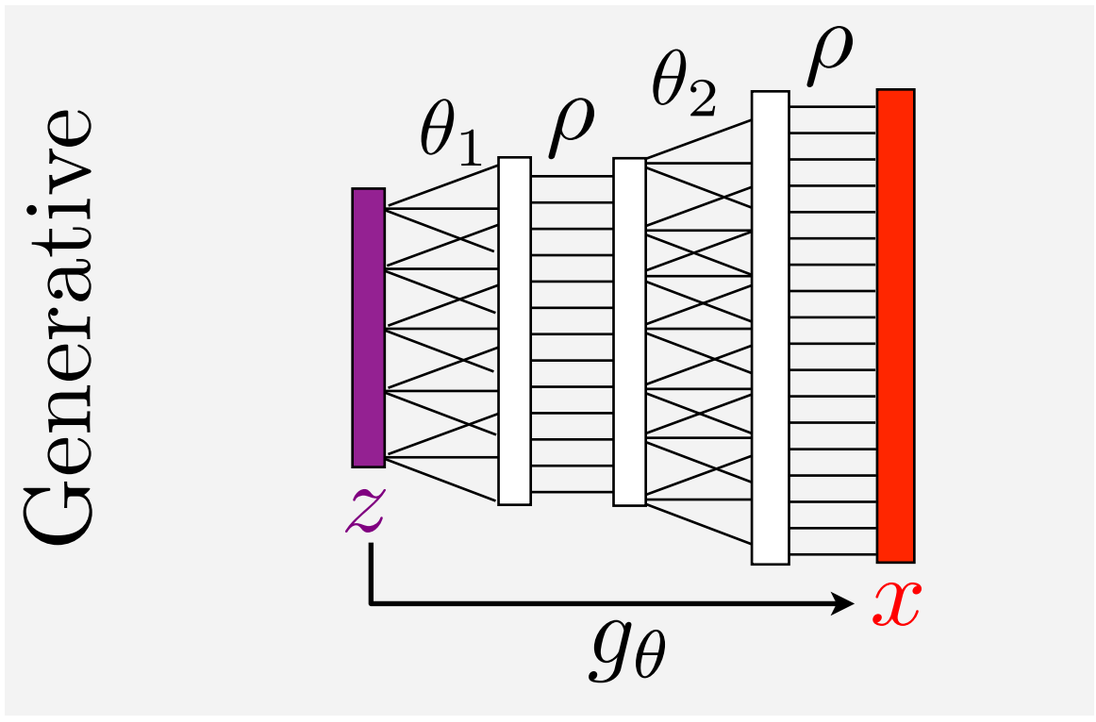
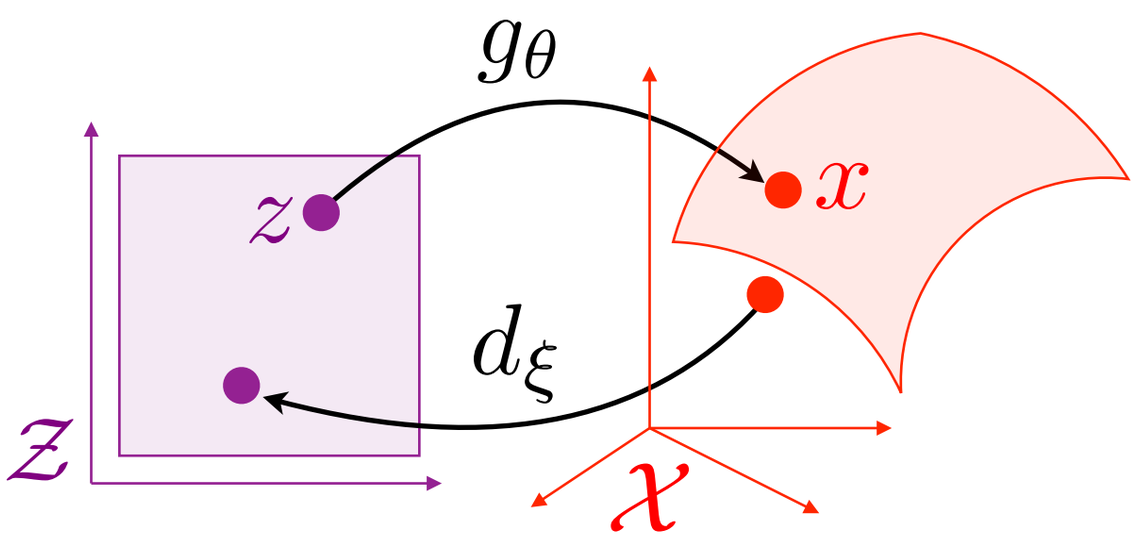
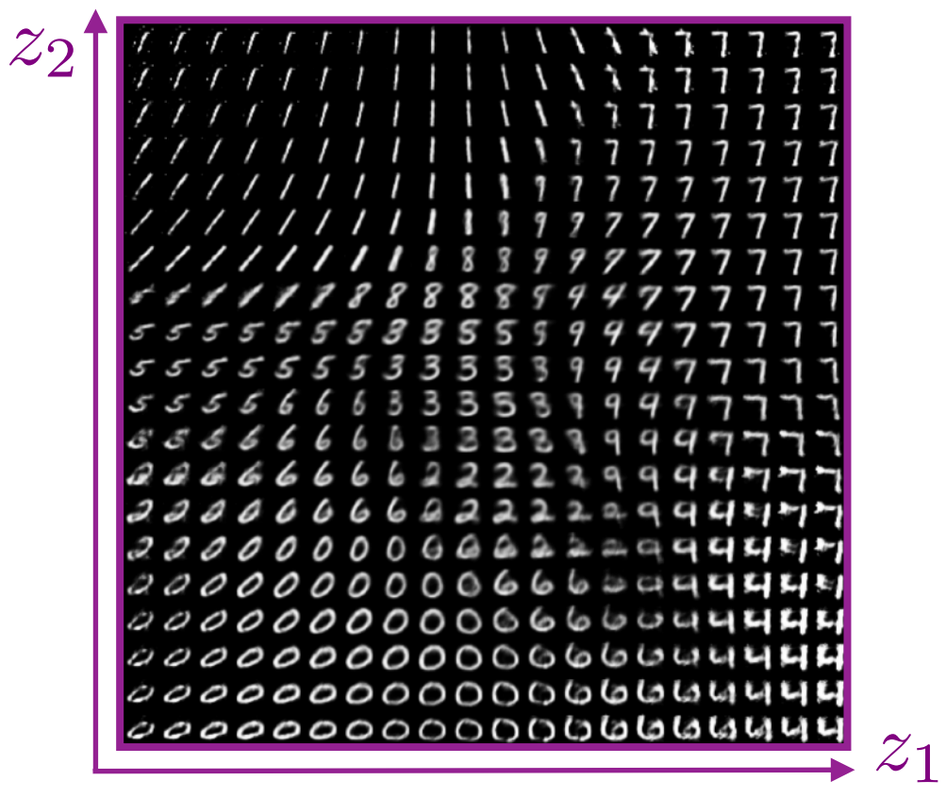




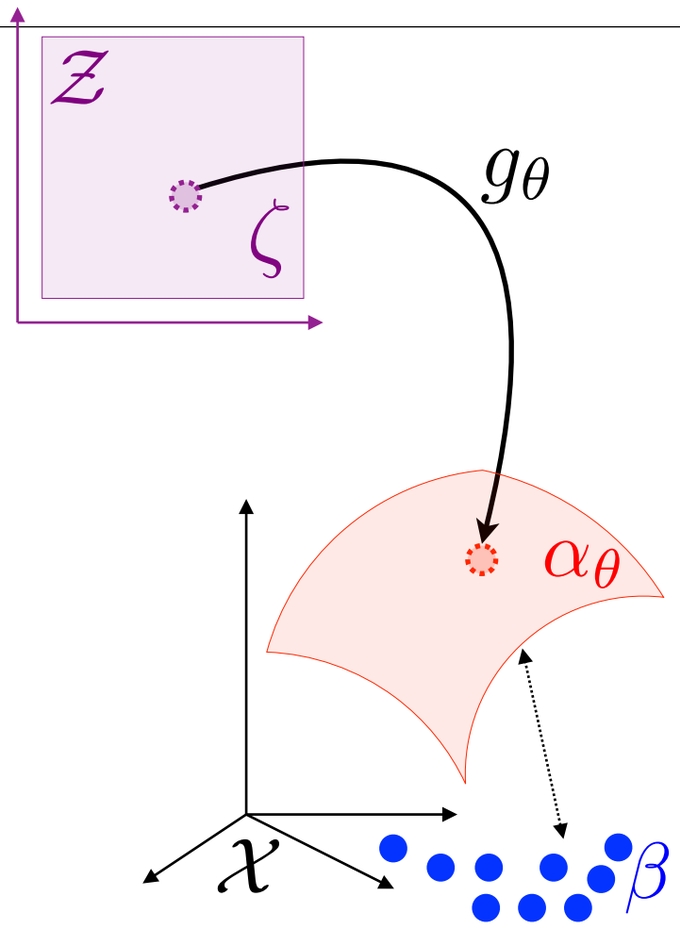




Examples of Images Generation

Inputs β

Generated α_θ



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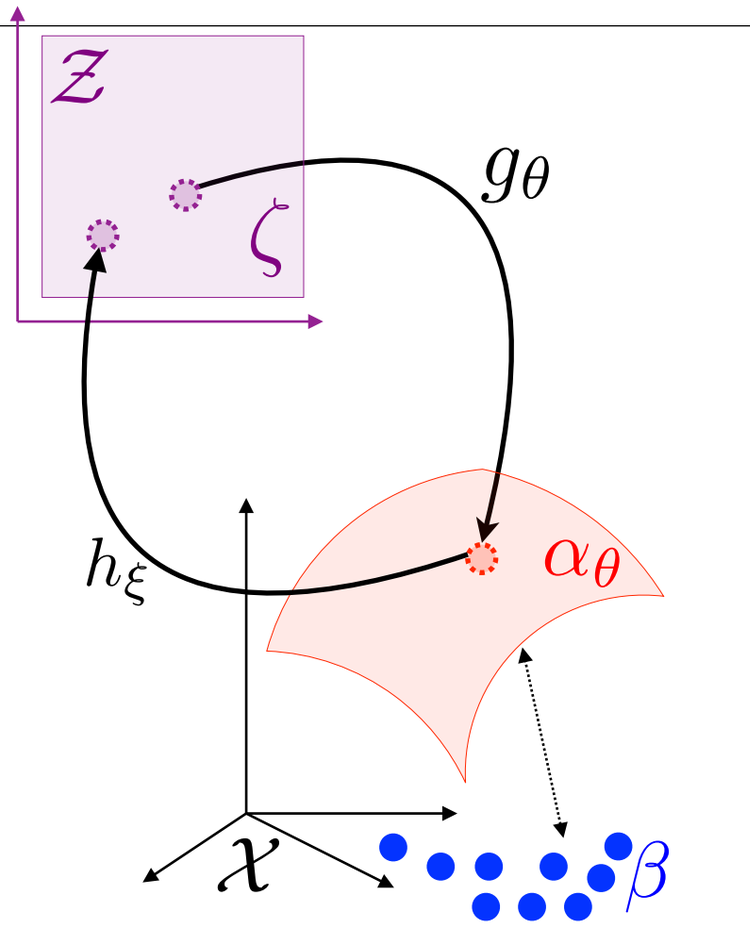
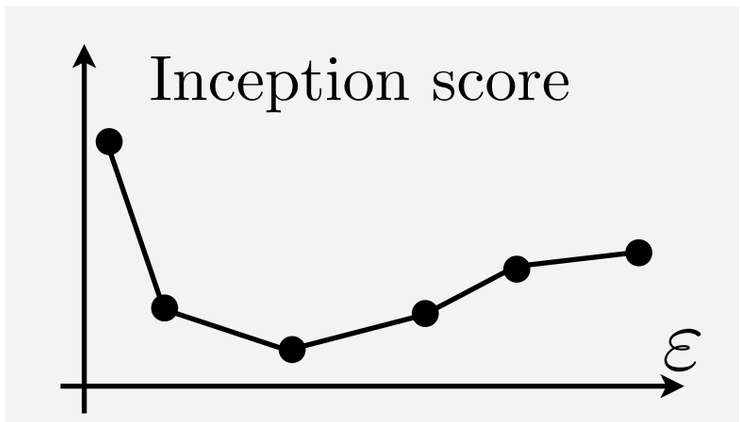




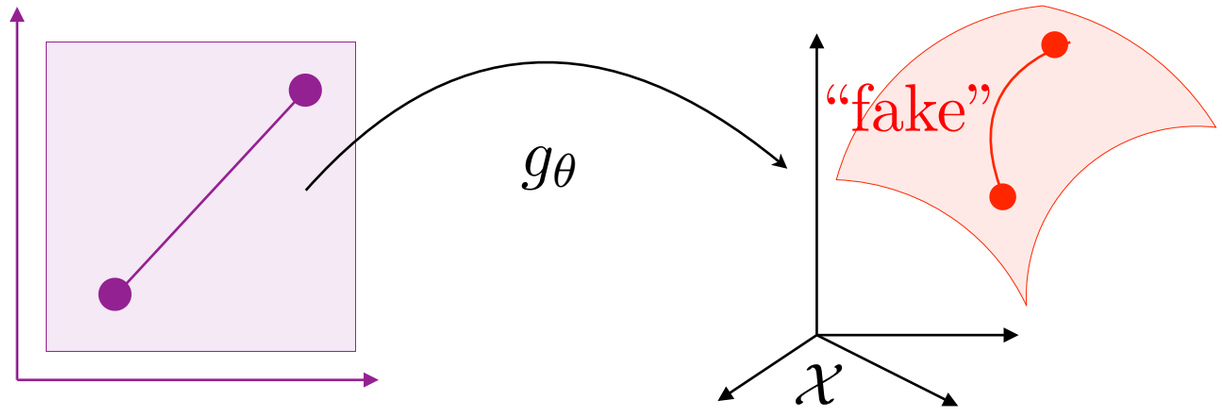
$\rightarrow$ Need to learn the metric $d(x, y) = \|h_\xi(x) - h_\xi(y)\|$ (GANs)

$\rightarrow$ Influence of ε?

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

Progressive Growing of GANs for Improved Quality, Stability, and Variation

Tero Karras, Timo Aila, Samuli Laine, Jaakko Lehtinen, ICLR 2018



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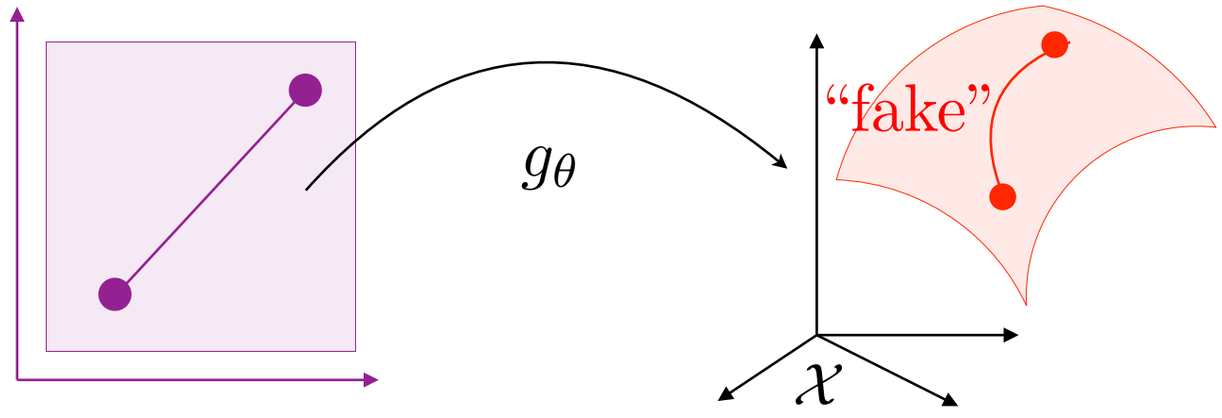
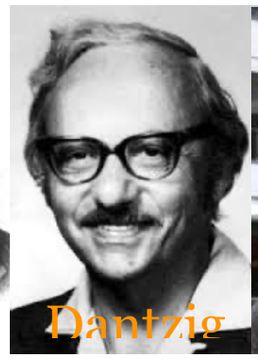
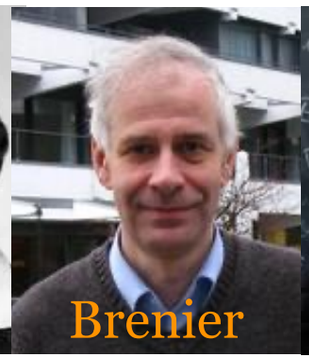
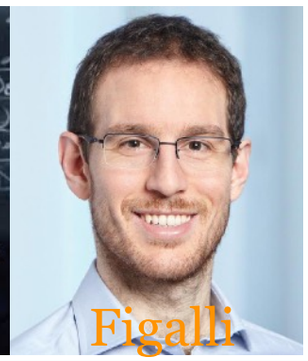


Conclusion



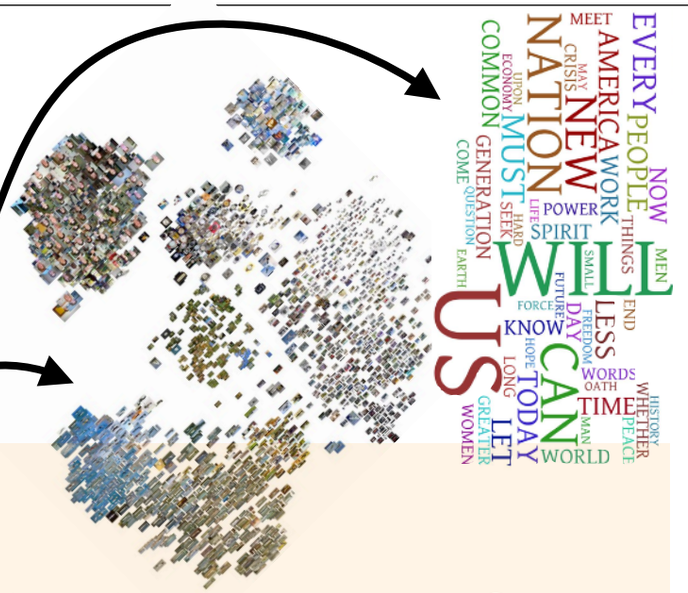


Toward high-dimensional OT:

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

$\rightarrow$ Performance quality measures for unsupervised learning?

Conclusion



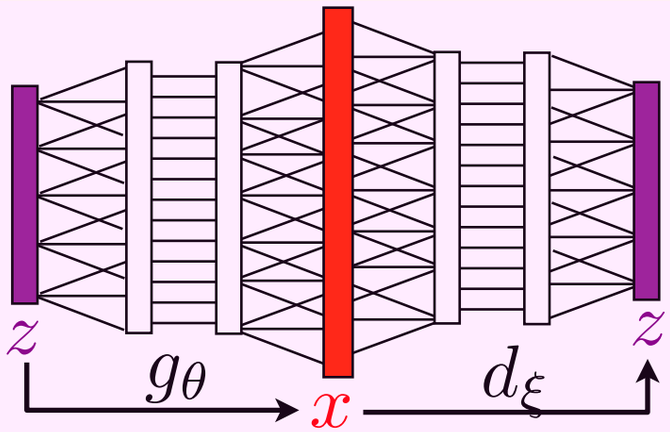
Toward high-dimensional OT:

→ Scalable geometrical loss functions in high dimension?

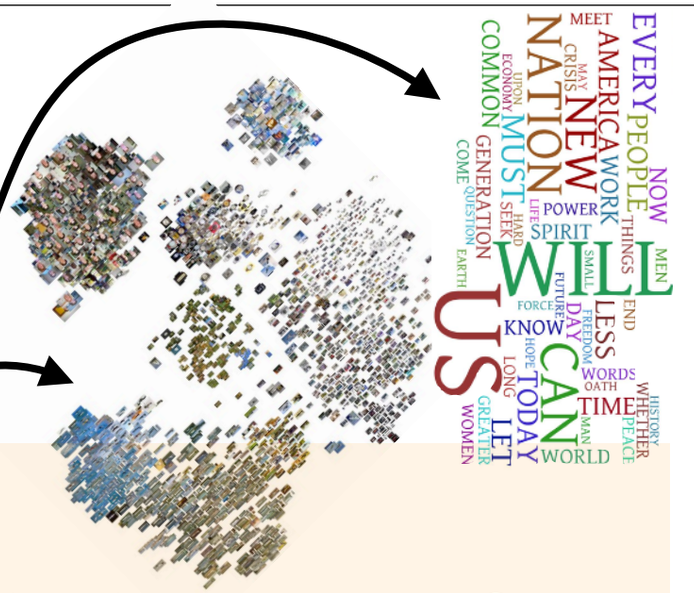
→ Performance quality measures for unsupervised learning?

Metric learning for OT:

→ Adversarial training to leverage multi scale priors?



Conclusion



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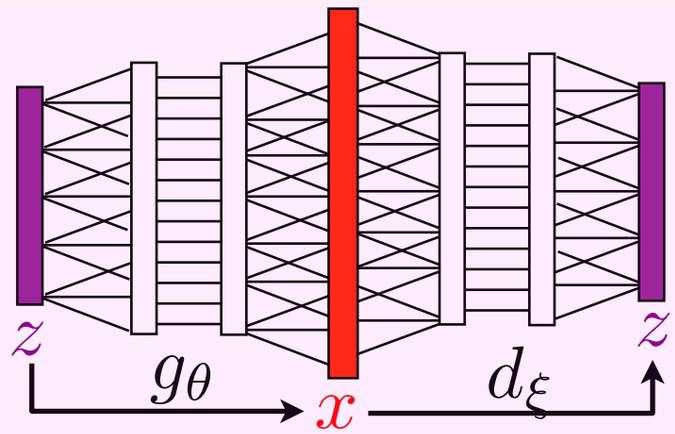

Beyond comparing measures:

→ Learning for surfaces, graphs, metric spaces?

→ Using Gromov-Wasserstein geometry?