

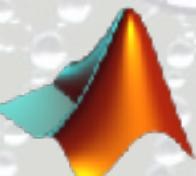
Numerical Optimal Transport

<http://optimaltransport.github.io>

Entropic Regularization

Gabriel Peyré

www.numerical-tours.com



ENS

ÉCOLE NORMALE
SUPÉRIEURE

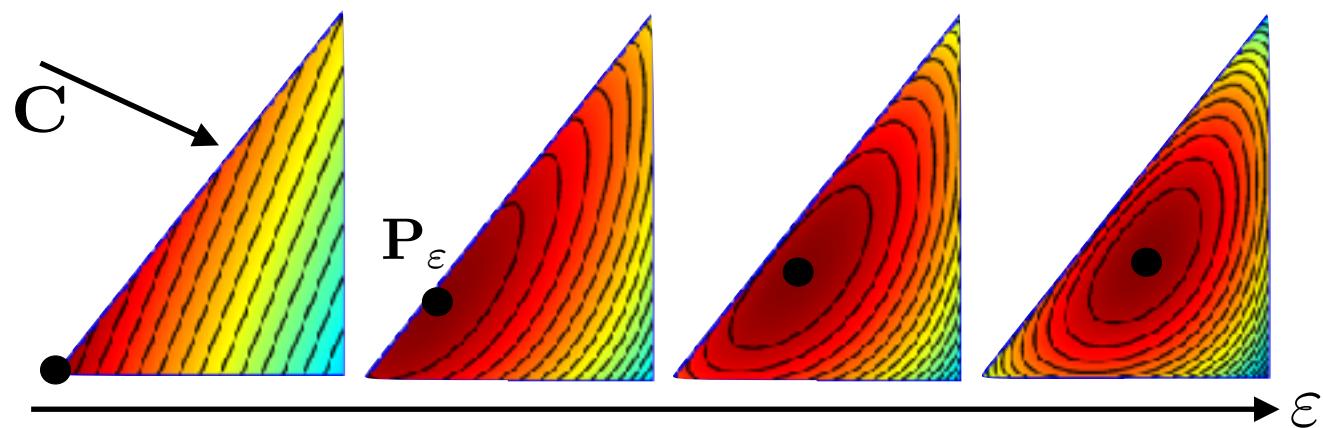
Overview

- **Entropic Regularization and Sinkhorn**
- Convergence Analysis
- Barycenters

Entropic Regularization

Entropy: $H(\mathbf{P}) \stackrel{\text{def.}}{=} -\sum_{i,j} \mathbf{P}_{i,j} (\log(\mathbf{P}_{i,j}) - 1)$

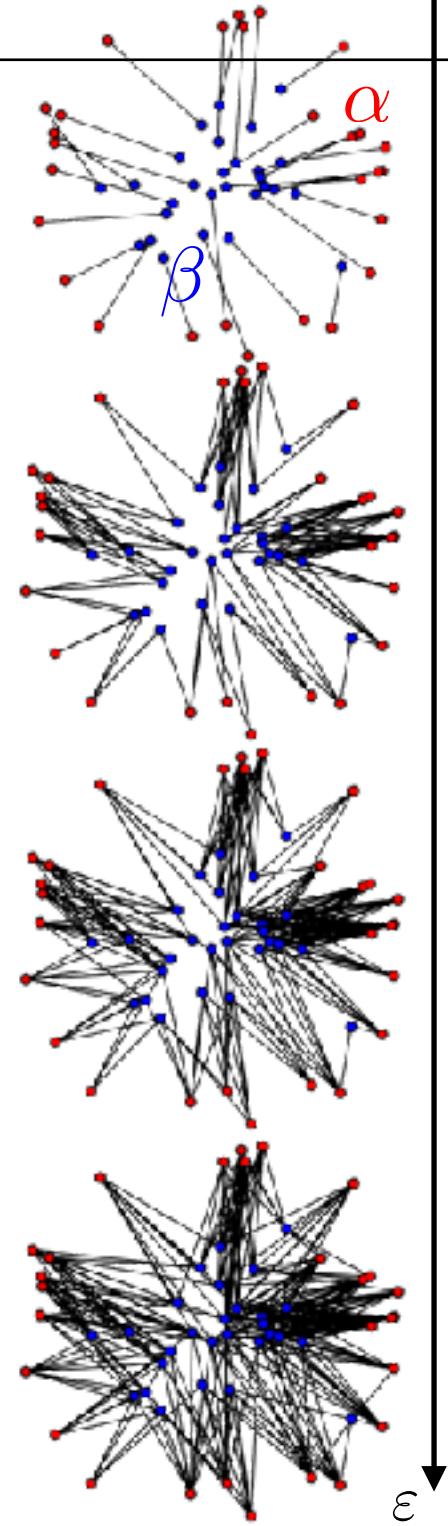
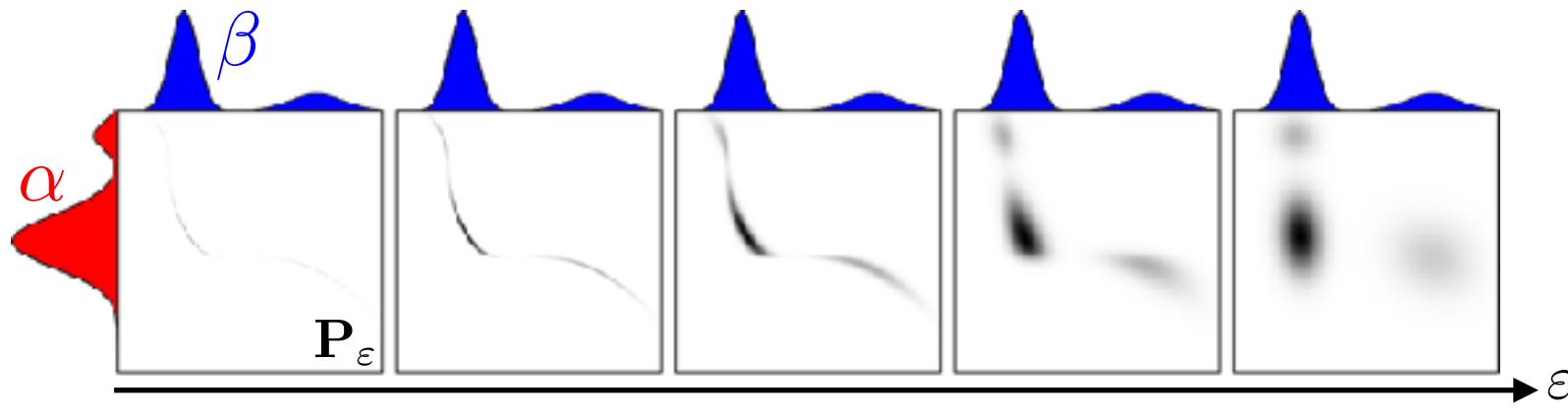
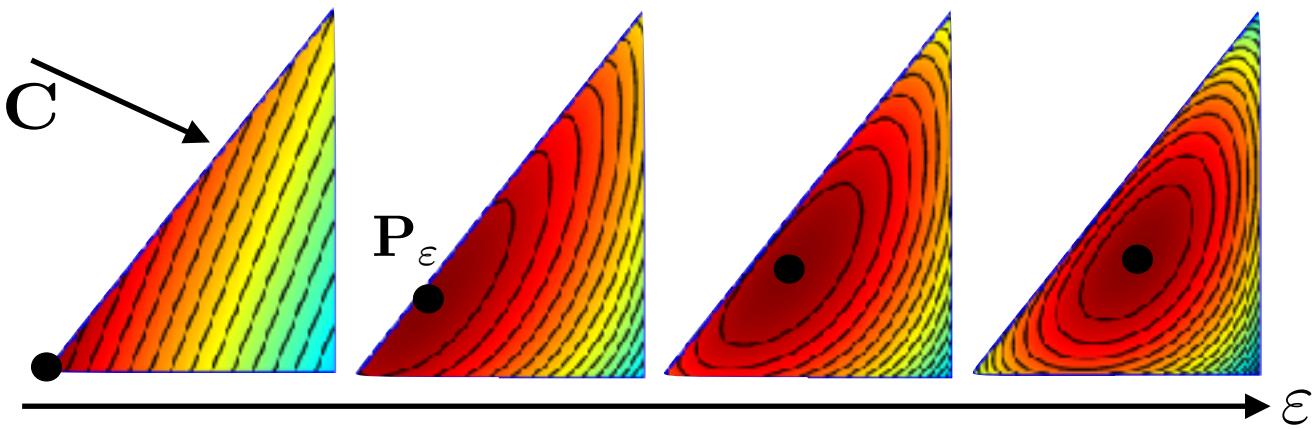
$$L_C^\varepsilon(\mathbf{a}, \mathbf{b}) \stackrel{\text{def.}}{=} \min_{\mathbf{P} \in \mathbf{U}(\mathbf{a}, \mathbf{b})} \langle \mathbf{P}, \mathbf{C} \rangle - \varepsilon H(\mathbf{P})$$



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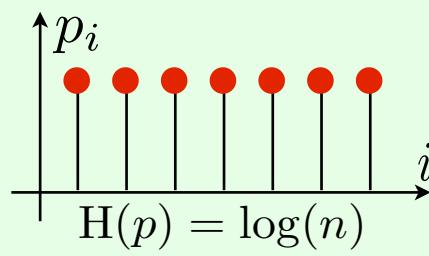
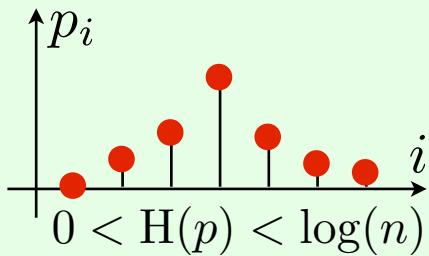
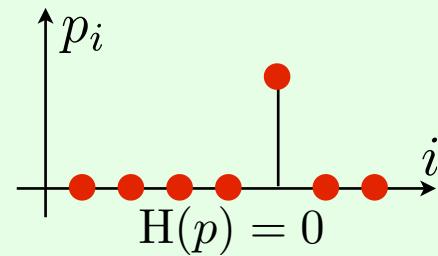
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Entropies

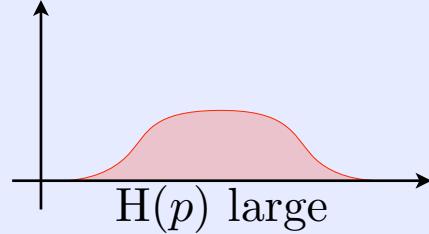
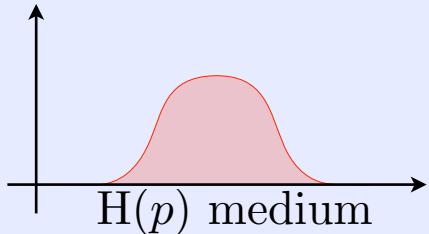
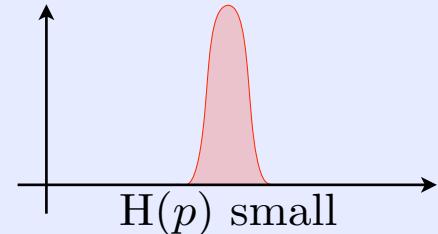
Discrete

$$p_i \geqslant 0, \sum_{i=1}^n p_i = 1 \quad H(p) \stackrel{\text{def.}}{=} -\sum_i p_i \log(p_i)$$



Continuous

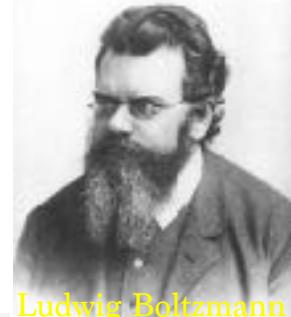
$$p(x) \geqslant 0, \int_{\mathbb{R}^d} p(x) = 1 \quad H(p) \stackrel{\text{def.}}{=} -\int_{\mathbb{R}^d} p(x) \log(p(x)) dx$$



General

Relative entropy (Kullback-Leibler)

$$\text{Measures } (\mu, \nu): \quad \text{KL}(\mu|\nu) \stackrel{\text{def.}}{=} \int_{\mathcal{X}} \log \left(\frac{d\mu}{d\nu}(x) \right) d\mu(x)$$



Arbitrary Measures

Relative-entropy:

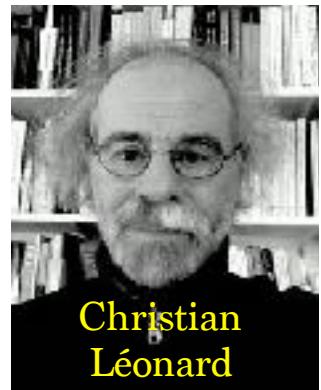
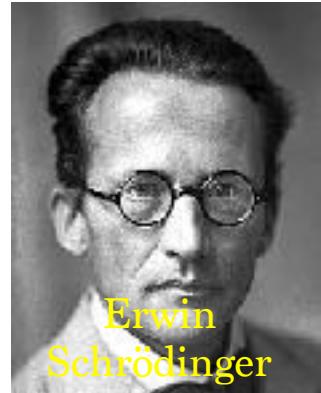
$$\text{KL}(\pi|\xi) \stackrel{\text{def.}}{=} \int_{\mathcal{X} \times \mathcal{Y}} \log \left(\frac{d\pi}{d\xi}(x, y) \right) d\pi(x, y) + \int_{\mathcal{X} \times \mathcal{Y}} (d\xi(x, y) - d\pi(x, y))$$

Schrödinger's problem: [1931]

$$\mathcal{L}_c^\varepsilon(\alpha, \beta) \stackrel{\text{def.}}{=} \min_{\pi \in \mathcal{U}(\alpha, \beta)} \int_{X \times Y} c(x, y) d\pi(x, y) + \varepsilon \text{KL}(\pi | \alpha \otimes \beta)$$

$$\min_{(X, Y)} \{ \mathbb{E}(c(X, Y)) + \varepsilon \text{I}(X, Y) ; X \sim \alpha, Y \sim \beta \}$$

Mutual information



Erwin
Schrödinger

Christian
Léonard

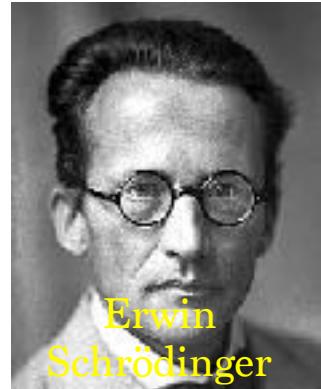
Arbitrary Measures

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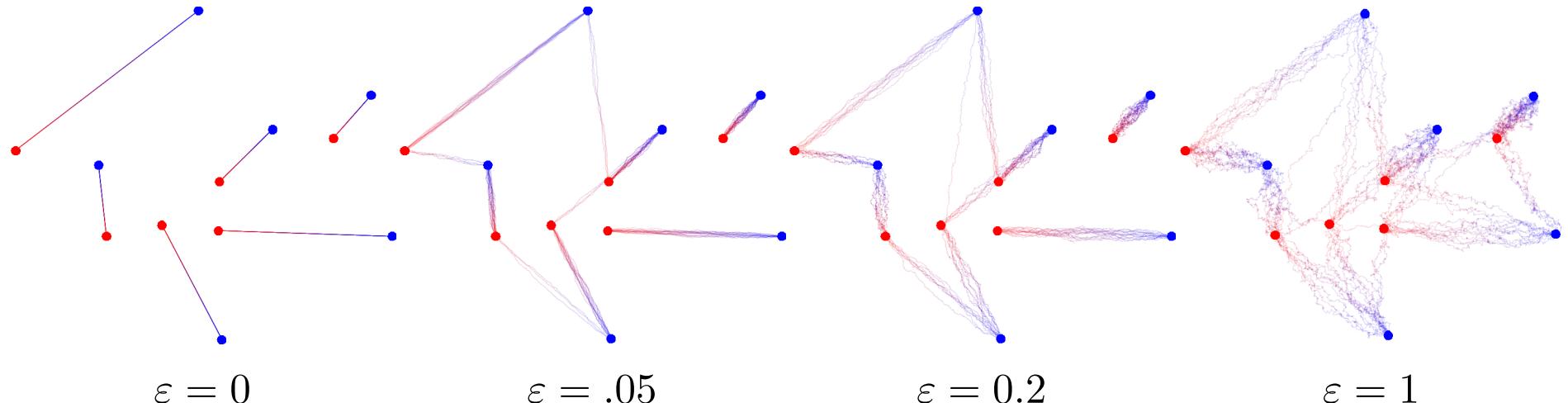
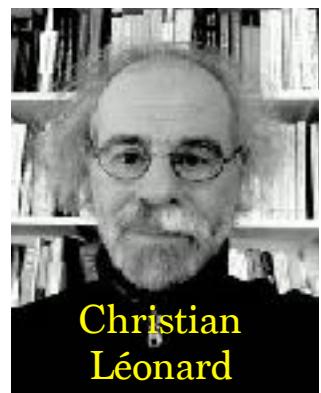
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Mutual information



Brownian Bridge

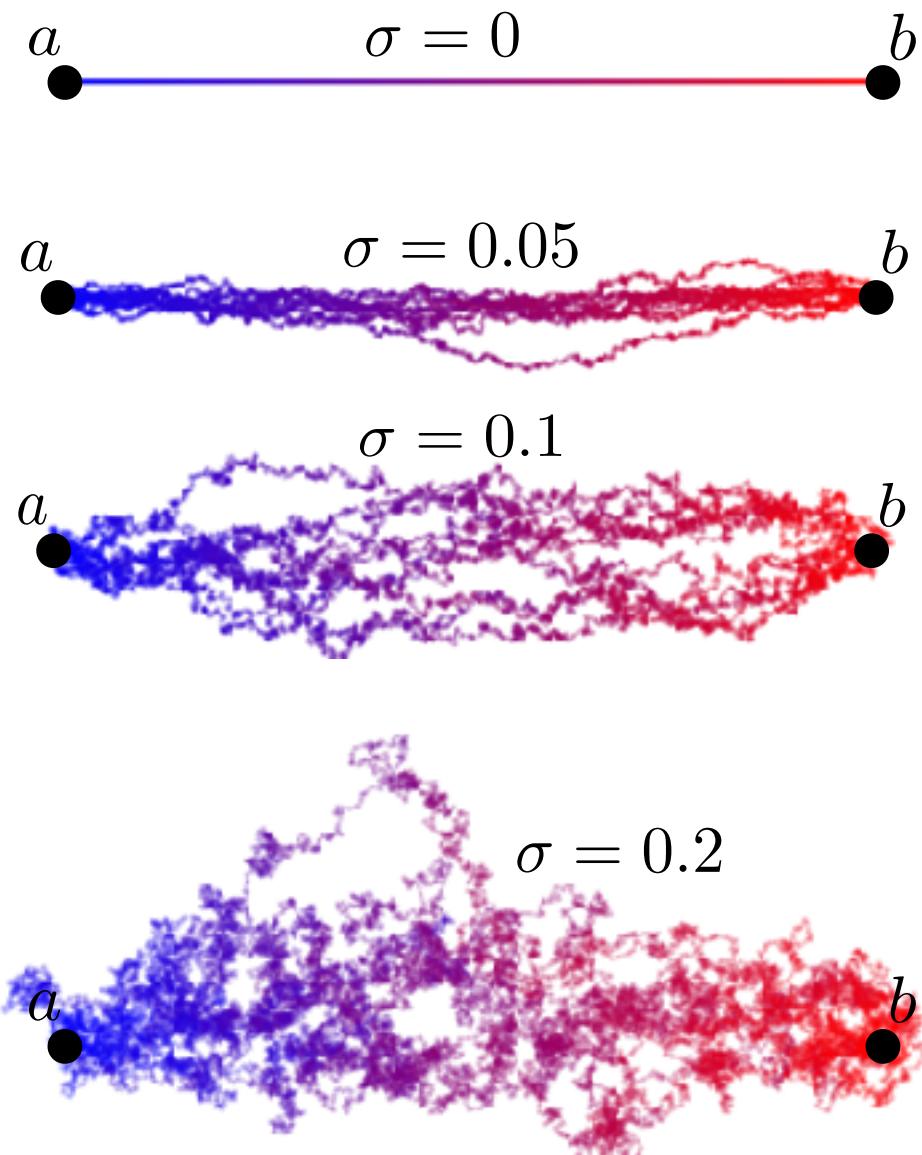
Random walk: $x_{k+1} = x_k + \frac{\sigma}{\sqrt{K}} \varepsilon_k$
 $\varepsilon_k \sim \mathcal{N}(0, \text{Id}_{\mathbb{R}^2})$

Brownian motion / Wiener process:

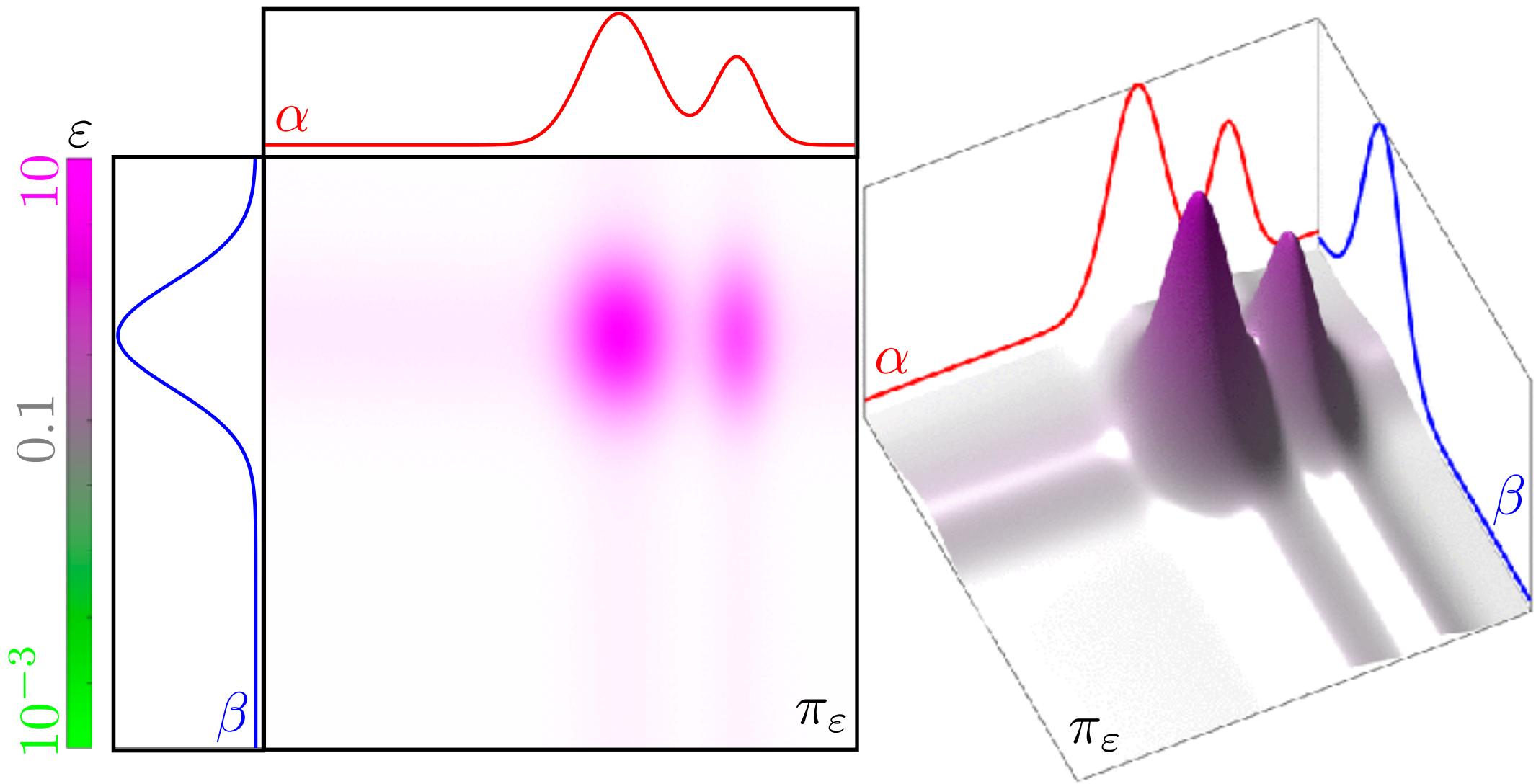
$$x_k \xrightarrow[k/K \rightarrow t]{K \rightarrow +\infty} W_t$$

Brownian bridge between $(a, b) \in \mathbb{C}^2$:

$$a + (b - a) \frac{x(t) - x(0)}{x(1) - x(0)}$$



Impact of Regularization



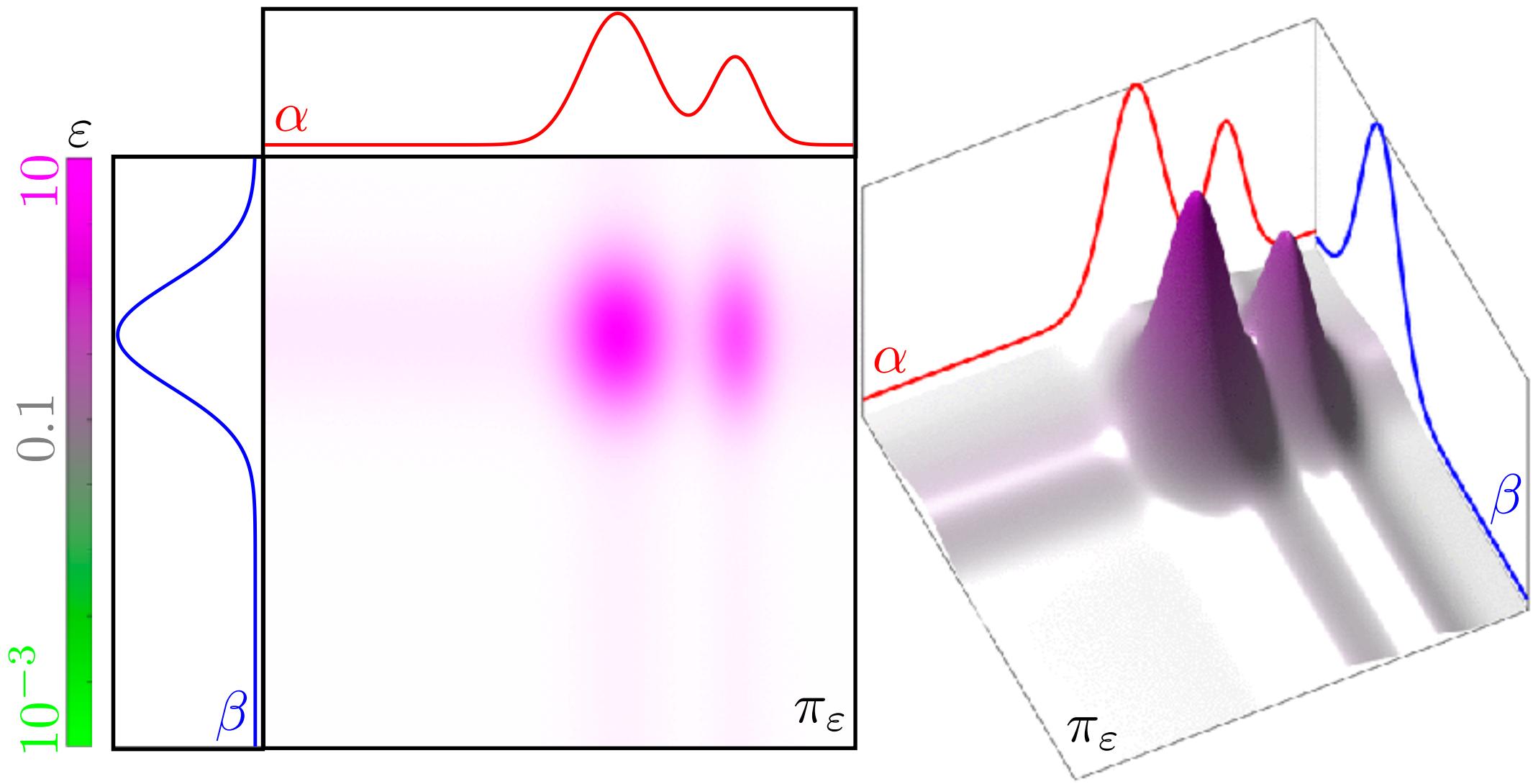
$$\pi_\varepsilon = \operatorname{argmin}_\pi \left\{ \int_{\mathbb{R}^2} \left(\|x - y\|^2 + \varepsilon \log \left(\frac{d\pi}{d\alpha d\beta}(x, y) \right) \right) d\pi(x, y) ; \; \pi_1 = \alpha, \pi_2 = \beta \right\}$$

Theorem:

$$\pi_\varepsilon \xrightarrow{\varepsilon \rightarrow +\infty} \alpha \otimes \beta$$

$$\pi_\varepsilon \xrightarrow{\varepsilon \rightarrow 0} \pi_{\text{OT}}$$

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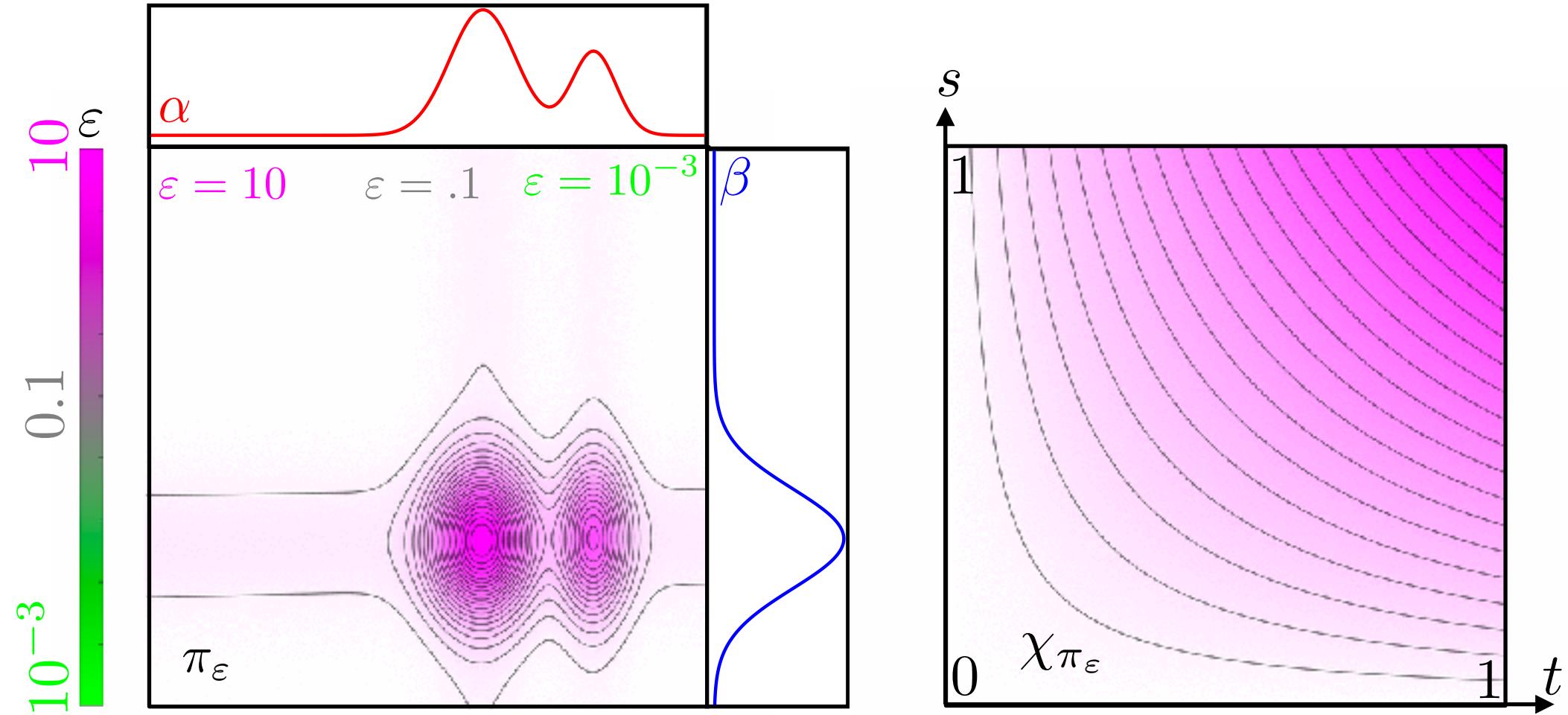
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Impact of Regularization

Cumulative: $C_\pi(x, y) \stackrel{\text{def.}}{=} \int_{-\infty}^x \int_{-\infty}^y d\pi(x, y)$

Copula: $\chi_\pi(s, t) \stackrel{\text{def.}}{=} C_\pi(C_\alpha^{-1}(s), C_\beta^{-1}(t))$

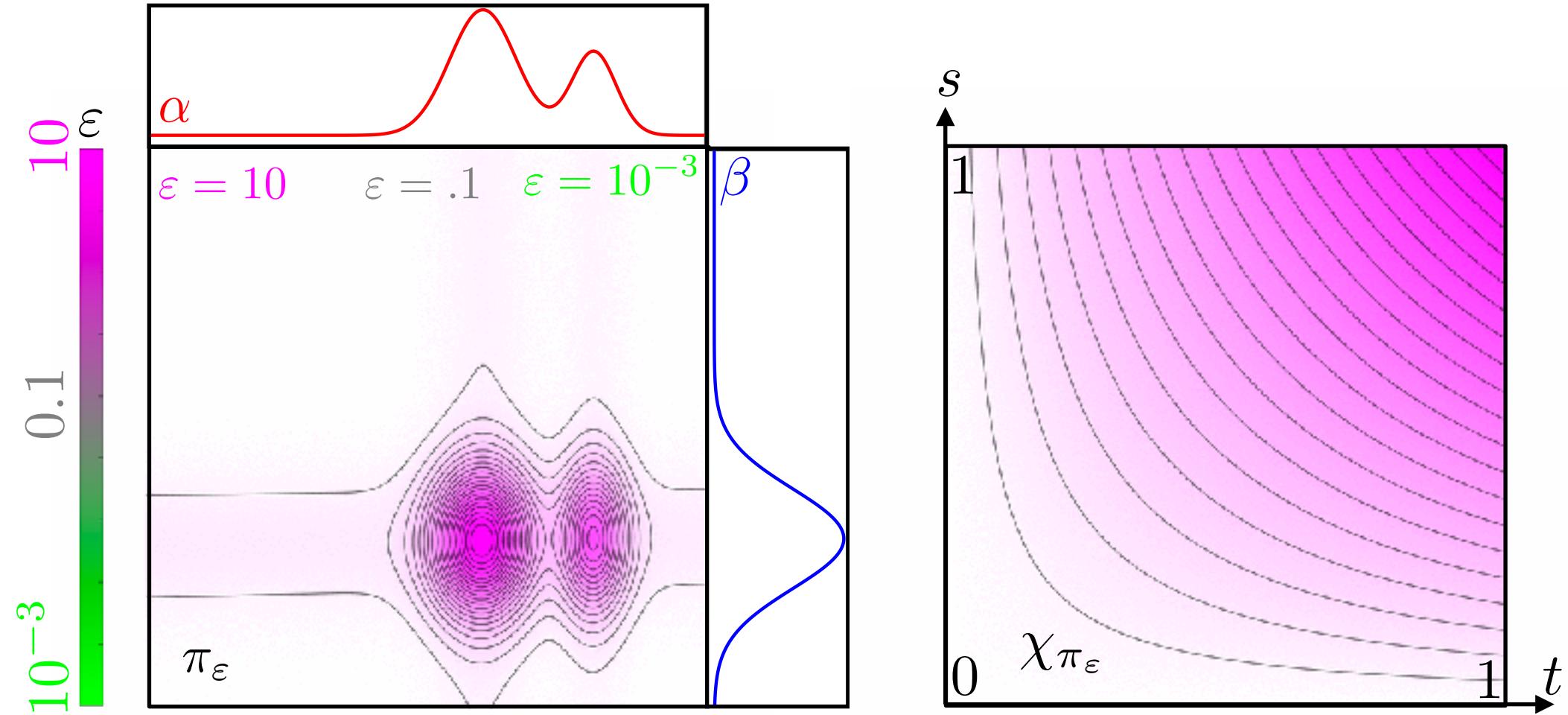


Theorem: $\chi_{\pi_\varepsilon}(s, t)$ $\begin{cases} \varepsilon \rightarrow 0 & \min(s, t) \\ \varepsilon \rightarrow +\infty & st \end{cases}$ (dependence)
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Sinkhorn's Algorithm

$$L_{\mathbf{C}}^{\varepsilon}(\mathbf{a}, \mathbf{b}) \stackrel{\text{def.}}{=} \min_{\mathbf{P} \in \mathbf{U}(\mathbf{a}, \mathbf{b})} \langle \mathbf{P}, \mathbf{C} \rangle - \varepsilon \mathbf{H}(\mathbf{P})$$

Proposition: $\forall (i, j) \in \llbracket n \rrbracket \times \llbracket m \rrbracket, \quad \mathbf{P}_{i,j} = \mathbf{u}_i \mathbf{K}_{i,j} \mathbf{v}_j$

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

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

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$$\mathbf{u}^{(\ell+1)} \stackrel{\text{def.}}{=} \frac{\mathbf{a}}{\mathbf{K}\mathbf{v}^{(\ell)}} \quad \text{and} \quad \mathbf{v}^{(\ell+1)} \stackrel{\text{def.}}{=} \frac{\mathbf{b}}{\mathbf{K}^T \mathbf{u}^{(\ell+1)}}$$

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Only matrix/vector multiplications.

Matrix-vectors

$$\mathbf{K} \begin{array}{|c|} \hline \text{v}^1 \\ \hline \end{array}, \dots, \mathbf{K} \begin{array}{|c|} \hline \text{v}^q \\ \hline \end{array}$$

parallelization
GPU

Matrix-matrix

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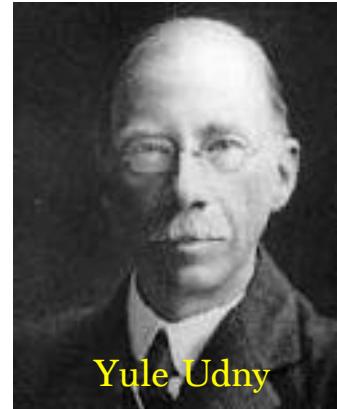
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→ Convolution on regular grids, separable kernels.

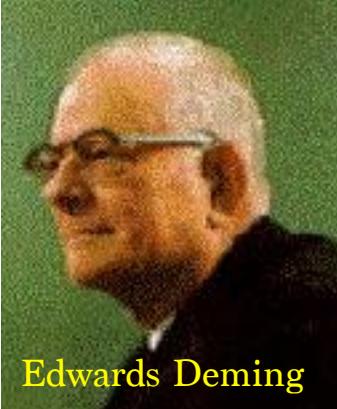
Sinkhorn, IPFP, RAS, ...



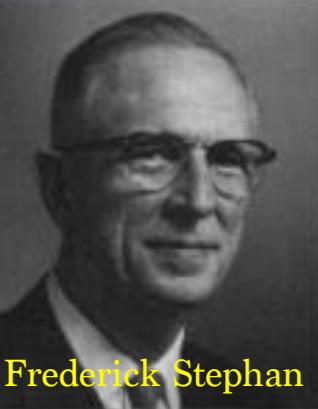
Richard Dennis Sinkhorn



Yule Udney



Edwards Deming



Frederick Stephan

Many names:

Sinkhorn algorithm

DAD scaling

Iterative proportional fitting

Biproportional fitting

RAS algorithm

Matrix scaling

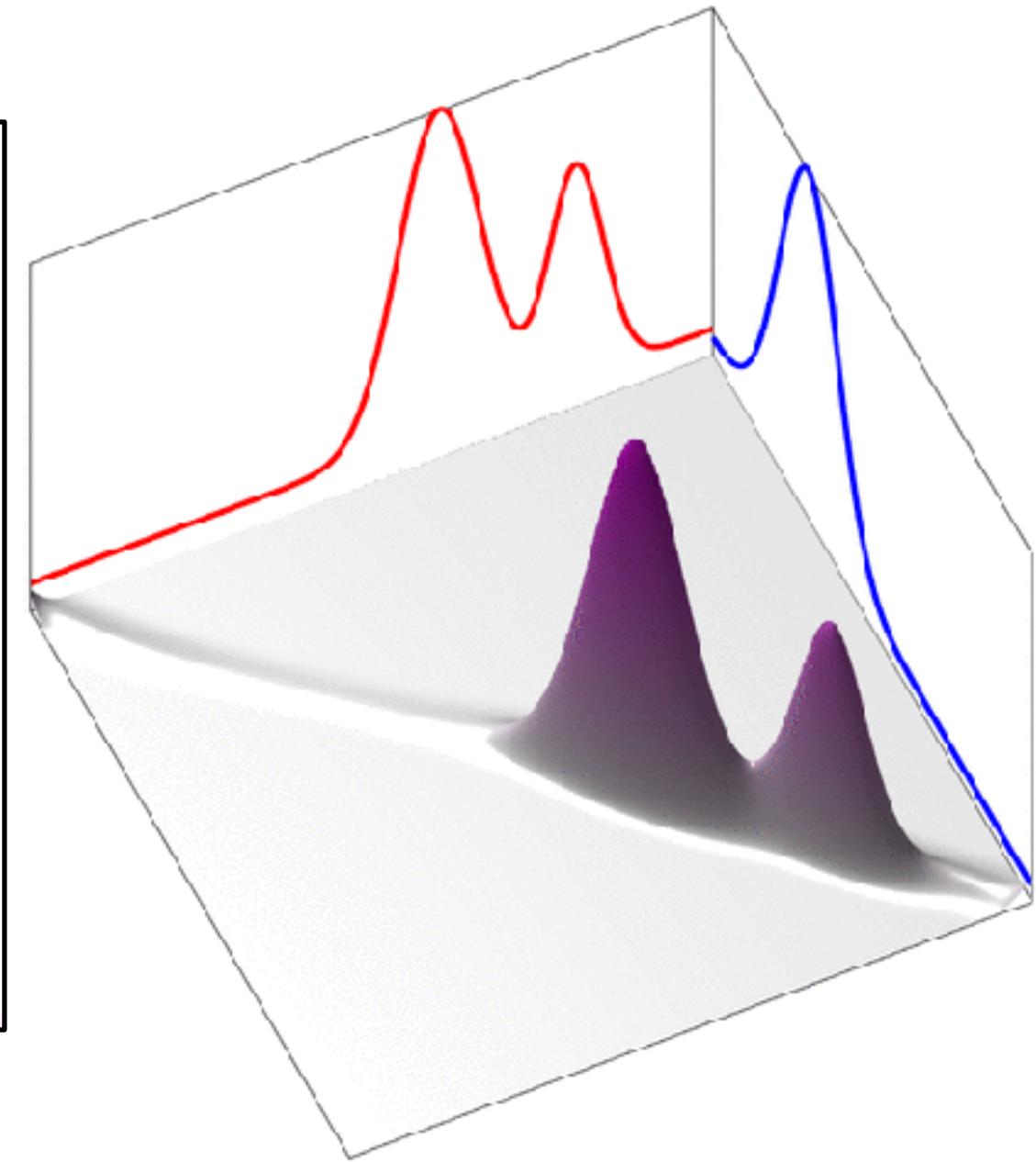
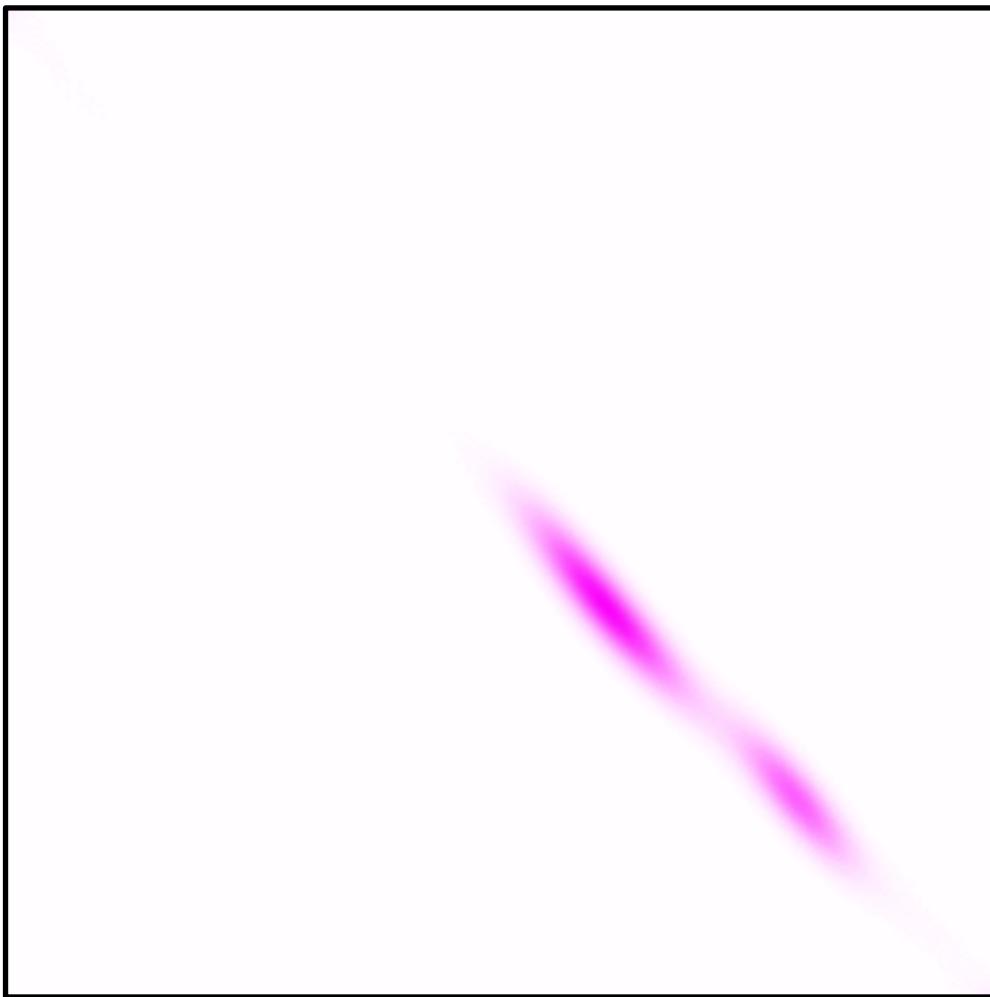
Udny 1912

Kruithof, 1937

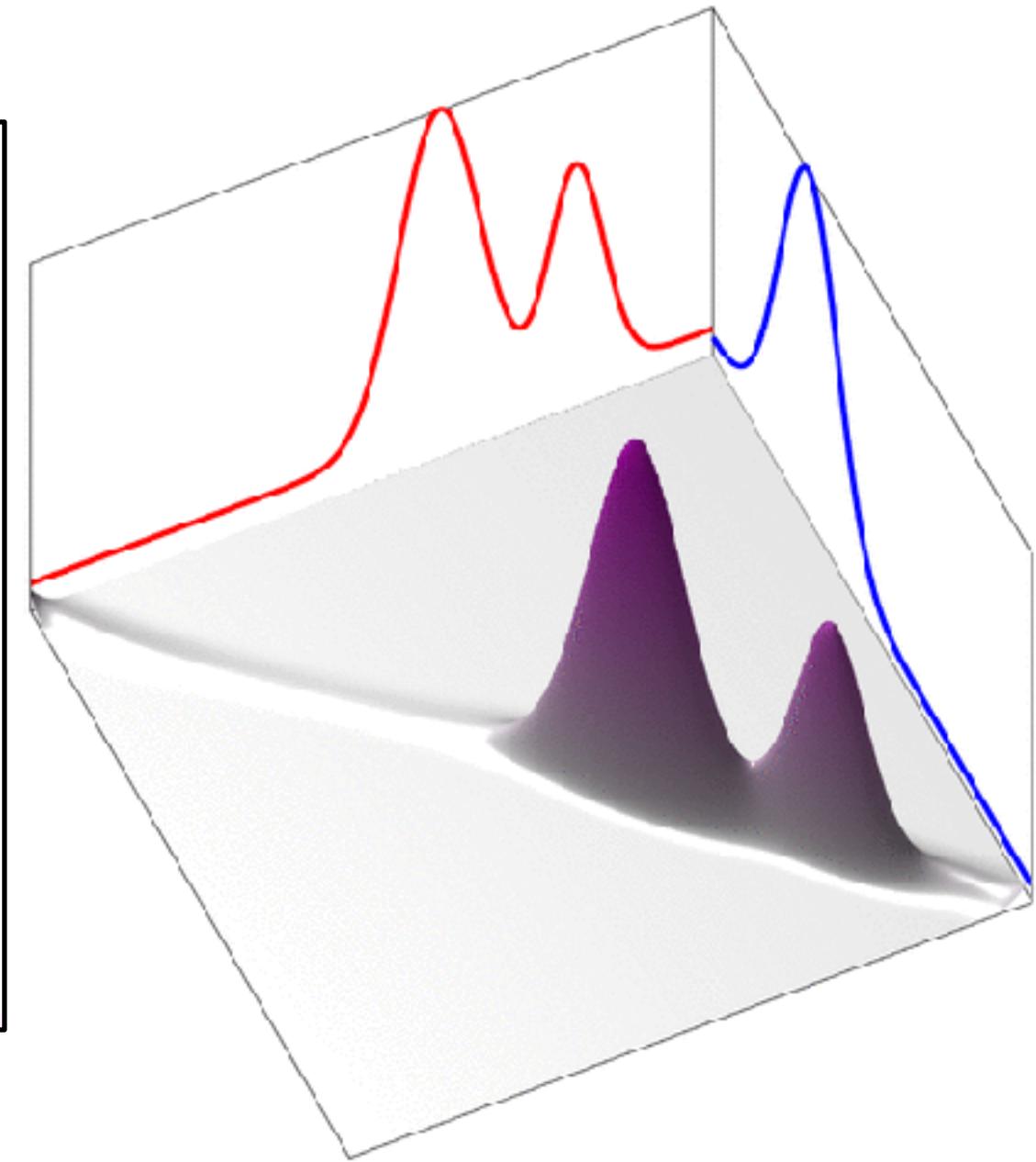
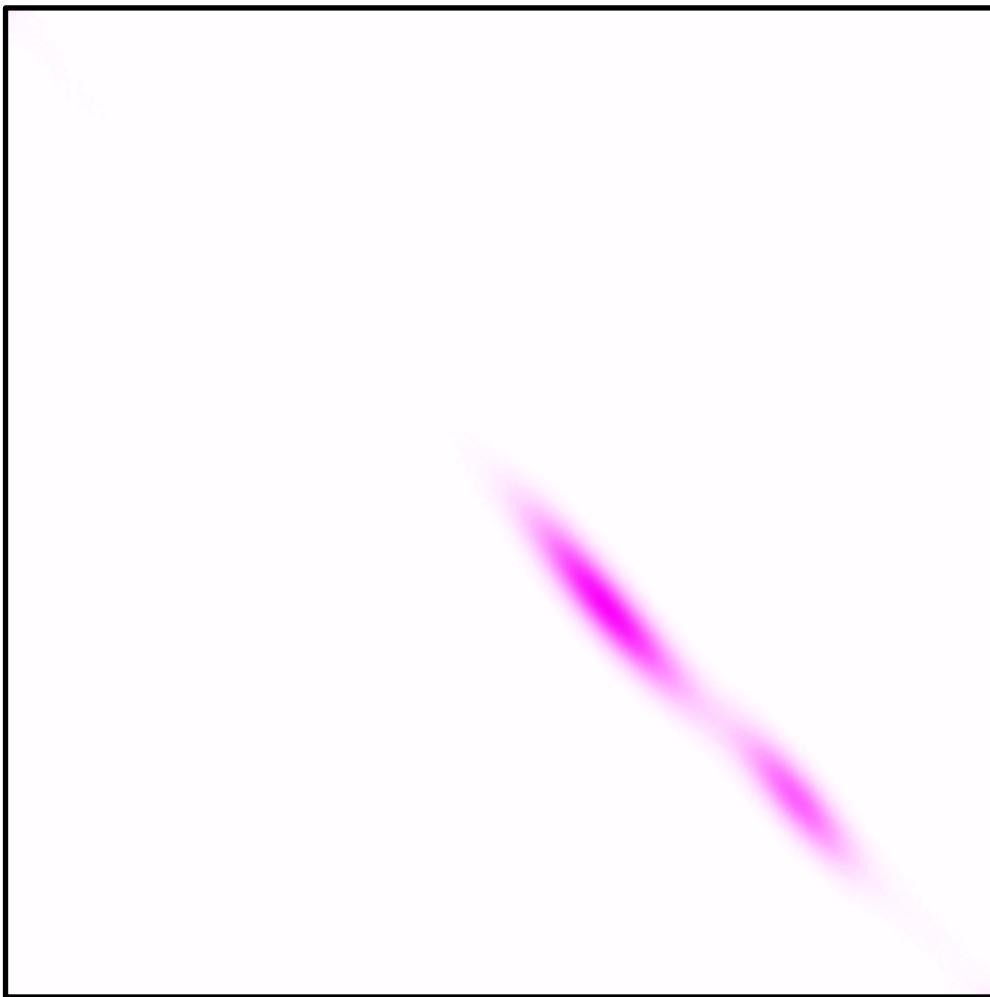
Deming and Stephan in 1940

Sinkhorn 1964

Sinkhorn Evolution

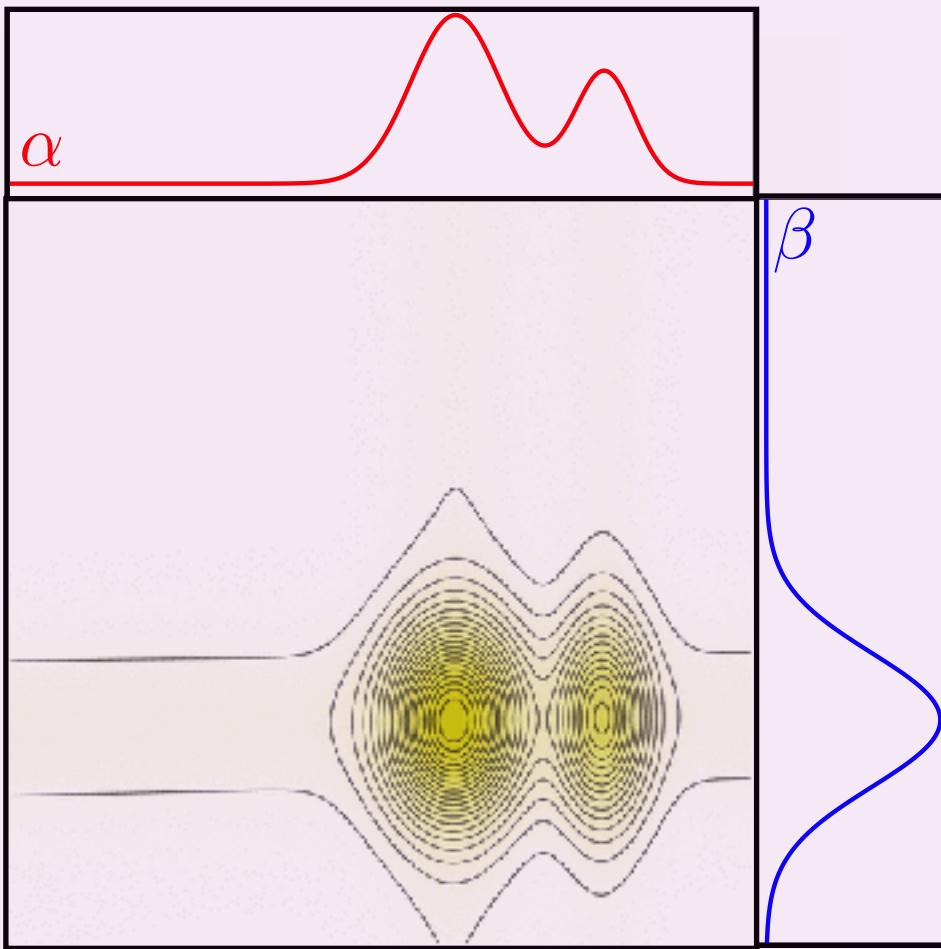


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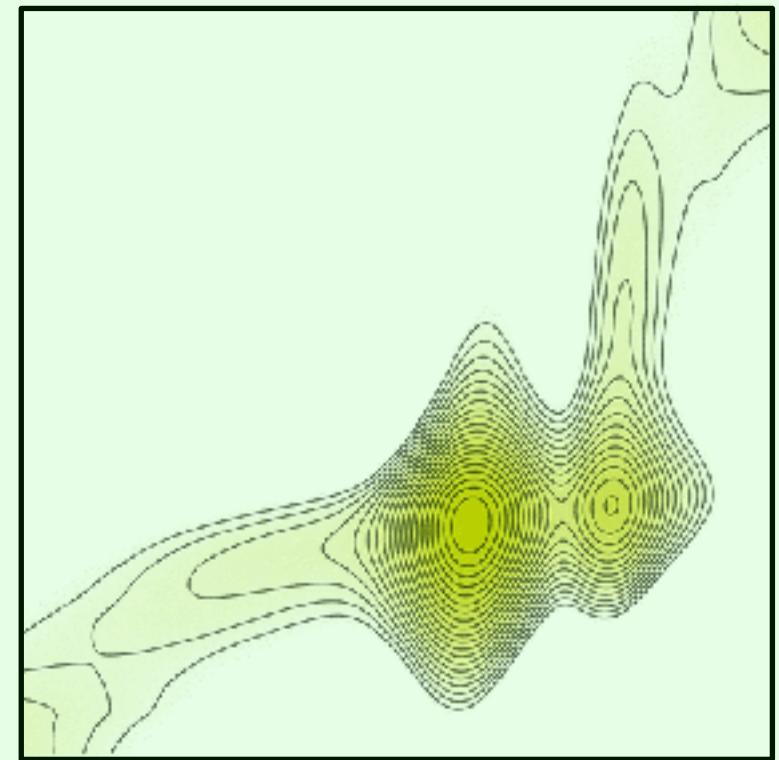
Other Regularizations

$$\min_{\pi} \left\{ \int_{\mathbb{R}^2} \|x - y\|^2 d\pi(x, y) + \varepsilon R(\pi) ; \pi_1 = \alpha, \pi_2 = \beta \right\}$$



$$R(\pi) = \int \log \left(\frac{d\pi}{dxdy} \right) d\pi(x, y)$$

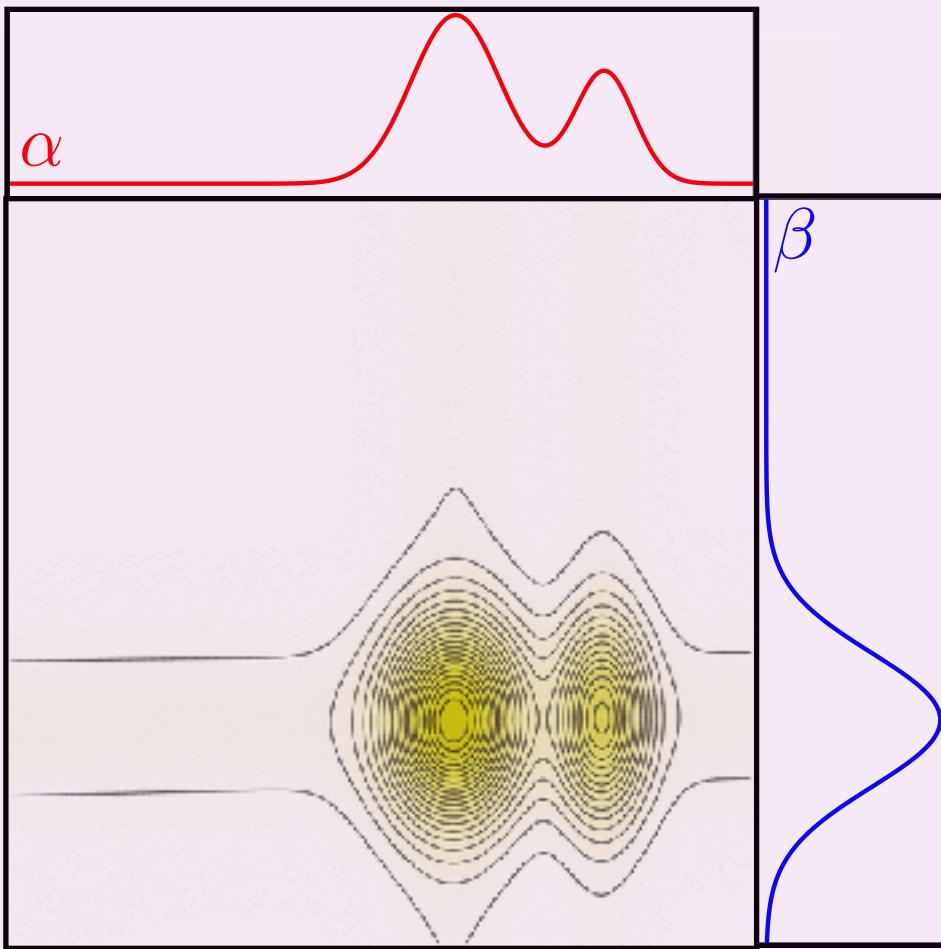
Dykstra's algorithm



$$R(\pi) = \int \left(\frac{d\pi}{dxdy} \right)^2 dx dy$$

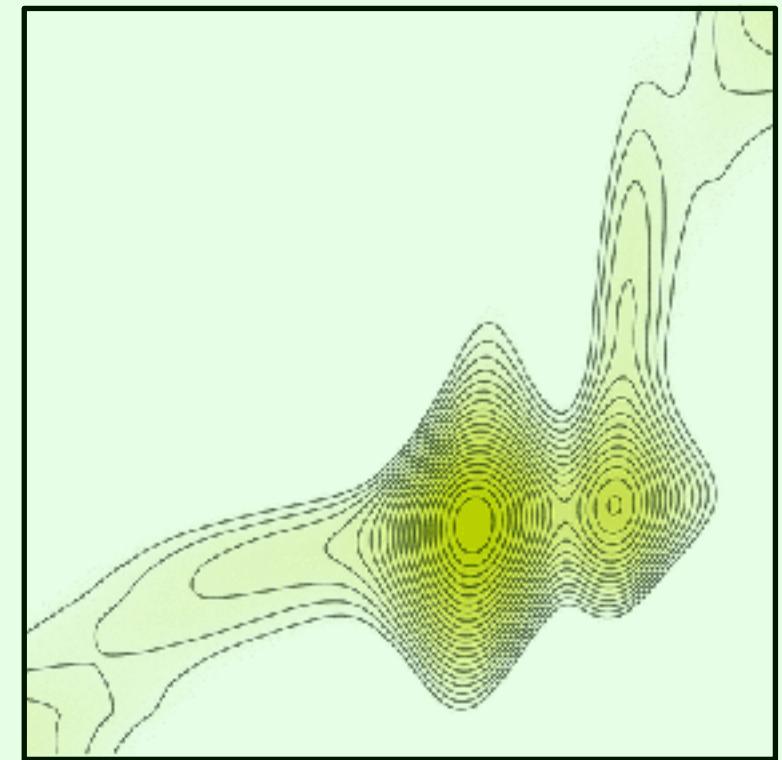
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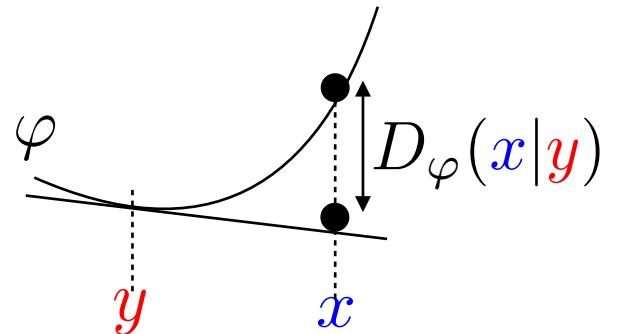
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Bregman Divergences

Bregman divergence: φ convex

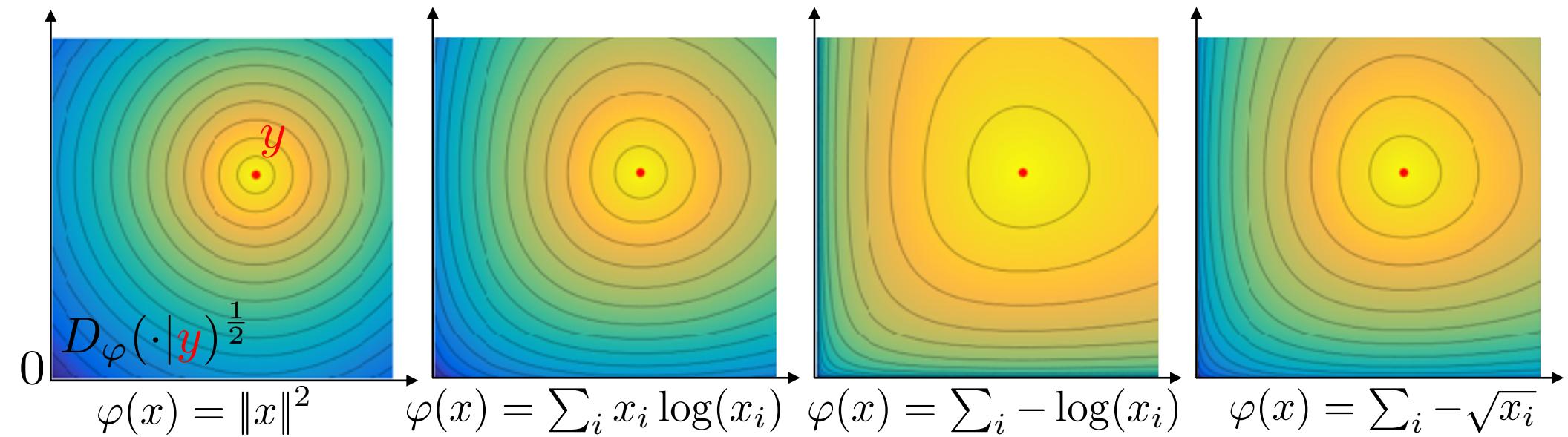
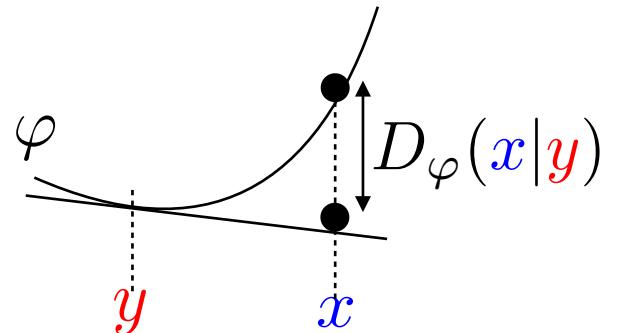
$$D_\varphi(\mathbf{x}|\mathbf{y}) \stackrel{\text{def.}}{=} \varphi(\mathbf{x}) - \varphi(\mathbf{y}) - \langle \mathbf{x} - \mathbf{y}, \nabla \varphi(\mathbf{y}) \rangle$$



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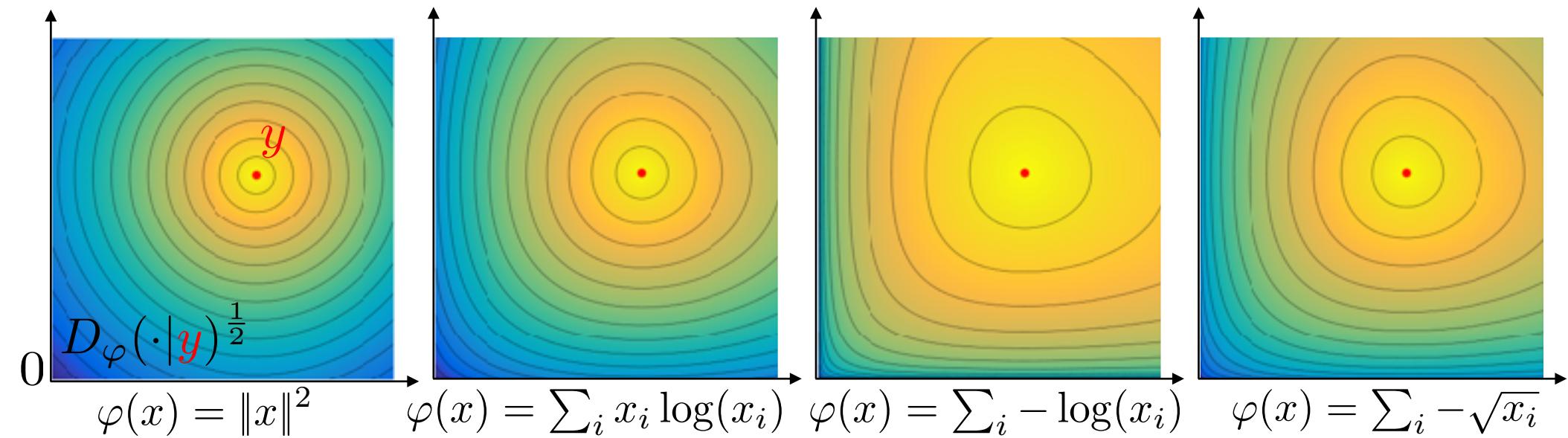
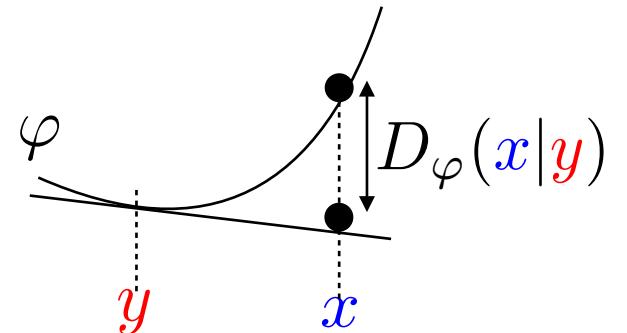
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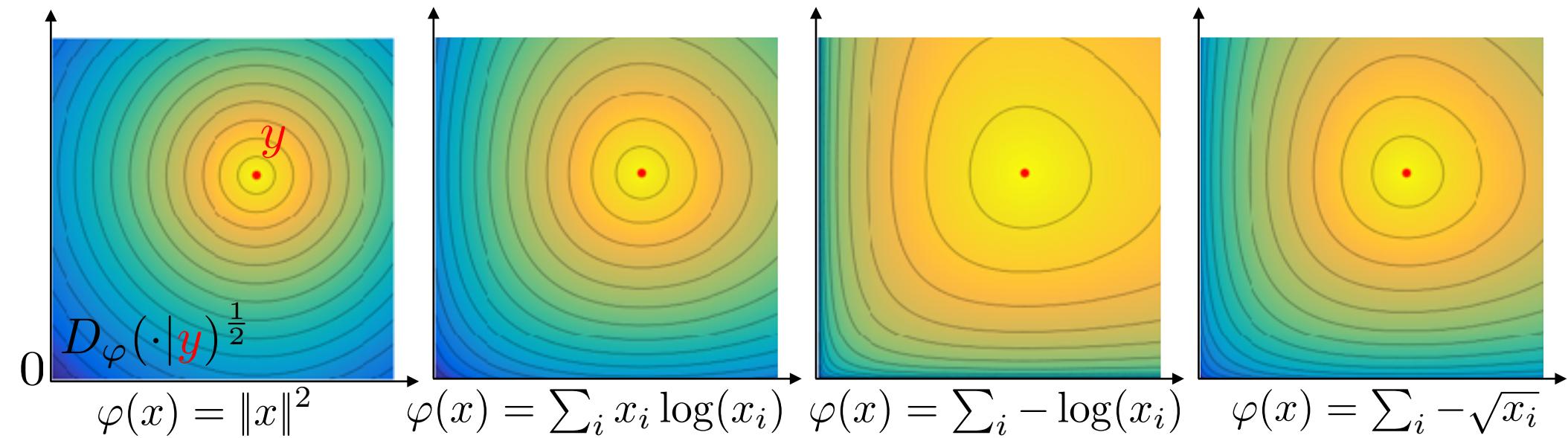
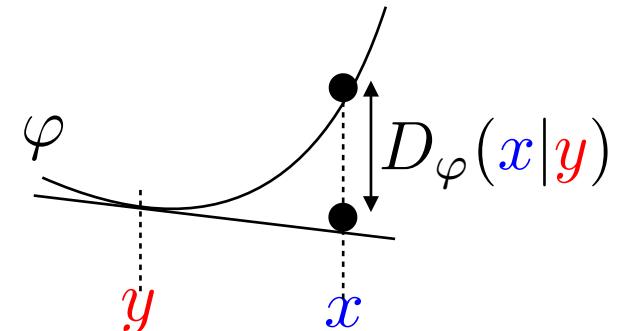


Locally Euclidean:
$$\left. \begin{aligned} & D_\varphi(x|x + \varepsilon) \\ & D_\varphi(x + \varepsilon|x) \end{aligned} \right\} = \frac{1}{2} \langle \partial^2 \varphi(x) \varepsilon, \varepsilon \rangle + o(\|\varepsilon\|^2)$$

Bregman Divergences

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Usually do not work for Radon Measures. Need to use f-divergences

Bregman Iterative Projections

KL divergence:

$$\text{KL}(\mathbf{P}|\mathbf{K}) \stackrel{\text{def.}}{=} \sum_{i,j} \mathbf{P}_{i,j} \log \left(\frac{\mathbf{P}_{i,j}}{\mathbf{K}_{i,j}} \right) - \mathbf{P}_{i,j} + \mathbf{K}_{i,j}$$

$$\text{KL}(\mathbf{P}|\mathbf{K}) = D_\varphi(\mathbf{P}|\mathbf{K}) \quad \text{for} \quad \varphi(\mathbf{P}) = \sum_{i,j} \mathbf{P}_{i,j} \log(\mathbf{P}_{i,j})$$

Proposition :

$$\min_{\mathbf{P} \in \mathbf{U}(\mathbf{a}, \mathbf{b})} \langle \mathbf{P}, \mathbf{C} \rangle - \varepsilon \mathbf{H}(\mathbf{P}) \iff \min_{\mathbf{P} \in \mathbf{U}(\mathbf{a}, \mathbf{b})} \varepsilon \text{KL}(\mathbf{P}|\mathbf{K}) \quad \mathbf{K}_{i,j} \stackrel{\text{def.}}{=} e^{-\frac{\mathbf{C}_{i,j}}{\varepsilon}}$$

Bregman Iterative Projections

KL divergence:

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$$\text{KL}(\mathbf{P}|\mathbf{K}) = D_\varphi(\mathbf{P}|\mathbf{K}) \quad \text{for} \quad \varphi(\mathbf{P}) = \sum_{i,j} \mathbf{P}_{i,j} \log(\mathbf{P}_{i,j})$$

Proposition :

$$\min_{\mathbf{P} \in \mathbf{U}(\mathbf{a}, \mathbf{b})} \langle \mathbf{P}, \mathbf{C} \rangle - \varepsilon \mathbf{H}(\mathbf{P}) \iff \min_{\mathbf{P} \in \mathbf{U}(\mathbf{a}, \mathbf{b})} \varepsilon \text{KL}(\mathbf{P}|\mathbf{K}) \quad \mathbf{K}_{i,j} \stackrel{\text{def.}}{=} e^{-\frac{\mathbf{C}_{i,j}}{\varepsilon}}$$

$$\mathbf{U}(\mathbf{a}, \mathbf{b}) = \mathcal{C}_{\mathbf{a}}^1 \cup \mathcal{C}_{\mathbf{b}}^2$$

$$\mathcal{C}_{\mathbf{a}}^1 \stackrel{\text{def.}}{=} \{ \mathbf{P} : \mathbf{P} \mathbb{1}_m = \mathbf{a} \}$$

$$\mathcal{C}_{\mathbf{b}}^2 \stackrel{\text{def.}}{=} \left\{ \mathbf{P} : \mathbf{P}^T \mathbb{1}_m = \mathbf{b} \right\}$$

Bregman Iterative Projections

KL divergence:

$$\text{KL}(\mathbf{P}|\mathbf{K}) \stackrel{\text{def.}}{=} \sum_{i,j} \mathbf{P}_{i,j} \log \left(\frac{\mathbf{P}_{i,j}}{\mathbf{K}_{i,j}} \right) - \mathbf{P}_{i,j} + \mathbf{K}_{i,j}$$

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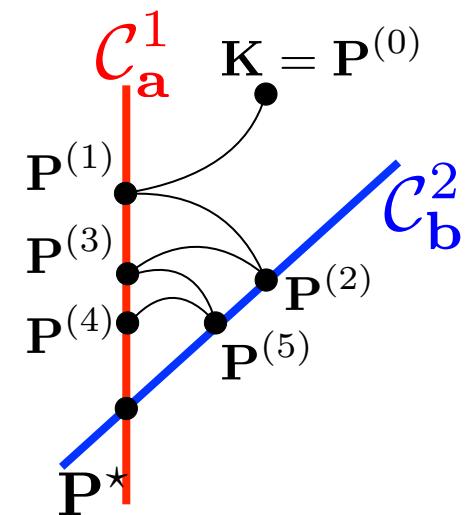
$$\min_{\mathbf{P} \in \mathbf{U}(\mathbf{a}, \mathbf{b})} \langle \mathbf{P}, \mathbf{C} \rangle - \varepsilon \mathbf{H}(\mathbf{P}) \iff \min_{\mathbf{P} \in \mathbf{U}(\mathbf{a}, \mathbf{b})} \varepsilon \text{KL}(\mathbf{P}|\mathbf{K}) \quad \mathbf{K}_{i,j} \stackrel{\text{def.}}{=} e^{-\frac{\mathbf{C}_{i,j}}{\varepsilon}}$$

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Iterative projections: $\mathbf{P}^{(\ell+1)} \stackrel{\text{def.}}{=} \text{Proj}_{\mathcal{C}_{\mathbf{a}}^1}^{\text{KL}}(\mathbf{P}^{(\ell)})$ and $\mathbf{P}^{(\ell+2)} \stackrel{\text{def.}}{=} \text{Proj}_{\mathcal{C}_{\mathbf{b}}^2}^{\text{KL}}(\mathbf{P}^{(\ell+1)})$

Theorem: $\mathbf{P}^{(\ell)} \rightarrow \mathbf{P}^* = \underset{\mathbf{P} \in \mathcal{C}_{\mathbf{a}}^1 \cap \mathcal{C}_{\mathbf{b}}^2}{\operatorname{argmin}} \text{KL}(\mathbf{P}|\mathbf{K})$
 For affine $(\mathcal{C}_{\mathbf{a}}^1, \mathcal{C}_{\mathbf{b}}^2)$,

[Bregman, 1967]



Bregman Iterative Projections

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Proposition :

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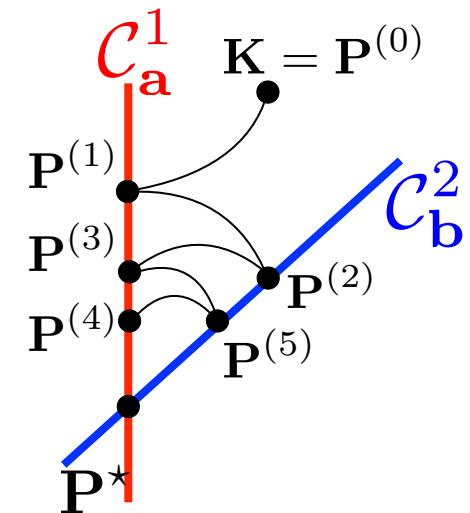
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Sinkhorn \iff iterative projections.

$$\mathbf{P}^{(2\ell)} \stackrel{\text{def.}}{=} \text{diag}(\mathbf{u}^{(\ell)}) \mathbf{K} \text{diag}(\mathbf{v}^{(\ell)}), \quad \mathbf{P}^{(2\ell+1)} \stackrel{\text{def.}}{=} \text{diag}(\mathbf{u}^{(\ell+1)}) \mathbf{K} \text{diag}(\mathbf{v}^{(\ell)})$$



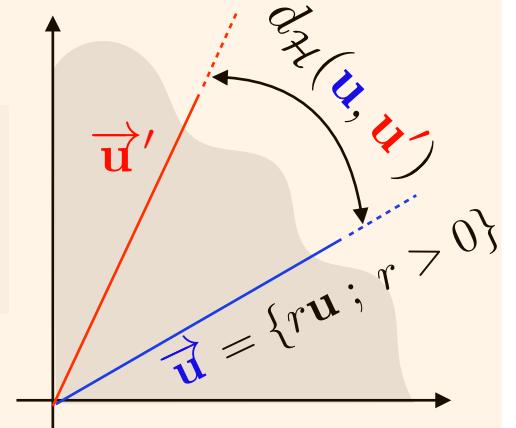
Hilbert Projective Metric

Hilbert's projective metric:



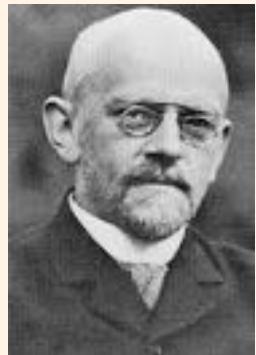
$$\forall (\mathbf{u}, \mathbf{u}') \in (\mathbb{R}_{+,*}^n)^2, \quad d_{\mathcal{H}}(\mathbf{u}, \mathbf{u}') \stackrel{\text{def.}}{=} \log \max_{i,i'} \frac{\mathbf{u}_i \mathbf{u}'_{i'}}{\mathbf{u}_{i'} \mathbf{u}'_i}.$$

$d_{\mathcal{H}}$ is a distance on the set of rays $\overrightarrow{\mathbf{u}}$.



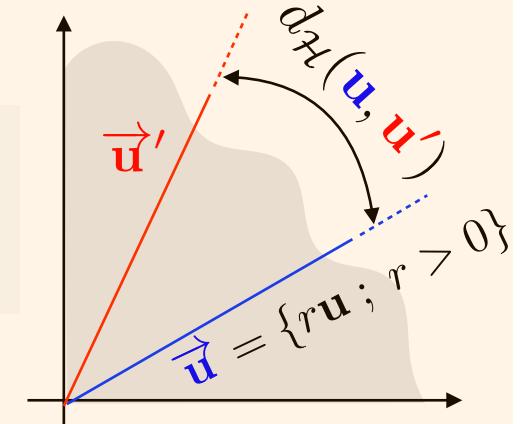
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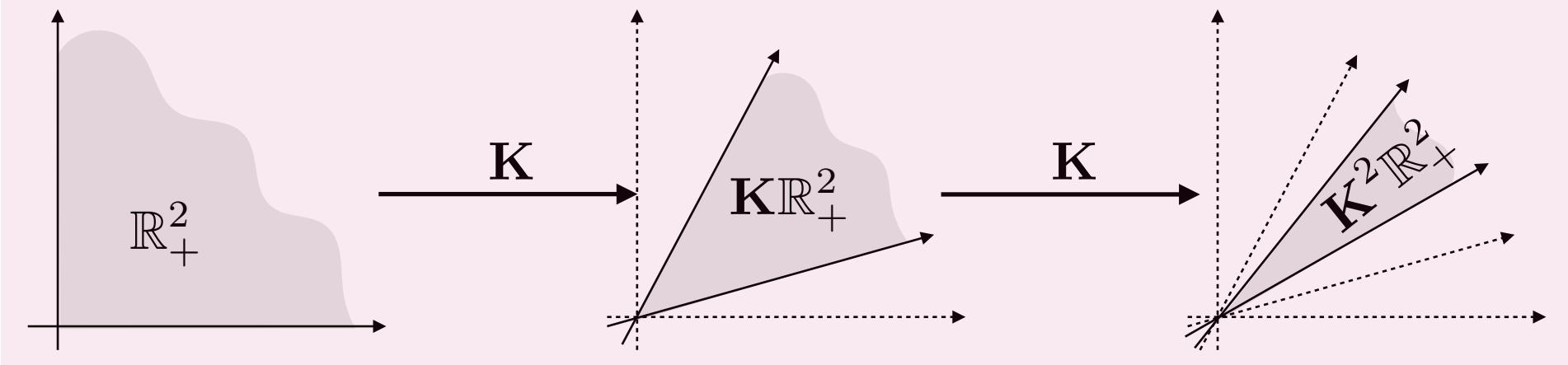


Birkhoff's contraction theorem:



Theorem 1.1. Let $\mathbf{K} \in \mathbb{R}_{+,*}^{n \times m}$, then for $(\mathbf{v}, \mathbf{v}') \in (\mathbb{R}_{+,*}^m)^2$

$$d_{\mathcal{H}}(\mathbf{K}\mathbf{v}, \mathbf{K}\mathbf{v}') \leq \lambda(\mathbf{K})d_{\mathcal{H}}(\mathbf{v}, \mathbf{v}') \text{ where } \begin{cases} \lambda(\mathbf{K}) \stackrel{\text{def.}}{=} \frac{\sqrt{\eta(\mathbf{K})}-1}{\sqrt{\eta(\mathbf{K})}+1} < 1 \\ \eta(\mathbf{K}) \stackrel{\text{def.}}{=} \max_{i,j,k,\ell} \frac{\mathbf{K}_{i,k} \mathbf{K}_{j,\ell}}{\mathbf{K}_{j,k} \mathbf{K}_{i,\ell}}. \end{cases}$$



Perron Frobenius

Simplex: $\Sigma_k = \{p \in \mathbb{R}_+^k ; \sum_i p_i = 1\}$

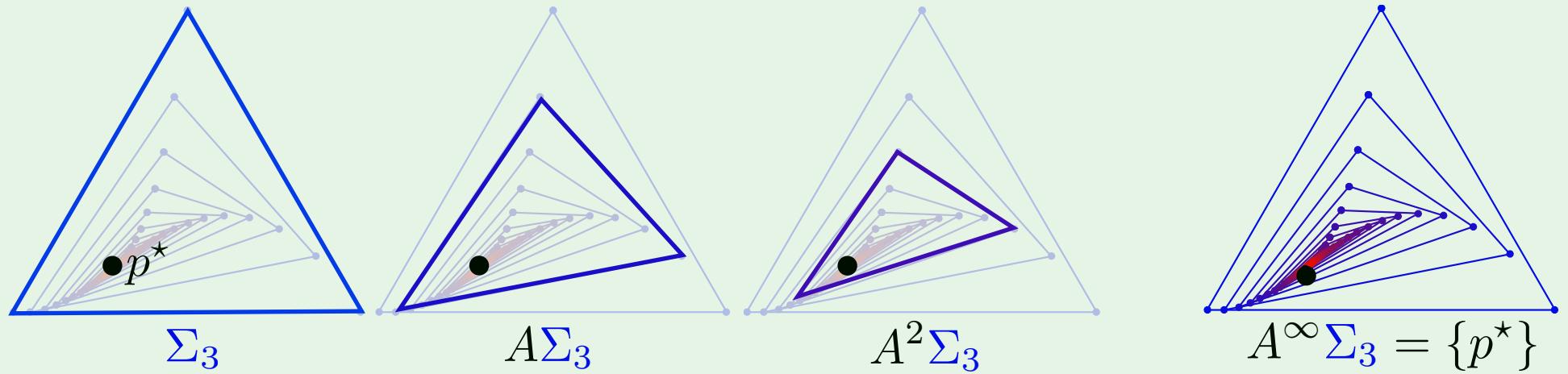
$$A : \Sigma_k \rightarrow \Sigma_k$$

Stochastic matrix: $A \in \mathbb{R}_+^n, A^\top \mathbf{1}_k = \mathbf{1}_k$

Theorem: [Perron-Frobenius]

If $A > 0$, $\exists! p^*$, $Ap^* = p^*$.

$$\exists \rho \in [0, 1[, \|A^k p - p^*\| \leq \rho^k$$



Sinkhorn under Hilbert's Metric

Sinkhorn iterations:

$$\mathbf{u}^{(\ell+1)} \stackrel{\text{def.}}{=} \frac{\mathbf{a}}{\mathbf{K}\mathbf{v}^{(\ell)}} \quad \text{and} \quad \mathbf{v}^{(\ell+1)} \stackrel{\text{def.}}{=} \frac{\mathbf{b}}{\mathbf{K}^T \mathbf{u}^{(\ell+1)}}$$

[Franklin and Lorenz, 1989]

Theorem: One has $(\mathbf{u}^{(\ell)}, \mathbf{v}^{(\ell)}) \rightarrow (\mathbf{u}^*, \mathbf{v}^*)$

$$d_{\mathcal{H}}(\mathbf{u}^{(\ell)}, \mathbf{u}^*) = O(\lambda(\mathbf{K})^{2\ell}), \quad d_{\mathcal{H}}(\mathbf{v}^{(\ell)}, \mathbf{v}^*) = O(\lambda(\mathbf{K})^{2\ell}).$$

$$d_{\mathcal{H}}(\mathbf{u}^{(\ell)}, \mathbf{u}^*) \leq \frac{d_{\mathcal{H}}(\mathbf{P}^{(\ell)} \mathbb{1}_m, \mathbf{a})}{1 - \lambda(\mathbf{K})^2}$$

$$d_{\mathcal{H}}(\mathbf{v}^{(\ell)}, \mathbf{v}^*) \leq \frac{d_{\mathcal{H}}(\mathbf{P}^{(\ell), \top} \mathbb{1}_n, \mathbf{b})}{1 - \lambda(\mathbf{K})^2}$$

$$\|\log(\mathbf{P}^{(\ell)}) - \log(\mathbf{P}^*)\|_\infty \leq d_{\mathcal{H}}(\mathbf{u}^{(\ell)}, \mathbf{u}^*) + d_{\mathcal{H}}(\mathbf{v}^{(\ell)}, \mathbf{v}^*)$$

Local Analysis of Sinkhorn

Sinkhorn fixed point: $\mathbf{f}^{(\ell+1)} = \Phi(\mathbf{f}^{(\ell)})$

$$\Phi \stackrel{\text{def.}}{=} \Phi_2 \odot \Phi_1 \quad \text{where} \quad \begin{cases} \Phi_1(\mathbf{f}) = \varepsilon \log \mathbf{K}^T(e^{\mathbf{f}/\varepsilon}) - \log(\mathbf{b}), \\ \Phi_2(\mathbf{g}) = \varepsilon \log \mathbf{K}(e^{\mathbf{g}/\varepsilon}) - \log(\mathbf{a}). \end{cases}$$

Proposition: $\partial\Phi(\mathbf{f}) = \text{diag}(\mathbf{a})^{-1} \odot \mathbf{P} \odot \text{diag}(\mathbf{b})^{-1} \odot \mathbf{P}^T$.

For ℓ large enough, $\|\mathbf{f}^{(\ell)} - \mathbf{f}\| = O((1 - \kappa)^\ell)$

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Global rate: $\kappa \sim e^{-\frac{1}{\varepsilon}}$

[Franklin and Lorenz, 1989]

Local rate: $\kappa \sim \varepsilon$

[Robert Berman 2017]

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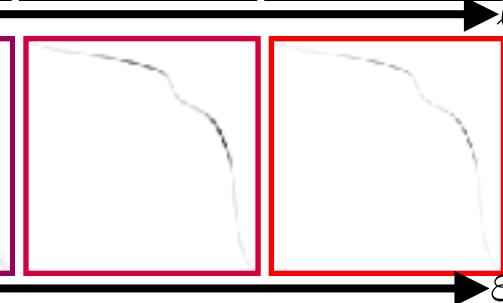
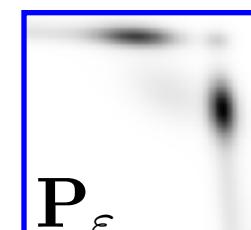
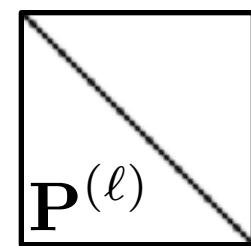
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$$\log(\|\mathbf{P}^{(\ell)} - \mathbf{P}_\varepsilon\|_1)$$

1000 2000 3000 4000 5000

ℓ

-2 -1.5 -1 -0.5 0

ε

Overview

- Entropic Regularization and Sinkhorn
- Convergence Analysis
- **Barycenters**

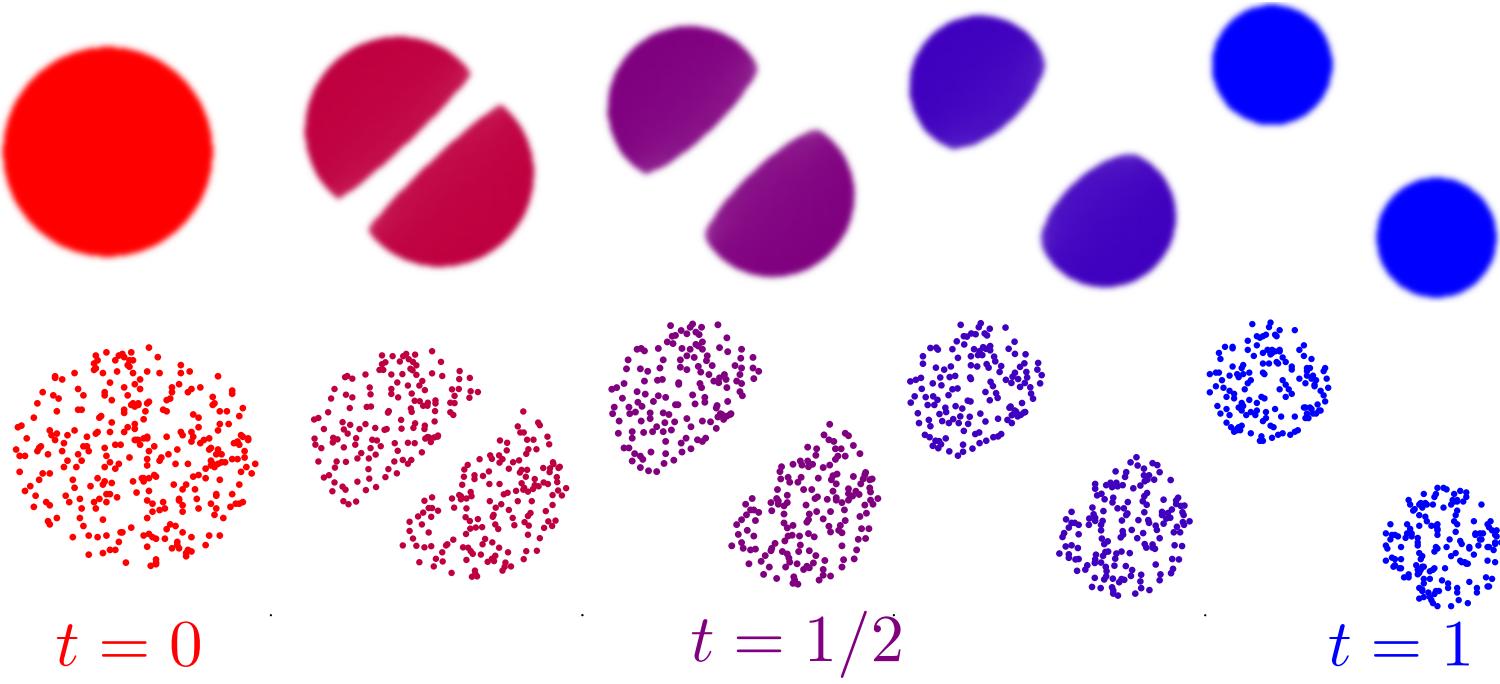
Displacement Interpolation

For $c(x, y) = \|x - y\|^2$, displacement interpolation geodesic:

$$\alpha_t \in \operatorname{argmin}_{\alpha} (1 - t) W_2^2(\alpha, \alpha_0) + t W_2^2(\alpha, \alpha_1)$$

Optimal coupling $\pi \in \mathcal{U}(\alpha_0, \alpha_1)$:

$$\alpha_t \stackrel{\text{def.}}{=} ((1 - t)P_{\mathcal{X}} + tP_{\mathcal{Y}}) \sharp \pi$$



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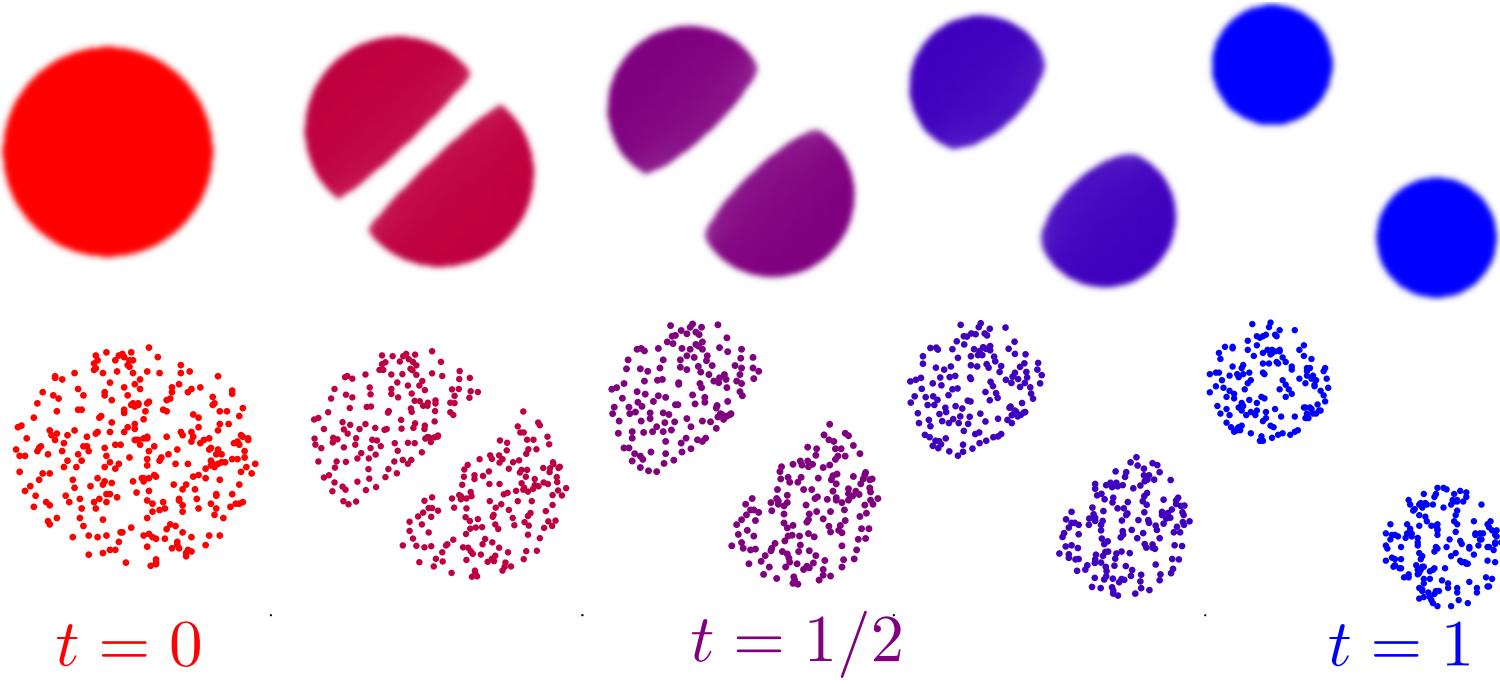
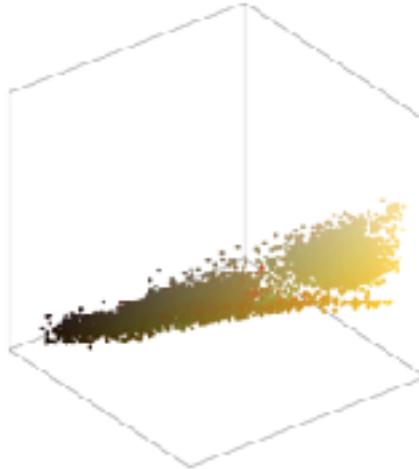


Image Color Palette Equalization



Optimal
transport

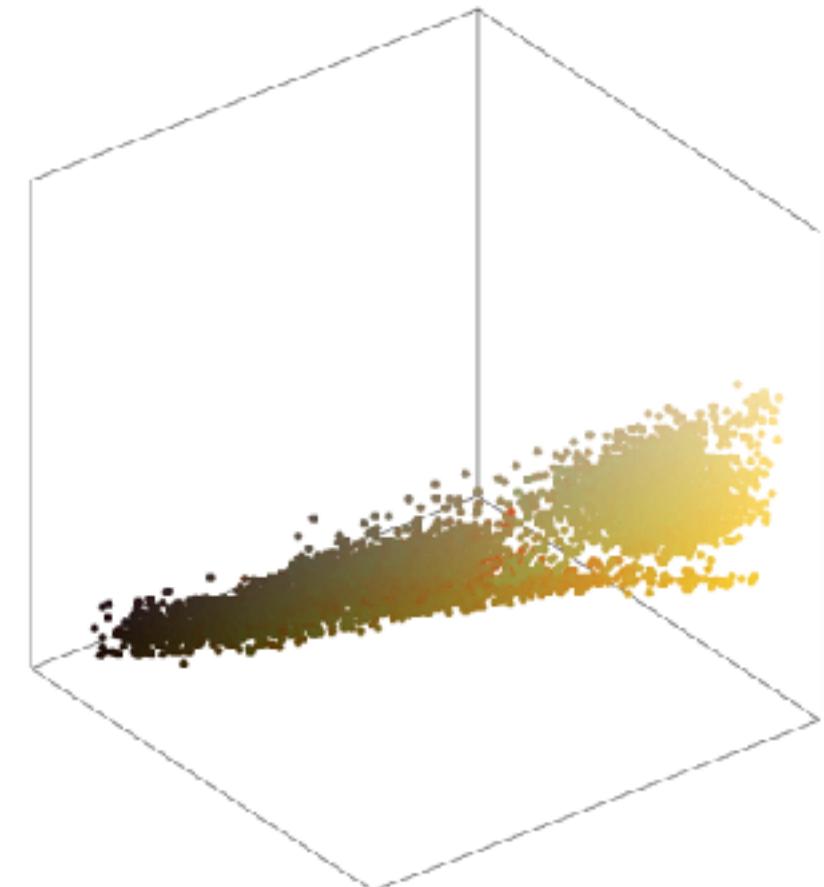
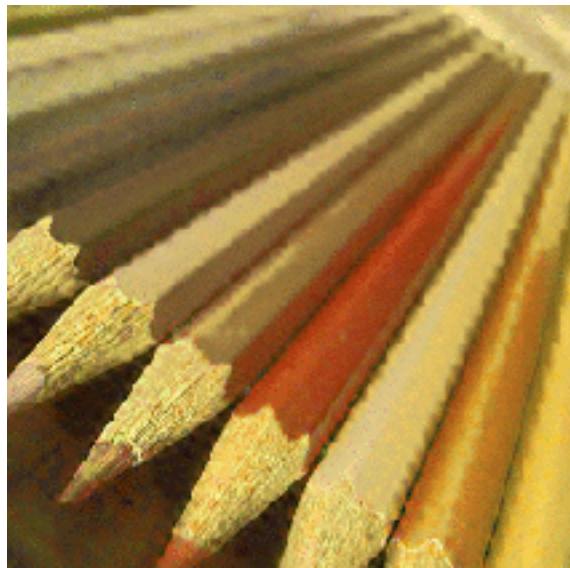
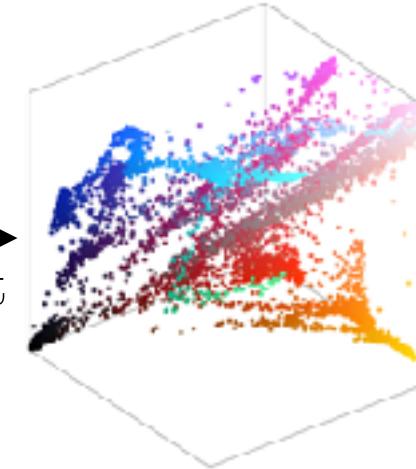
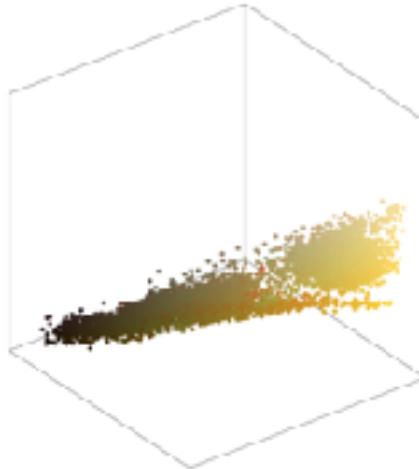
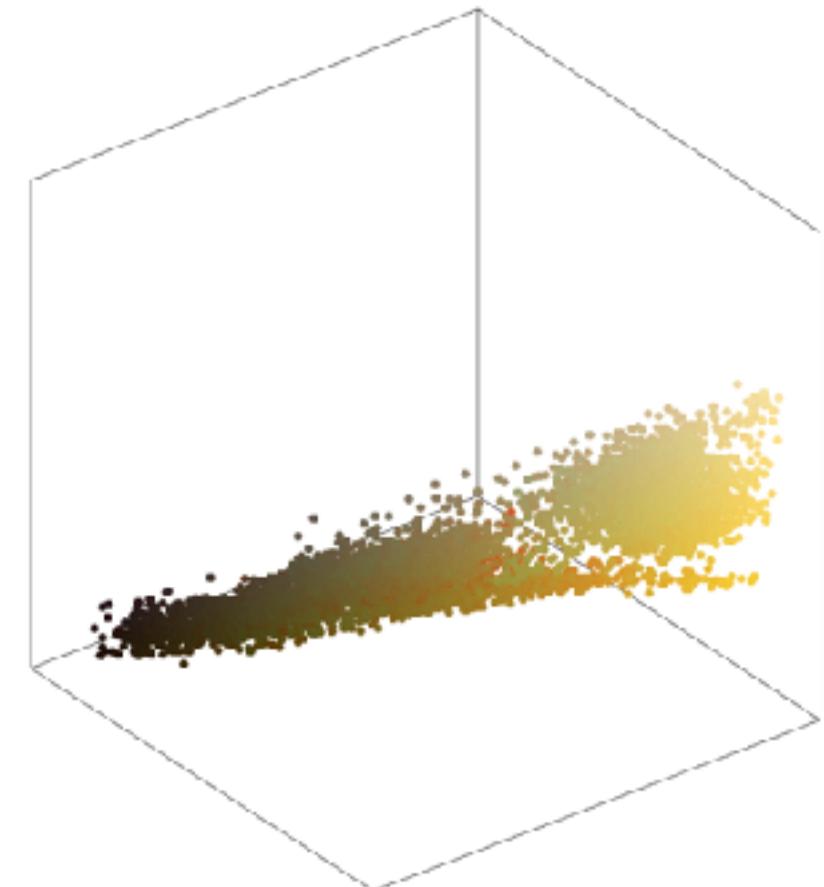
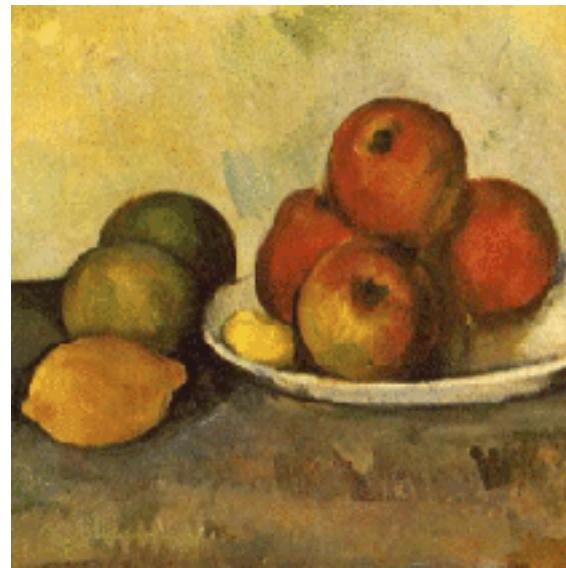
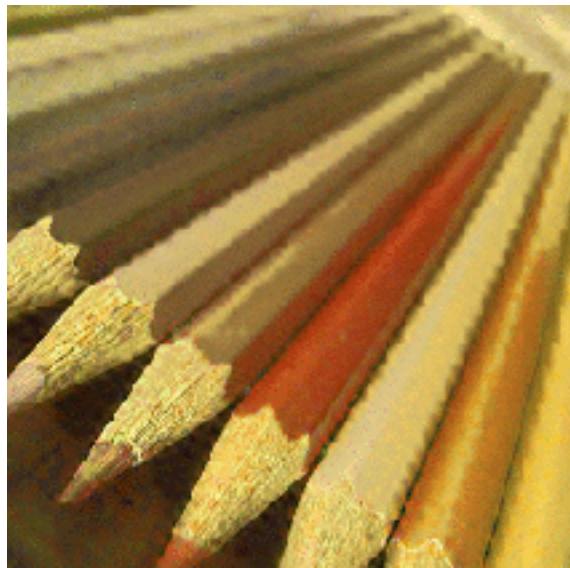
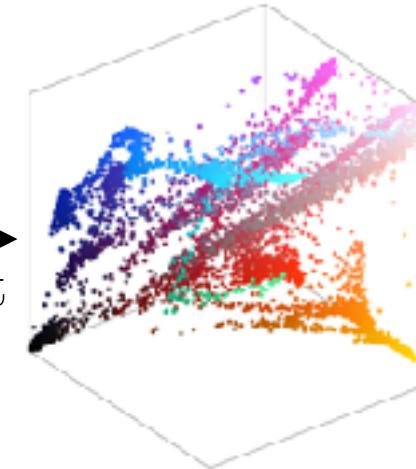


Image Color Palette Equalization



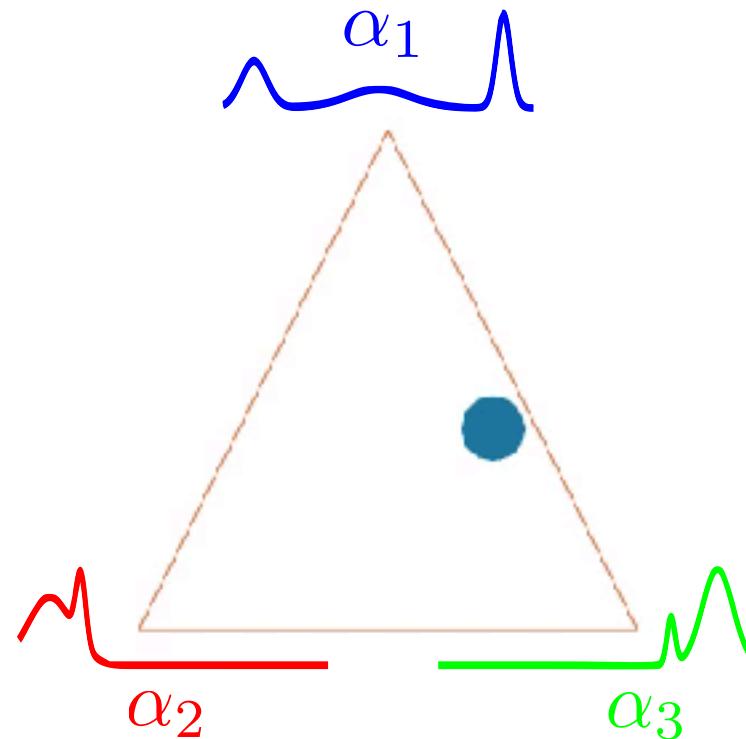
Optimal
transport



Wasserstein Barycenters

Barycenters of measures $(\alpha_s)_{s=1}^S$: $\sum_s \lambda_s = 1$

$$\alpha^* \in \operatorname{argmin}_{\alpha} \sum_s \lambda_s W_p^p(\alpha, \alpha_s)$$



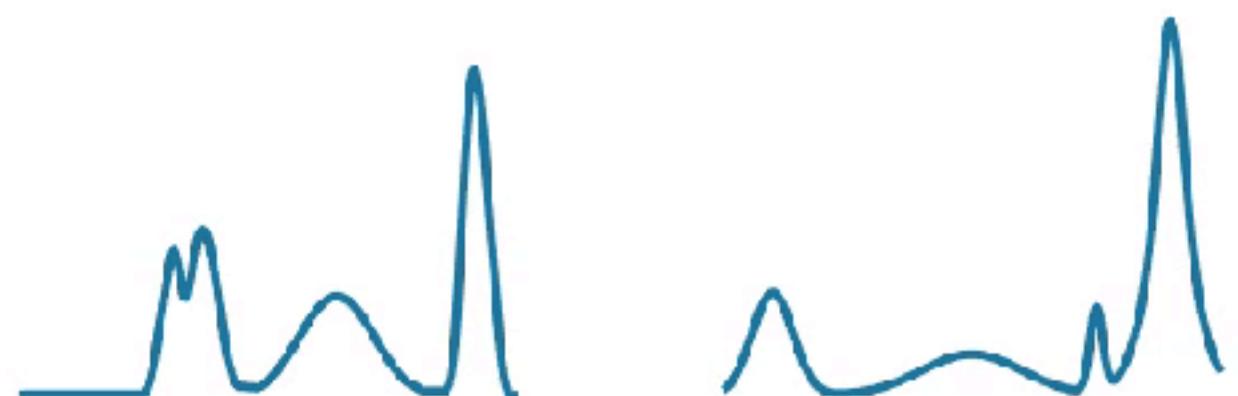
$$\lambda \in \Sigma_3$$

$$\min_{\alpha} \sum_s \lambda_s W_p^p(\alpha, \alpha_s)$$

Wasserstein

$$\sum_s \lambda_s \alpha_s$$

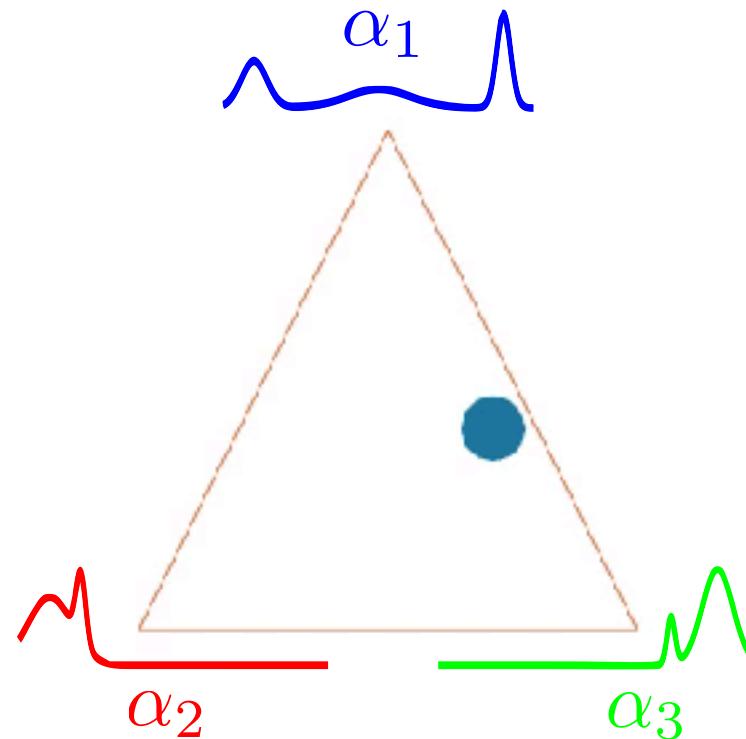
Euclidean



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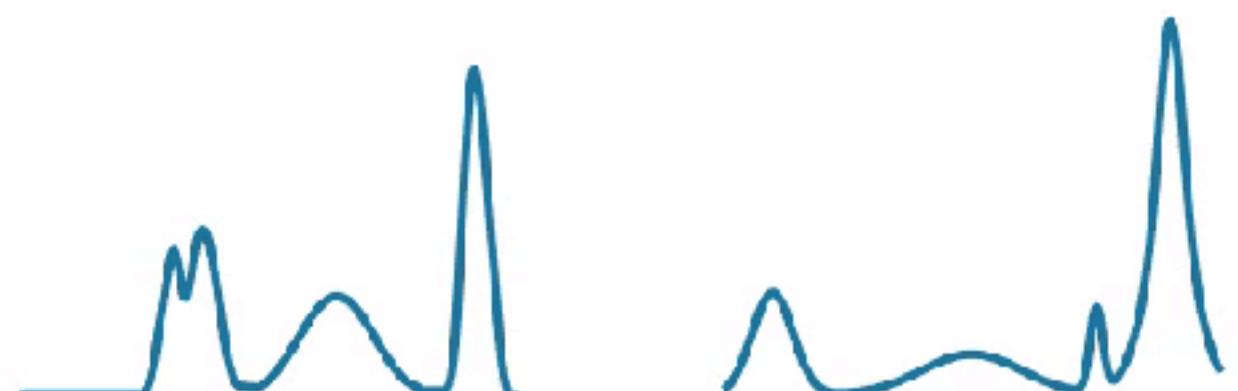
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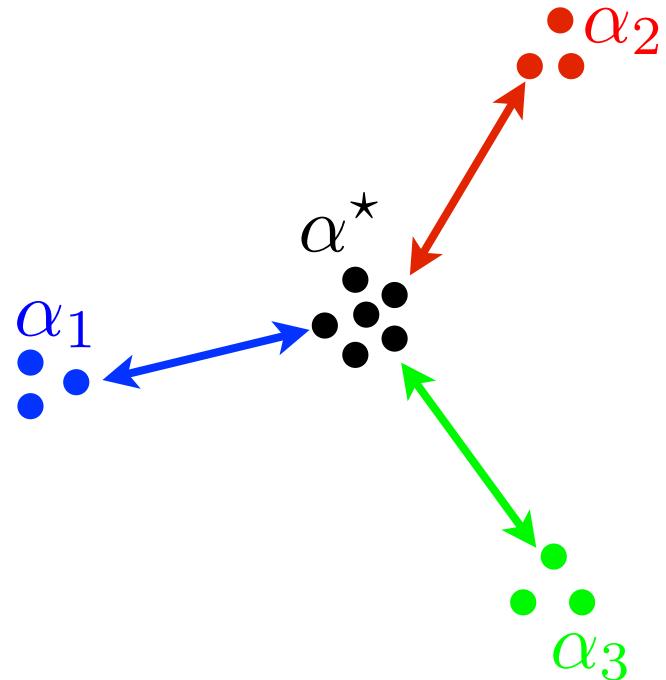


Wasserstein Barycenters

Generalizes usual barycenter:

If $\alpha_s = \delta_{x_s}$ then $\alpha^* = \delta_{x^*}$

$$x^* \in \operatorname{argmin}_x \sum_s \lambda_s d(x, x_s)^p$$



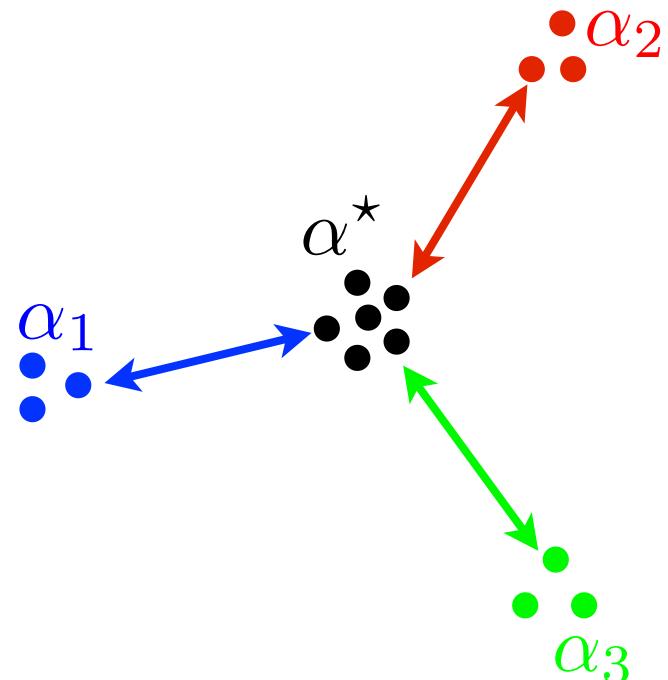
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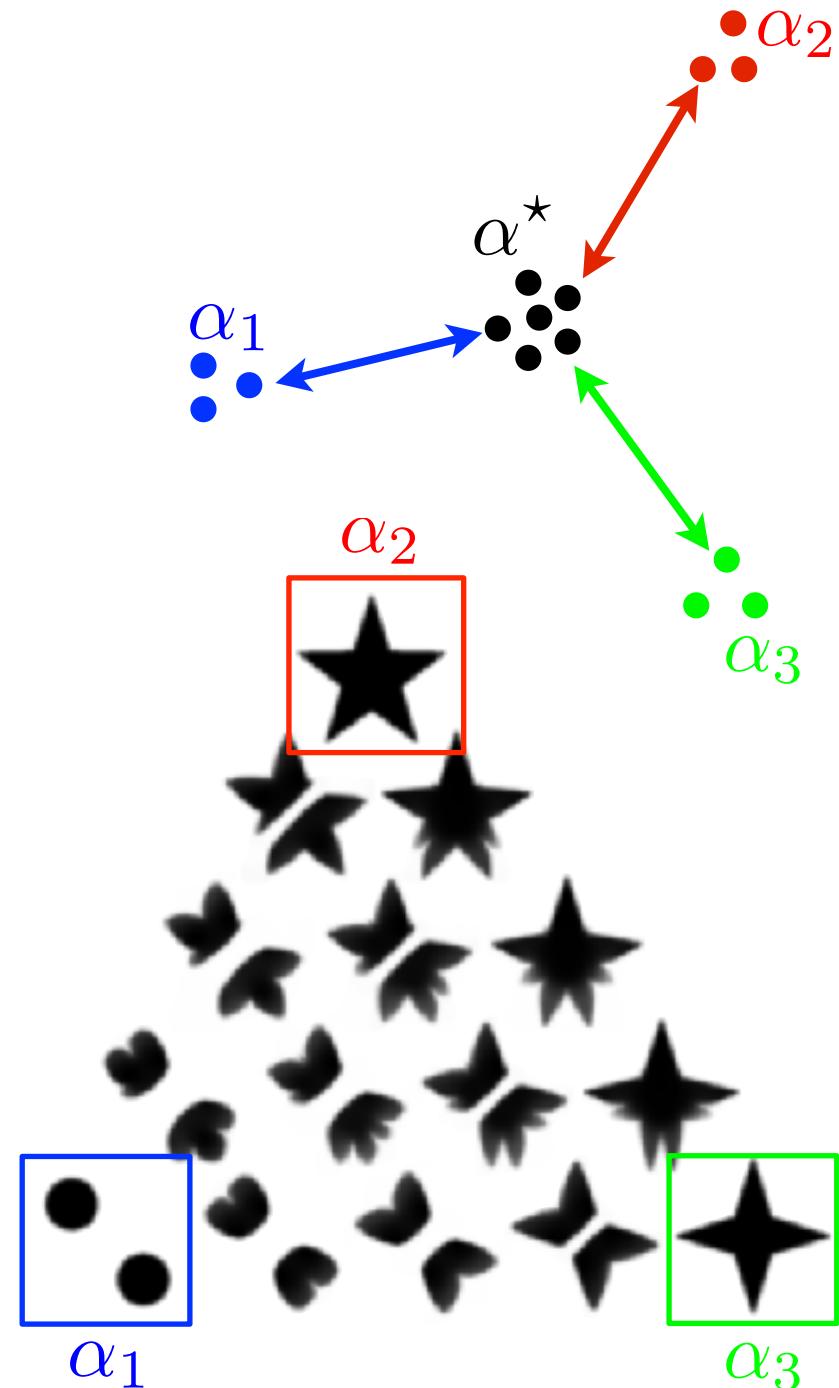
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Theorem: [Agueh, Carlier, 2010]

(for $c(x, y) = \|x - y\|^2$)

if α_1 has a density,
 α^* exists and is unique.



Barycenters of Gaussians

OT between $\alpha = \mathcal{N}(\mathbf{m}_\alpha, \Sigma_\alpha)$ $\beta = \mathcal{N}(\mathbf{m}_\beta, \Sigma_\beta)$

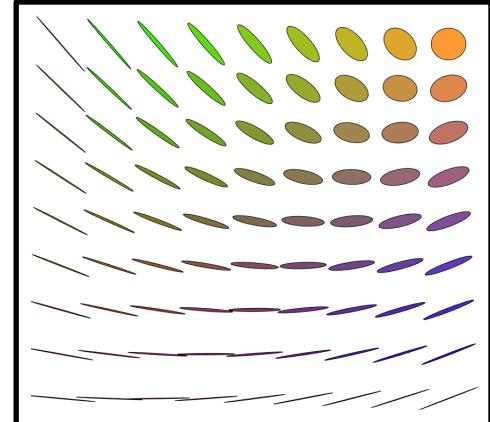
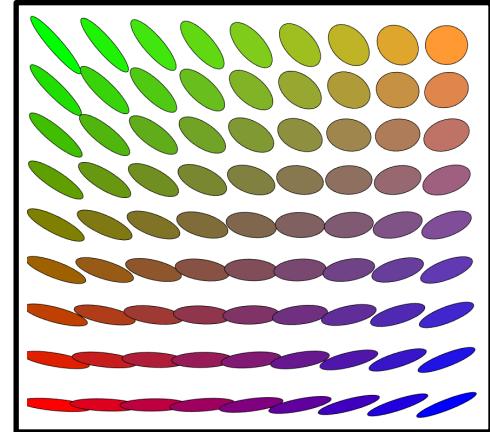
$$\mathcal{W}_2^2(\alpha, \beta) = \|\mathbf{m}_\alpha - \mathbf{m}_\beta\|^2 + \mathcal{B}(\Sigma_\alpha, \Sigma_\beta)^2 \quad \mathcal{B}(\Sigma_\alpha, \Sigma_\beta)^2 \stackrel{\text{def.}}{=} \text{tr} \left(\Sigma_\alpha + \Sigma_\beta - 2(\Sigma_\alpha^{1/2} \Sigma_\beta \Sigma_\alpha^{1/2})^{1/2} \right)$$

Proposition: barycenter is $\mathcal{N}(\mathbf{m}^\star, \Sigma^\star)$ and solves

[Carlier, Agueh, 2011]

$$\mathbf{m}^\star = \sum_s \lambda_s \mathbf{m}_s$$

$$\min_{\Sigma} \sum_s \lambda_s \mathcal{B}(\Sigma, \Sigma_s)^2$$



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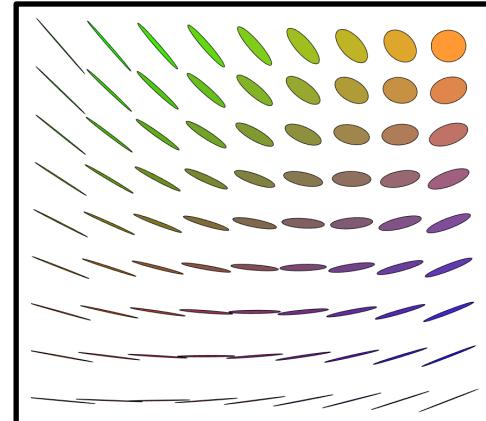
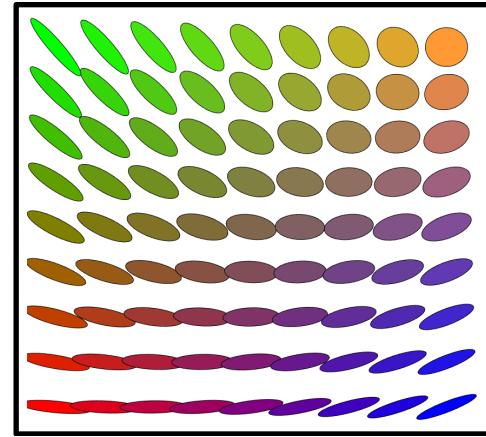
$$\min_{\Sigma} \sum_s \lambda_s \mathcal{B}(\Sigma, \Sigma_s)^2$$

Fixed point equation:

$$\Sigma^\star = \Psi(\Sigma^\star) \quad \text{where} \quad \Psi(\Sigma) \stackrel{\text{def.}}{=} \sum_s \lambda_s (\Sigma^{\frac{1}{2}} \Sigma_s \Sigma^{\frac{1}{2}})^{\frac{1}{2}}$$

→ empirically convergent.

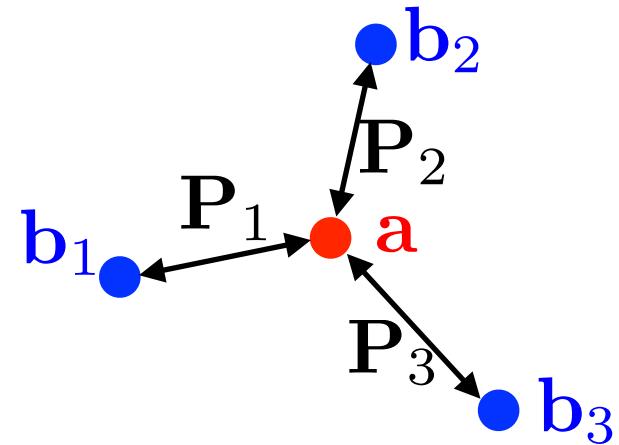
→ related provably convergent scheme by [Alvarez-Esteban et al 2016].



Regularized Barycenters

→ Need to fix a grid (Eulerian scheme).

$$L_C^\varepsilon(a, b) \stackrel{\text{def.}}{=} \min_{P \in U(a, b)} \langle P, C \rangle - \varepsilon H(P)$$



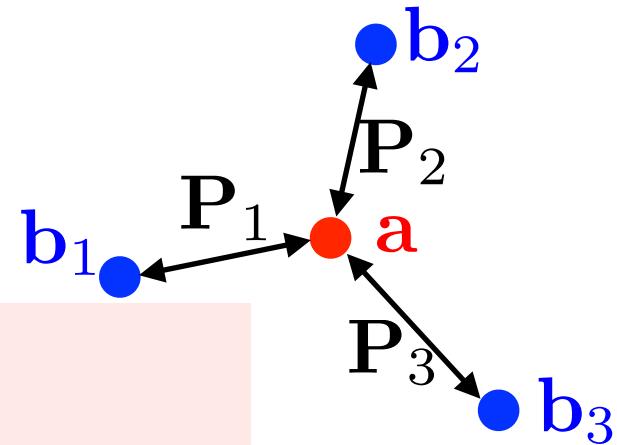
Regularized Barycenters

→ Need to fix a grid (Eulerian scheme).

$$L_C^\varepsilon(\mathbf{a}, \mathbf{b}) \stackrel{\text{def.}}{=} \min_{\mathbf{P} \in \mathbf{U}(\mathbf{a}, \mathbf{b})} \langle \mathbf{P}, \mathbf{C} \rangle - \varepsilon H(\mathbf{P})$$

Coupling re-writing:

$$\begin{aligned} & \min_{\mathbf{a} \in \Sigma_n} \sum_{s=1}^S \lambda_s L_{C_s}^\varepsilon(\mathbf{a}, \mathbf{b}_s) \\ = & \min_{(\mathbf{P}_s)_s} \left\{ \sum_s \lambda_s \varepsilon \mathbf{KL}(\mathbf{P}_s | \mathbf{K}_s) : \forall s, \mathbf{P}_s^T \mathbf{1}_m = \mathbf{b}_s, \mathbf{P}_1 \mathbf{1}_1 = \dots = \mathbf{P}_S \mathbf{1}_S \right\} \end{aligned}$$



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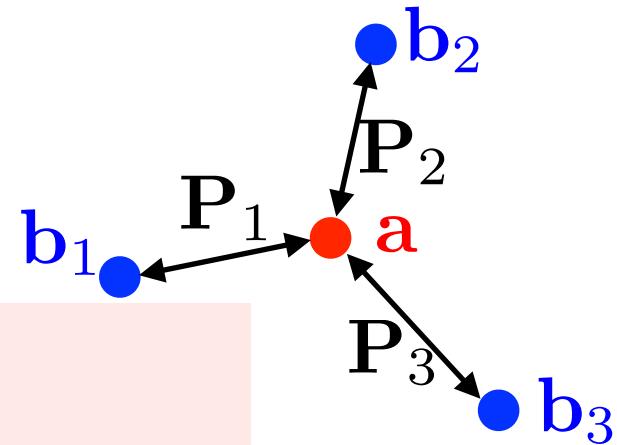
Coupling factorization: $\mathbf{P}_s = \text{diag}(\mathbf{u}_s) \mathbf{K} \text{diag}(\mathbf{v}_s)$

Sinkhorn-like

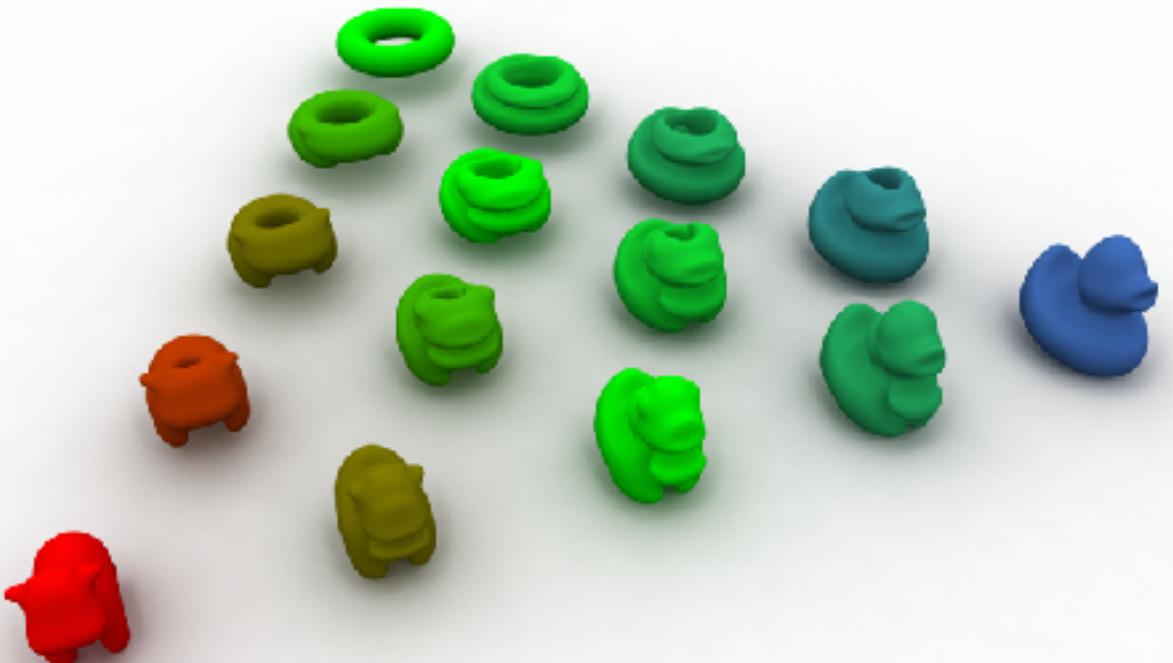
$$\forall s \in \llbracket 1, S \rrbracket, \quad \mathbf{v}_s^{(\ell+1)} \stackrel{\text{def.}}{=} \frac{\mathbf{b}_s}{\mathbf{K}_s^T \mathbf{u}_s^{(\ell)}}$$

$$\mathbf{a}^{(\ell+1)} \stackrel{\text{def.}}{=} \prod_s (\mathbf{K}_s \mathbf{v}_s^{(\ell+1)})^{\lambda_s}$$

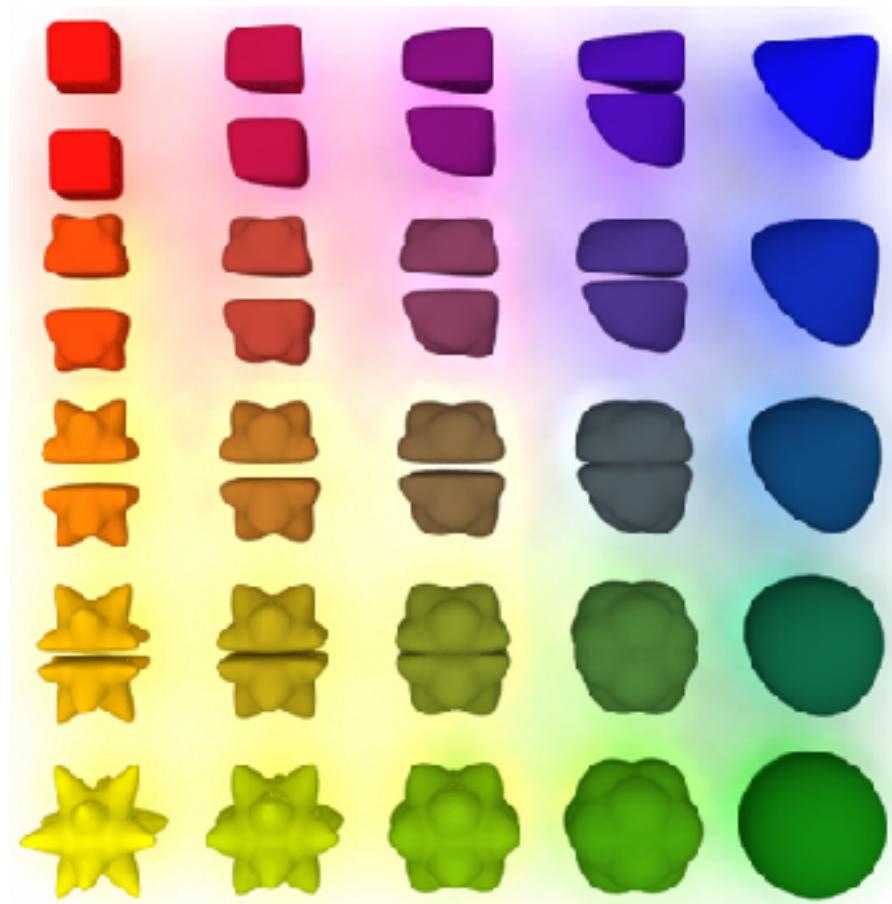
$$\forall s \in \llbracket 1, S \rrbracket, \quad \mathbf{u}_s^{(\ell+1)} \stackrel{\text{def.}}{=} \frac{\mathbf{a}^{(\ell+1)}}{\mathbf{K}_s \mathbf{v}_s^{(\ell+1)}}$$



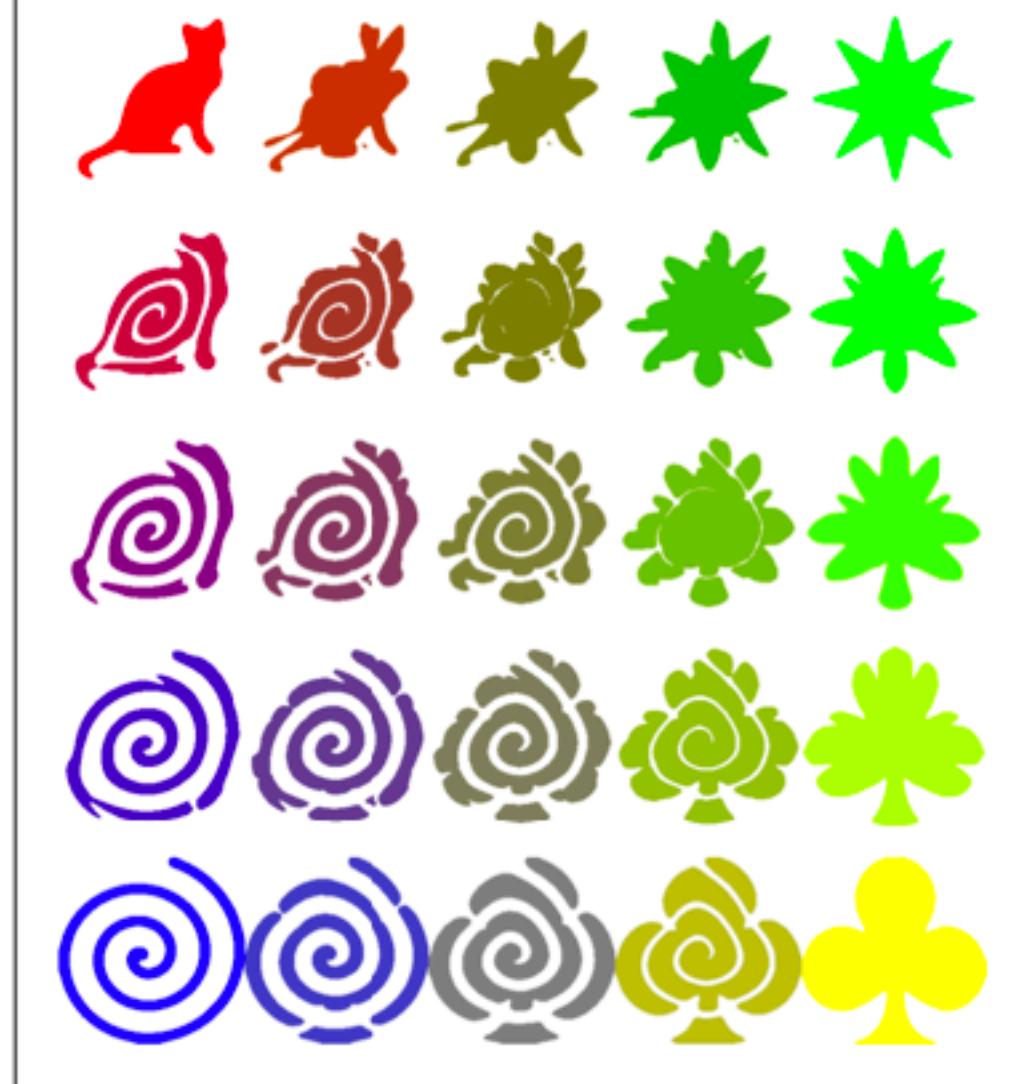
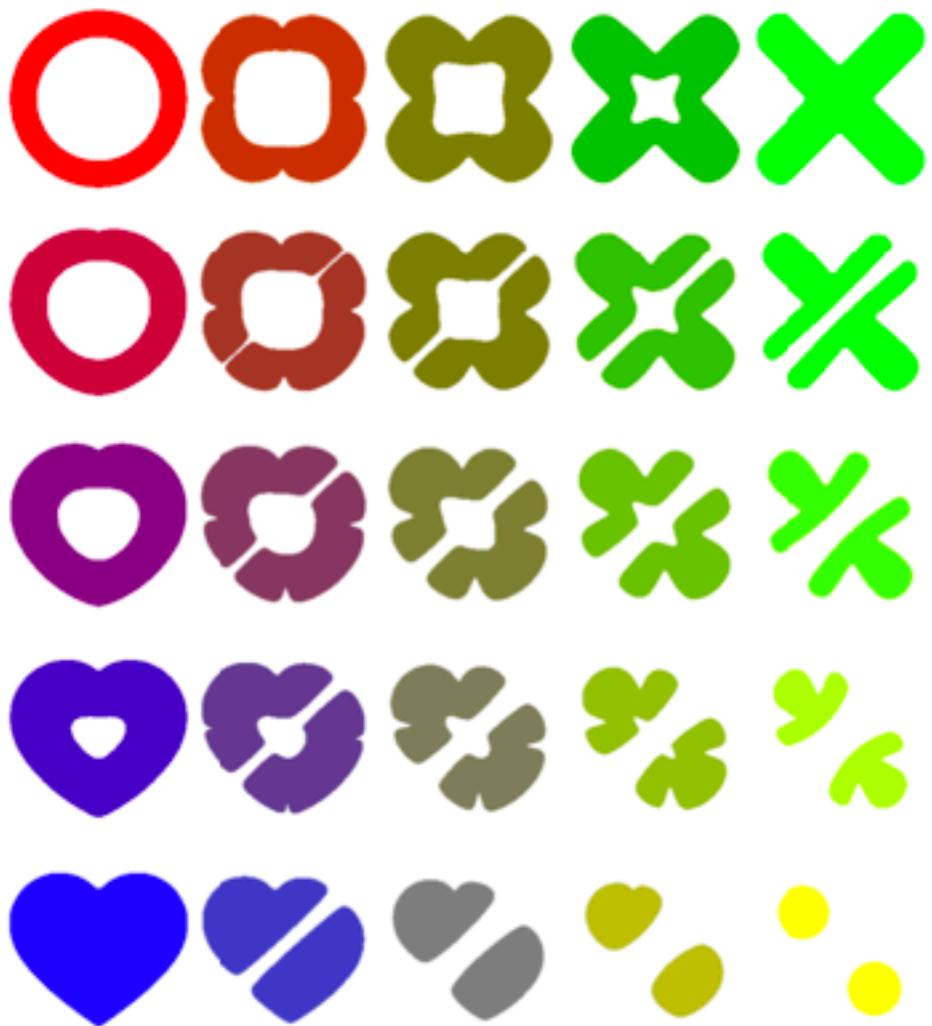
Examples



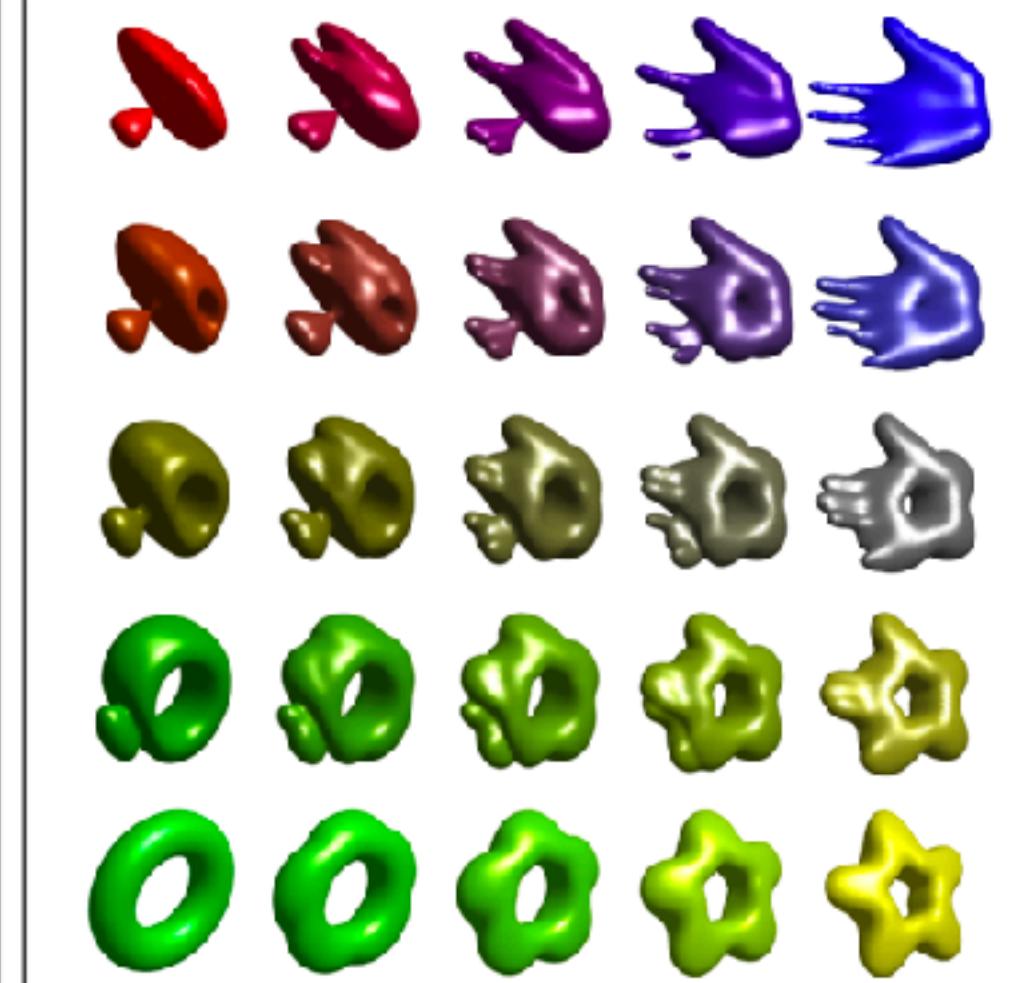
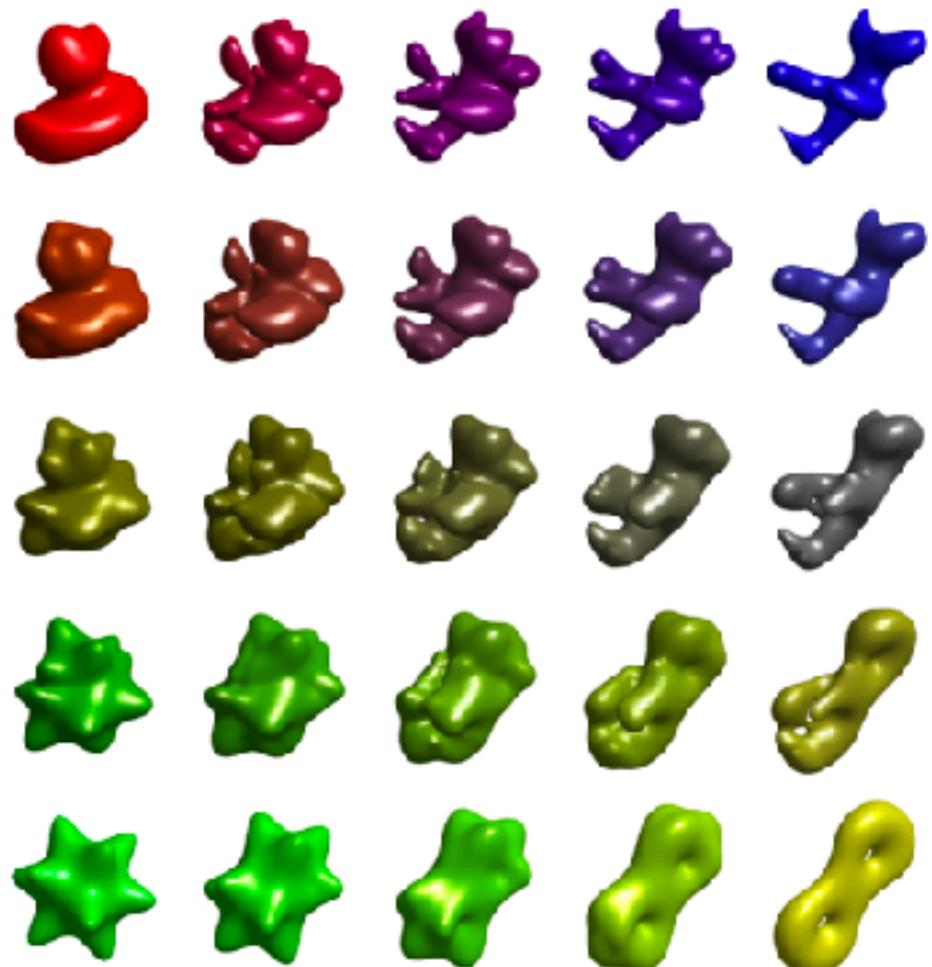
[Solomon et al, SIGGRAPH 2015]



Barycenters of 2D Shapes



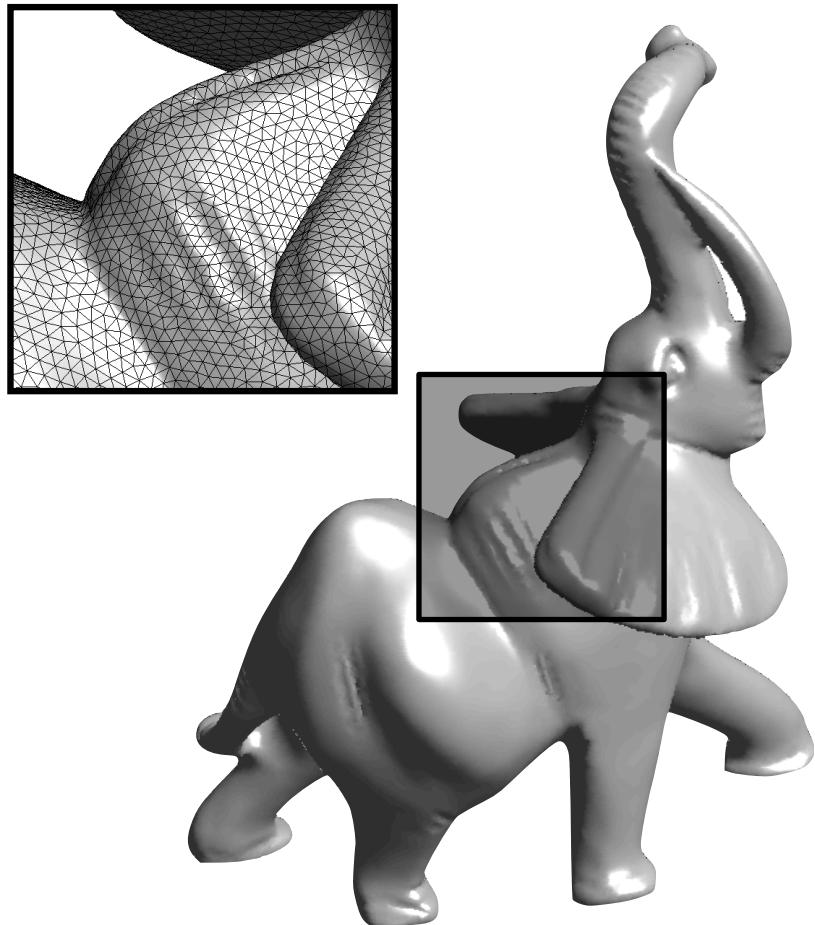
Barycenters of 3D Shapes



Optimal Transport on Surfaces

Triangulated mesh M .

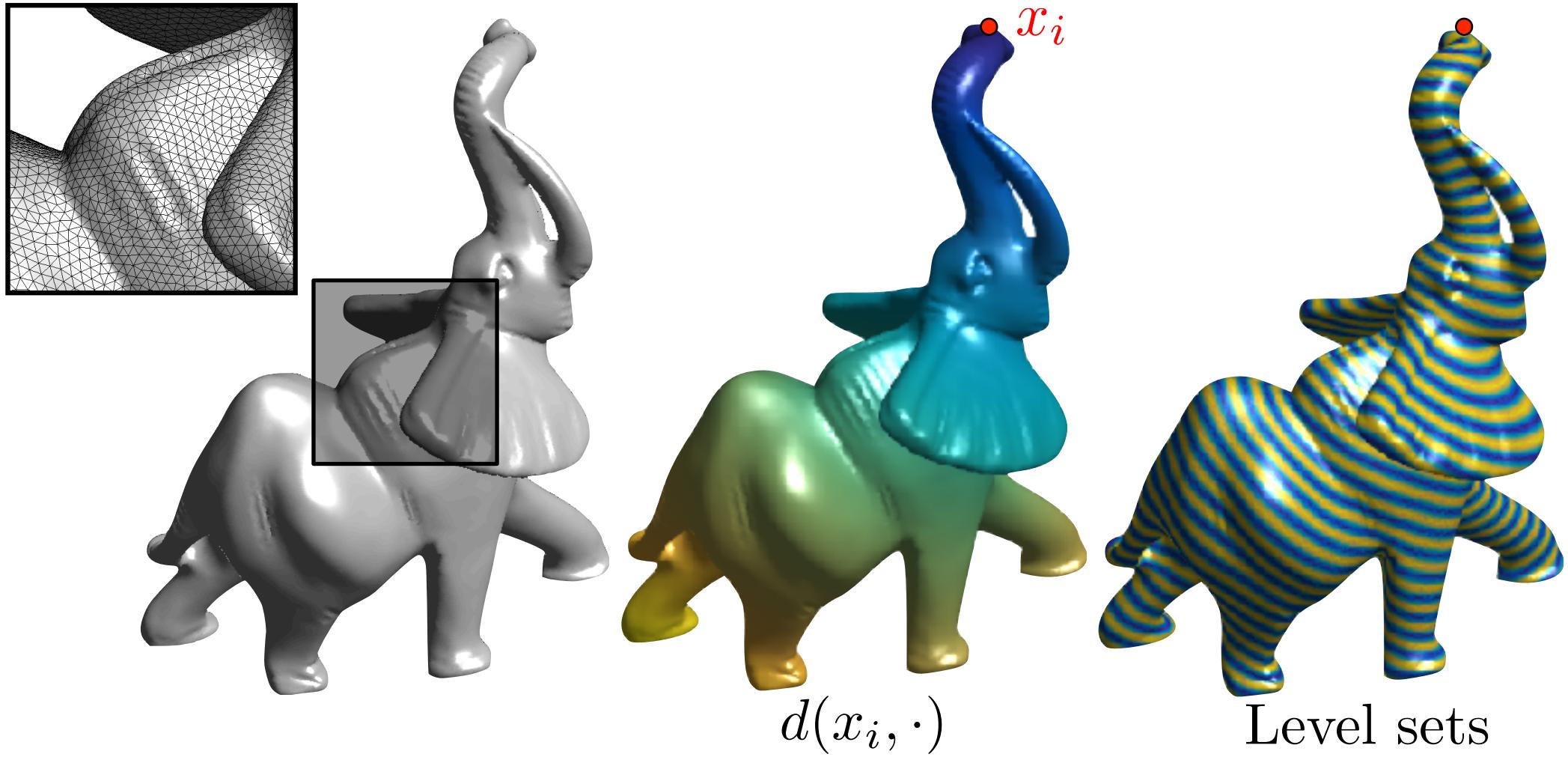
Geodesic distance d_M .



Optimal Transport on Surfaces

Triangulated mesh M . Geodesic distance d_M .

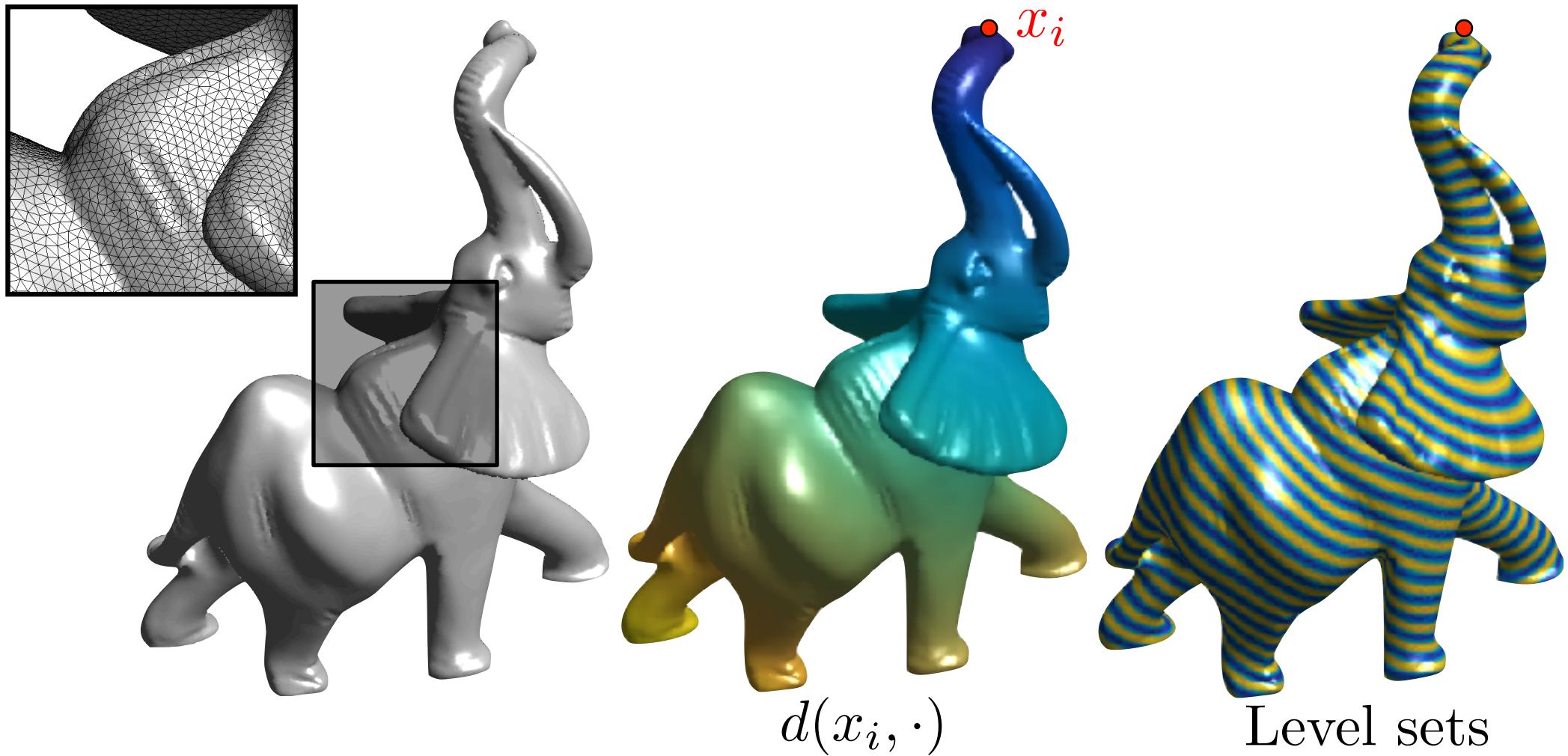
Ground cost: $c(x, y) = d_M(x, y)^\alpha$.



Optimal Transport on Surfaces

Triangulated mesh M . Geodesic distance d_M .

Ground cost: $c(x, y) = d_M(x, y)^\alpha$.

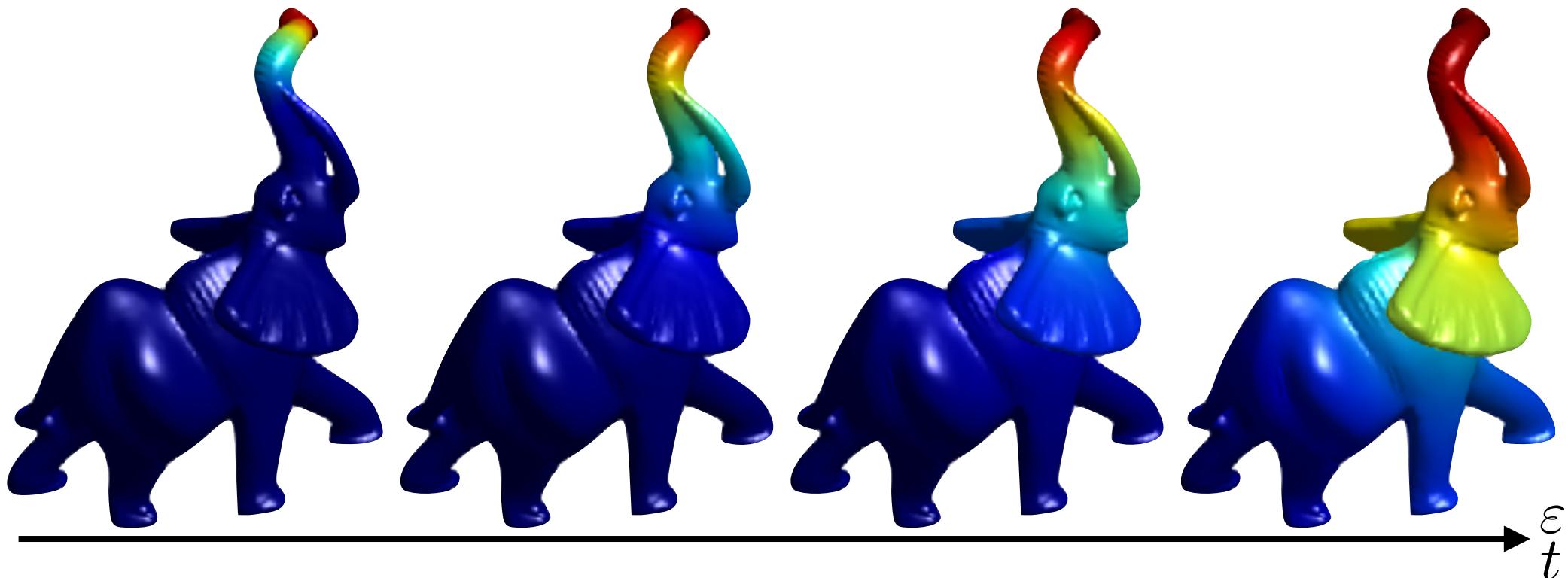


Computing c (Fast-Marching): $N^2 \log(N) \rightarrow$ too costly.

Entropic Transport on Surfaces

Heat equation on M : $\partial_t u_t(x, \cdot) = \Delta_M u_t(x, \cdot)$, $u_{t=0}(x, \cdot) = \delta_x$

Theorem: [Varadhan] $-\varepsilon \log(u_\varepsilon) \xrightarrow{\varepsilon \rightarrow 0} d_M^2$

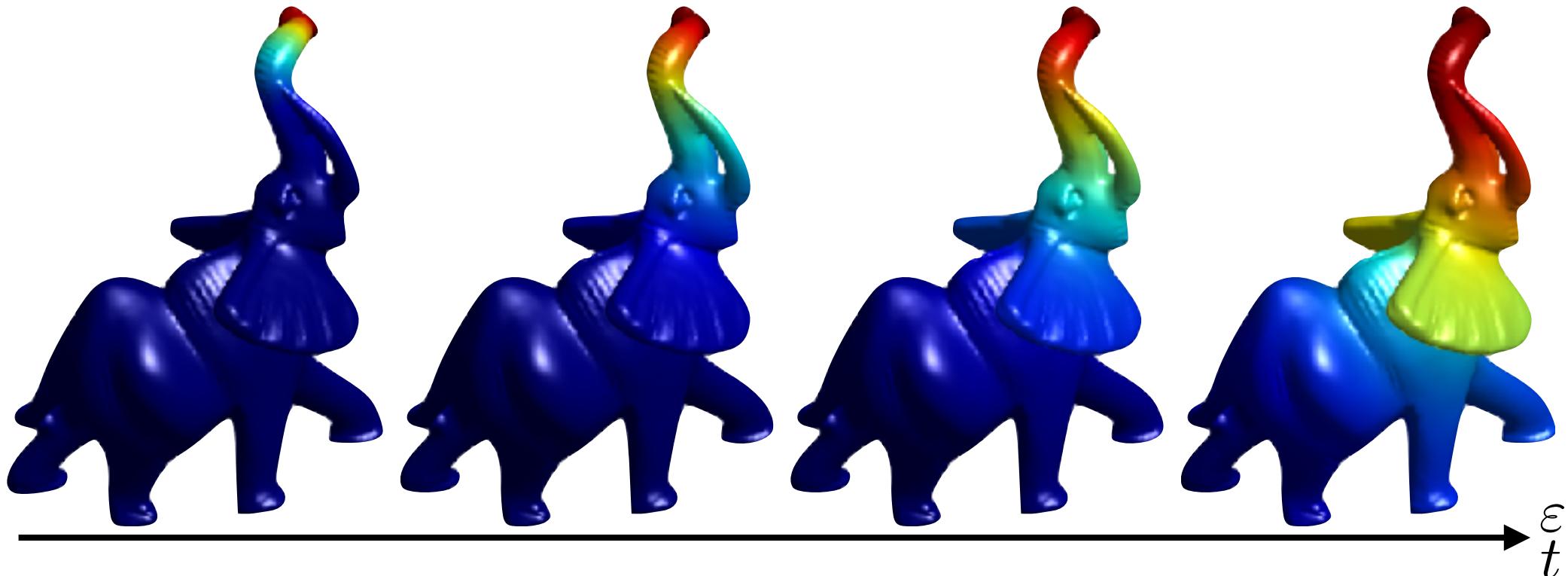


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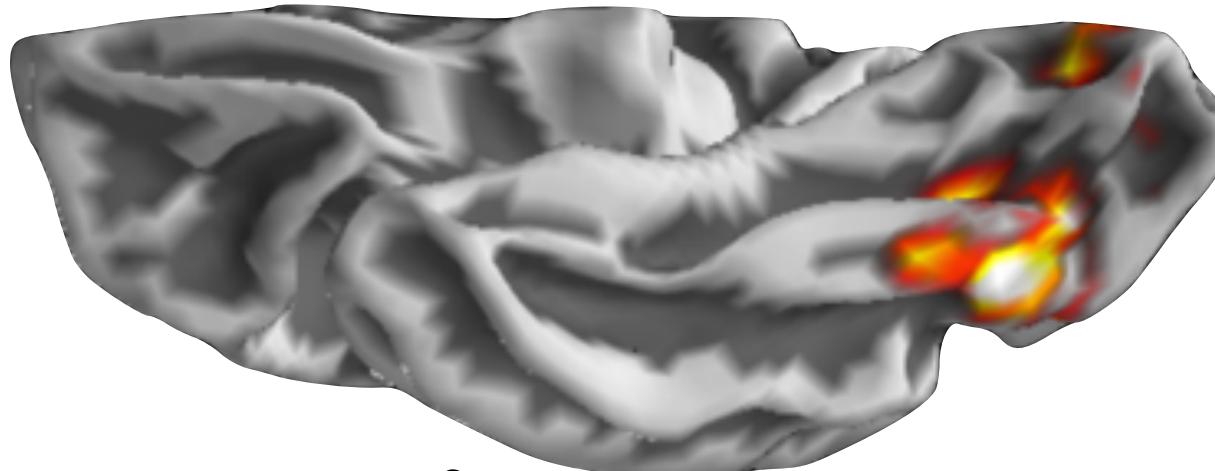
Theorem: [Varadhan] $-\varepsilon \log(u_\varepsilon) \xrightarrow{\varepsilon \rightarrow 0} d_M^2$

Sinkhorn kernel: $K \stackrel{\text{def.}}{=} e^{-\frac{d_M^2}{\varepsilon}} \approx u_\varepsilon \approx \left(\text{Id} - \frac{\varepsilon}{\ell} \Delta_M\right)^{-\ell}$

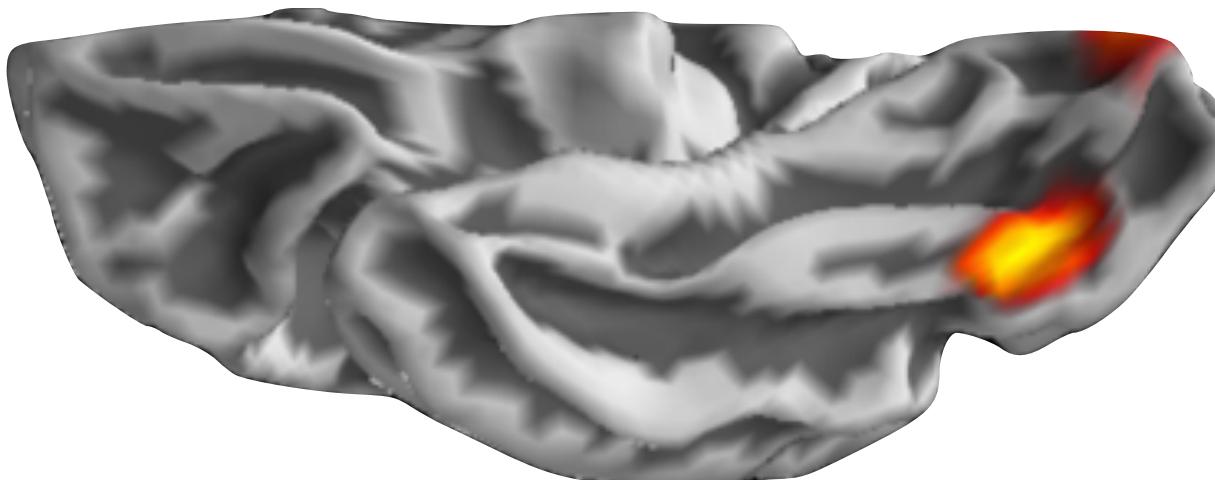


MRI Data Processing [with A. Gramfort]

Ground cost $c = d_M$: geodesic on cortical surface M .



L^2 barycenter



W_2^2 barycenter

Barycenters on a Surface

