Numerical Optimal Transport and Applications

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Joint works with:
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CEREMADE

DAUPHINE UNIVERSITÉ PARIS

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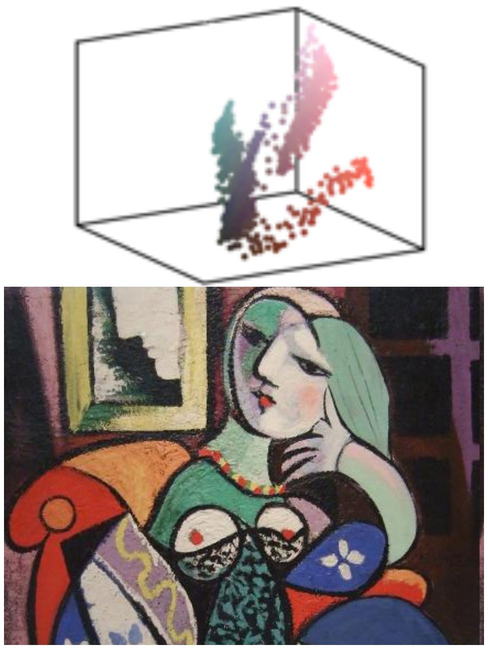
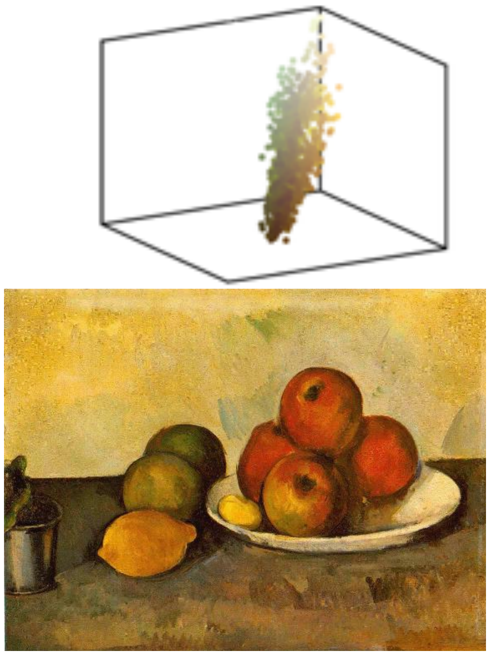
Histograms in Imaging and Machine Learning

Color histograms:





Input image

Histograms in Imaging and Machine Learning

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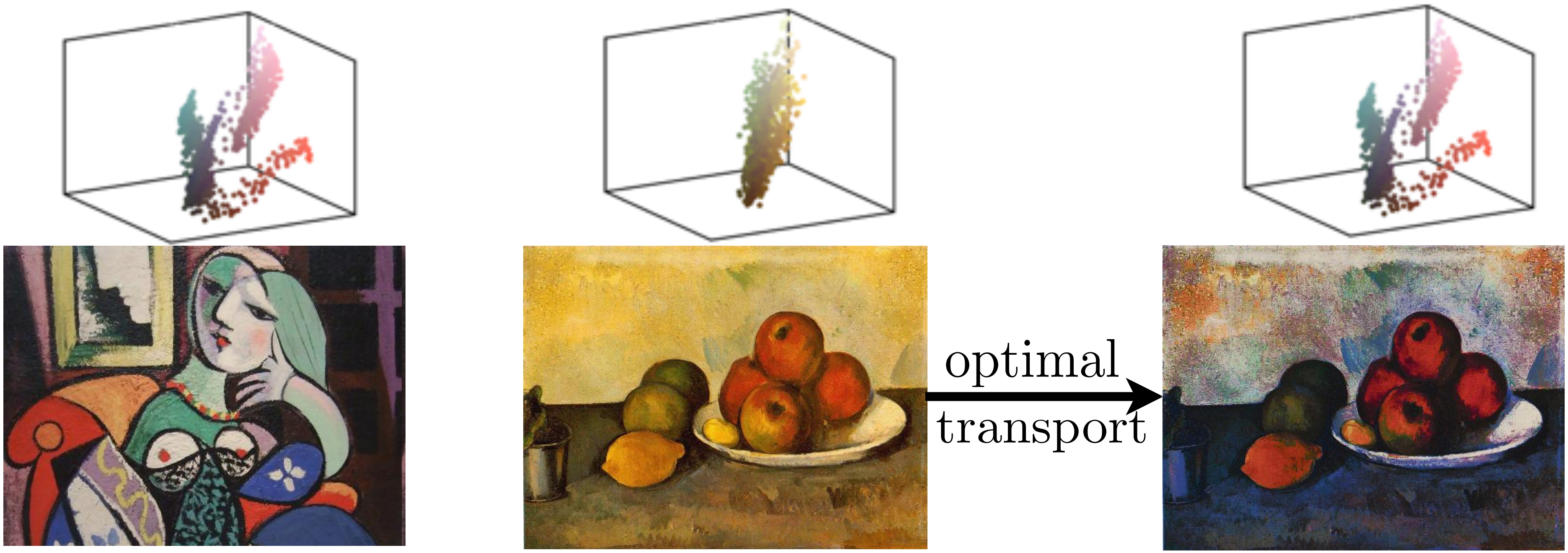

Input image

Modified image

Histograms in Imaging and Machine Learning

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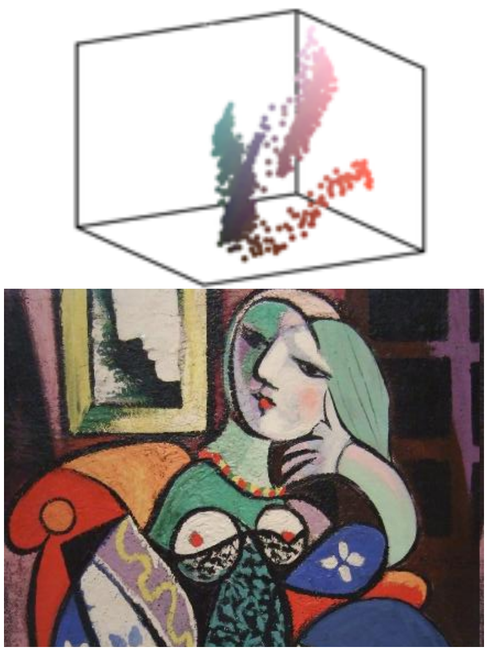
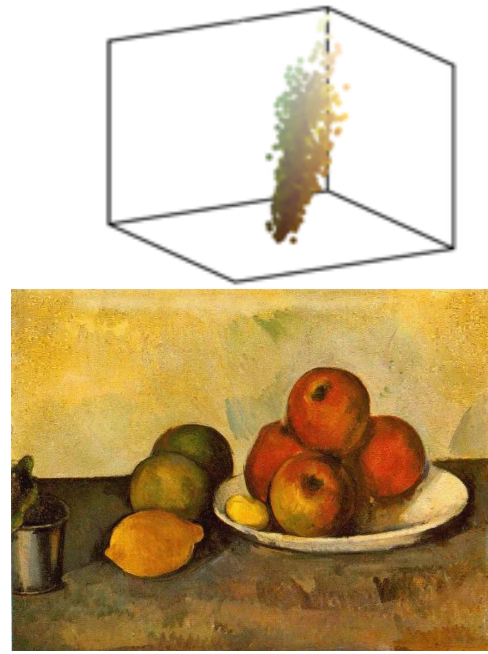
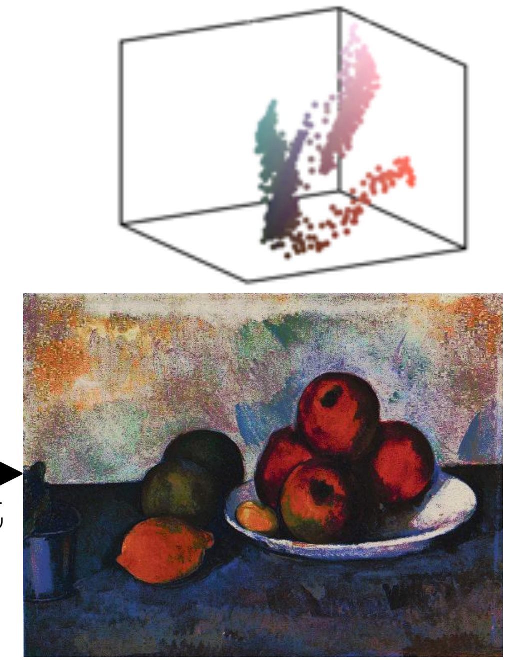




Input image

optimal

transport



Modified image

Bag of words:

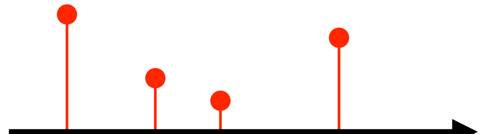
Overview

- Transportation-like Problems
- Regularized Transport
- Optimal Transport Barycenters
- Heat Kernel Approximation

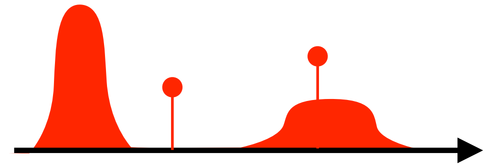
Radon Measures and Couplings

Positive Radon measures $\mathcal{M}_+(X)$: On a metric space (X, d).

$\mathrm{d}\mu(x) = f(x)\mathrm{d}x$



$\mu = \sum_i p_i \delta_{x_i}$



$X = \mathbb{R}$

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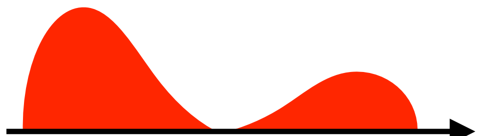

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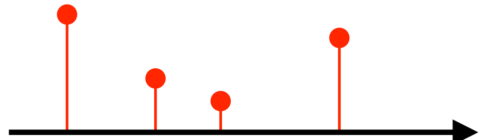

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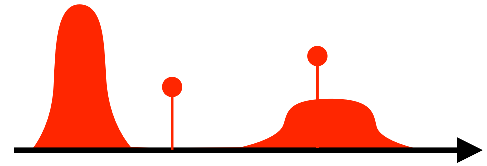

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Probability measures. $\mu(X) = 1$ $\int f = 1$ $\sum_i p_i = 1$

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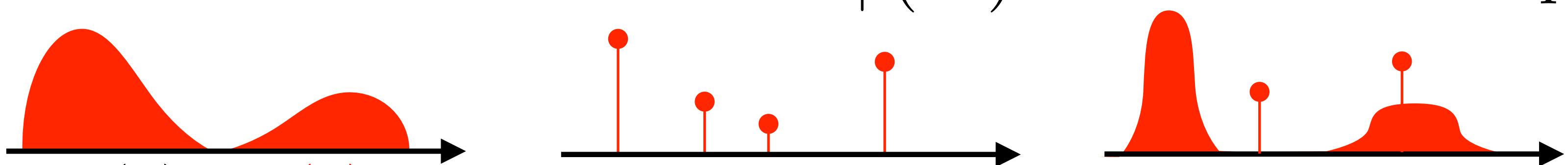

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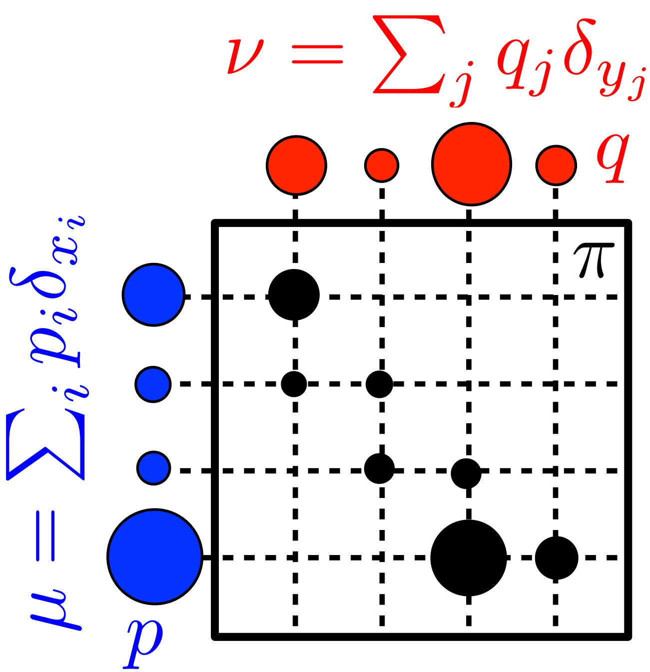
Couplings: $\Pi(\mu, \nu) \overset{\text{def.}}{=} \{\pi \in \mathcal{M}_+(X \times X) \; ; \; P_{1\sharp}\pi = \mu, P_{2\sharp}\pi = \nu\}$

Marginals: $P_{1\sharp}\pi(S) \overset{\text{def.}}{=} \pi(S, X)$ $\quad$ $P_{2\sharp}\pi(S) \overset{\text{def.}}{=} \pi(X, S)$



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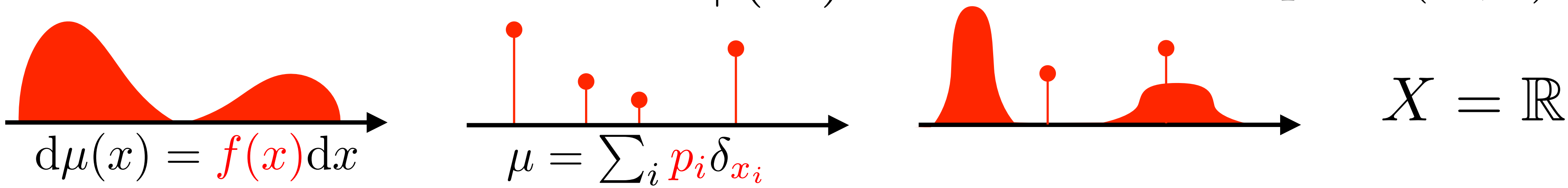

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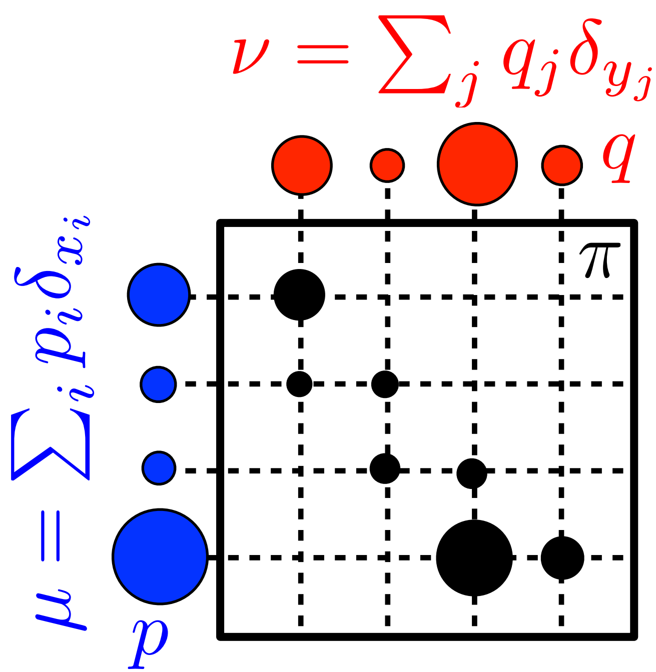

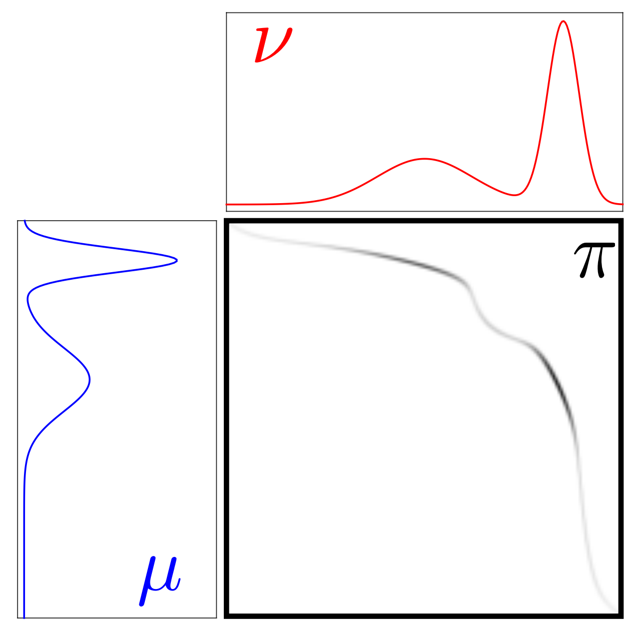

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Ground cost $c(x, y)$ on $X \times X$.

Optimal transport: [Kantorovitch 1942]

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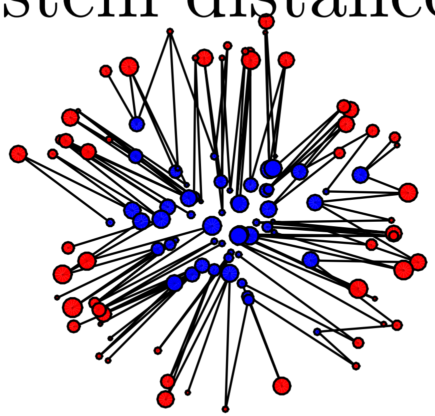

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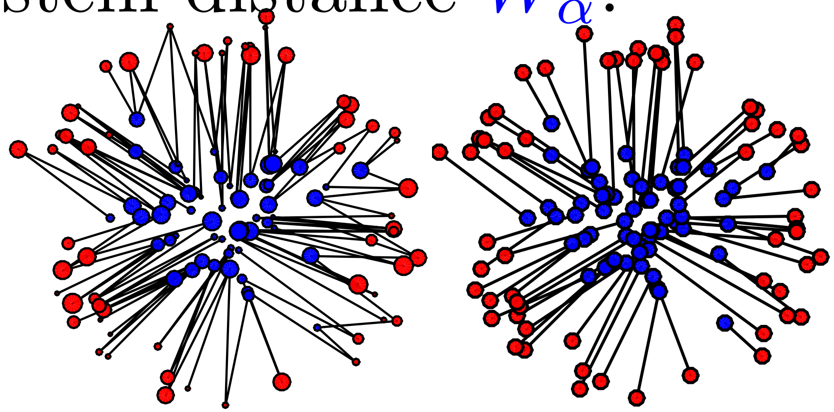

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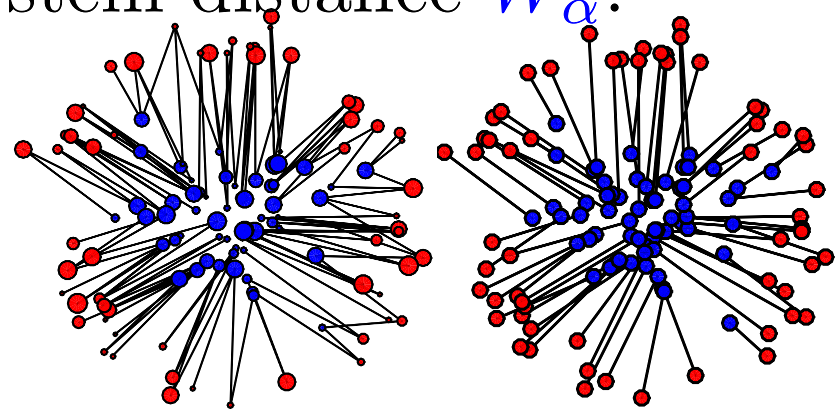

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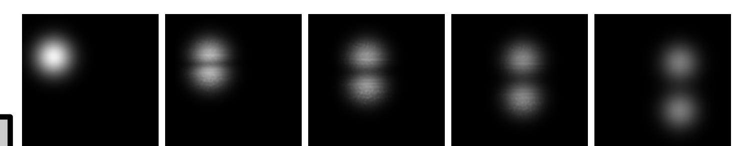

Monge-Ampère/Benamou-Brenier, $d = \|\cdot\|_2^2$.

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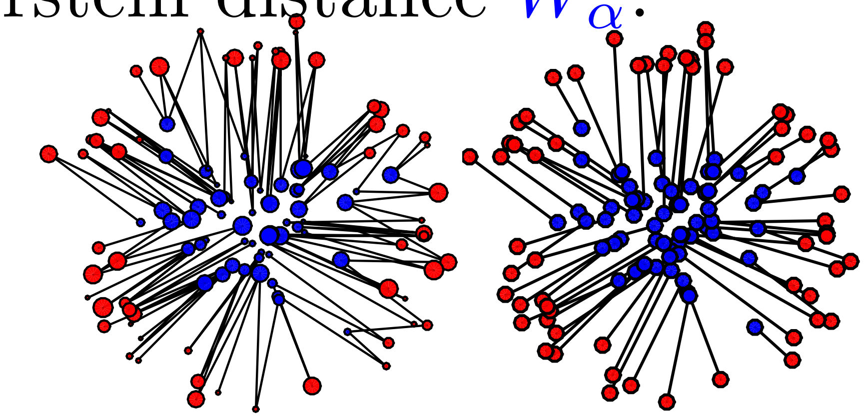

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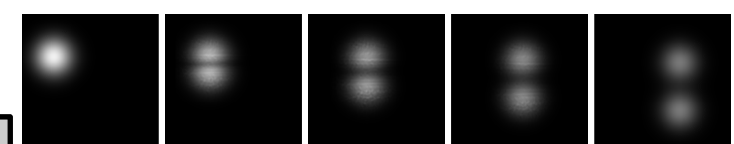

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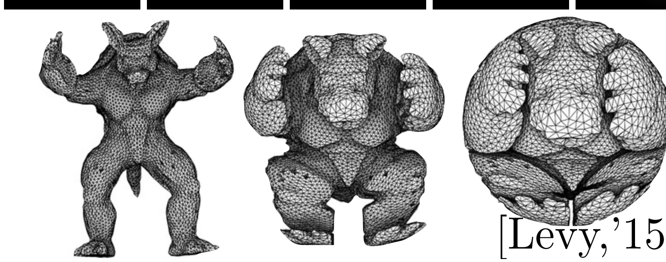
Semi-discrete: Laguerre cells, $d = \|\cdot\|_2^2$.



[Levy,'15]

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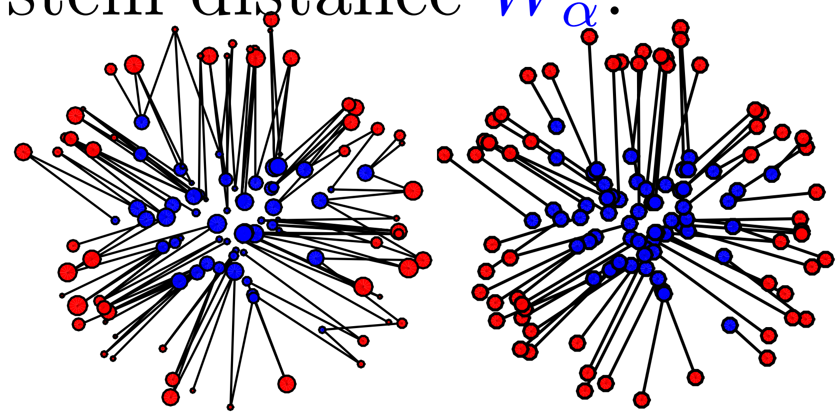

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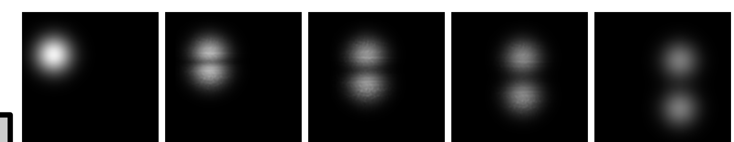

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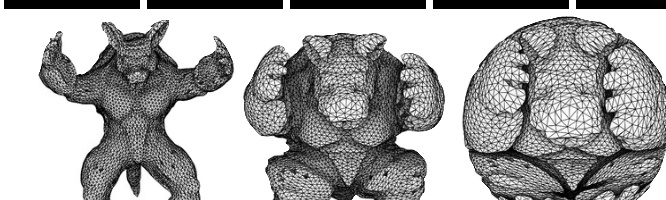

[Levy,'15]

Need for fast approximate algorithms for generic c.

Unbalanced Transport

$$(\mu, \nu) \in \mathcal{M}_+(X) \qquad \mathrm{KL}(\nu|\mu) \overset{\text{def.}}{=} \int_X \log\left(\frac{\mathrm{d}\nu}{\mathrm{d}\mu}\right) \mathrm{d}\mu + \int_X (\mathrm{d}\mu - \mathrm{d}\nu)$$

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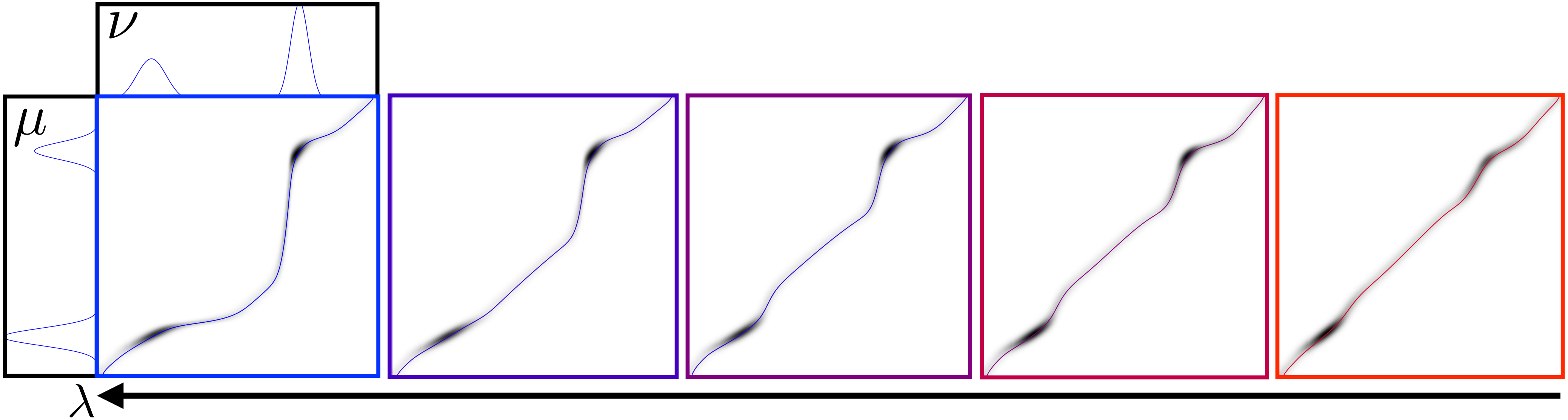

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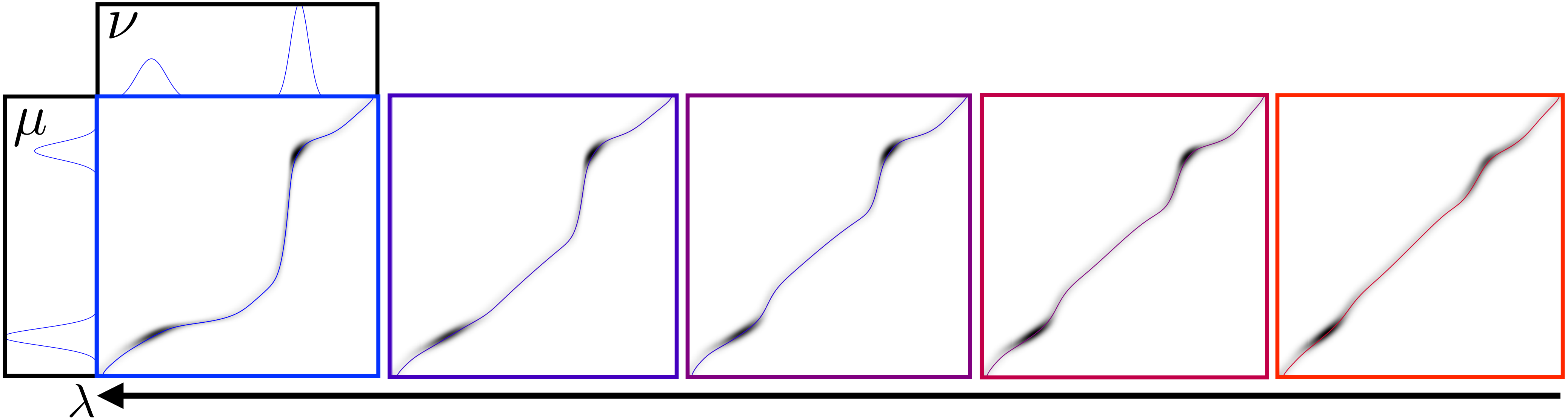
Proposition: If $c(x, y) = -\log(\cos(\min(\frac{d(x,y)}{\delta}, \frac{\pi}{2}))$
then $WF_c^{1/2}$ is a distance on $\mathcal{M}_+(X)$.

[Liereo, Mielke, Savaré 2015] [Chizat, Schmitzer, Peyré, Vialard 2015]



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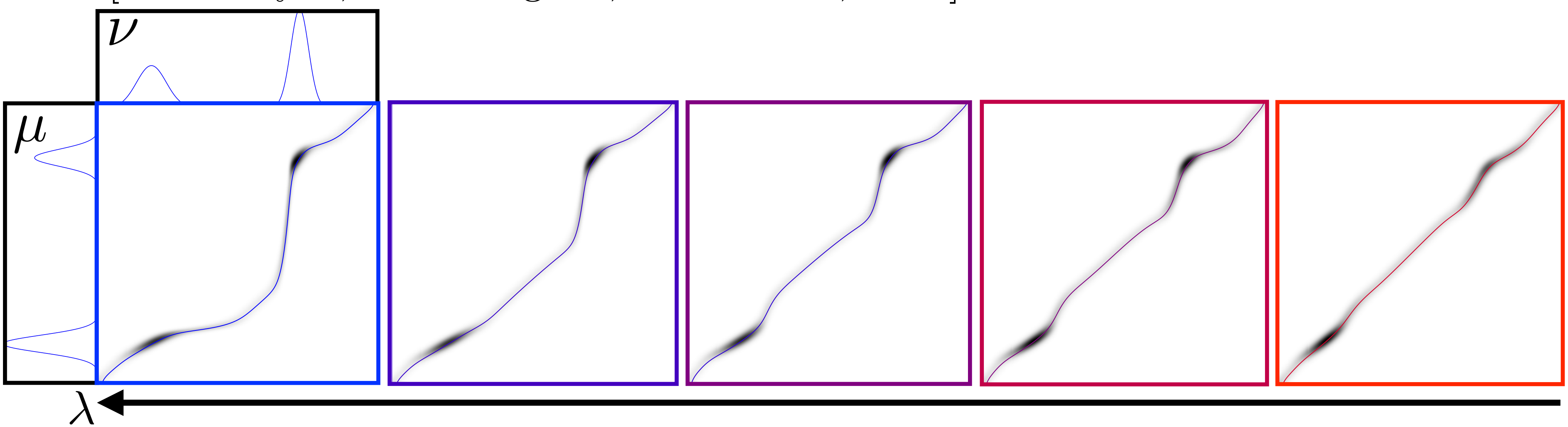
$\rightarrow$ "Dynamic" Benamou-Brenier formulation.

[Liereo, Mielke, Savaré 2015] [Chizat, Schmitzer, Peyré, Vialard 2015]
[Kondratyev, Monsaingeon, Vorotnikov, 2015]



Wasserstein Gradient Flows

Implicit Euler step: [Jordan, Kinderlehrer, Otto 1998]

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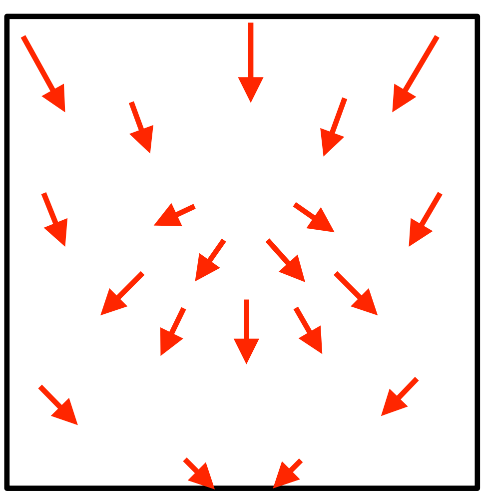
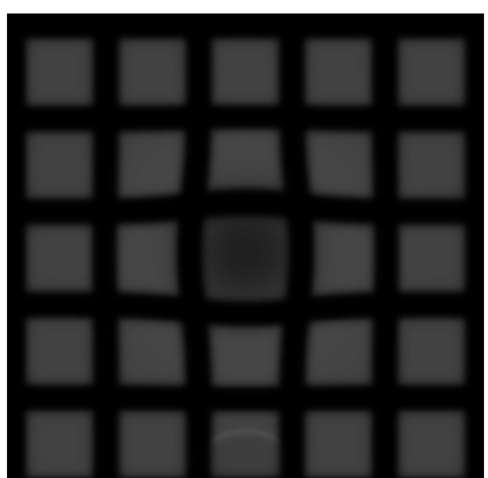
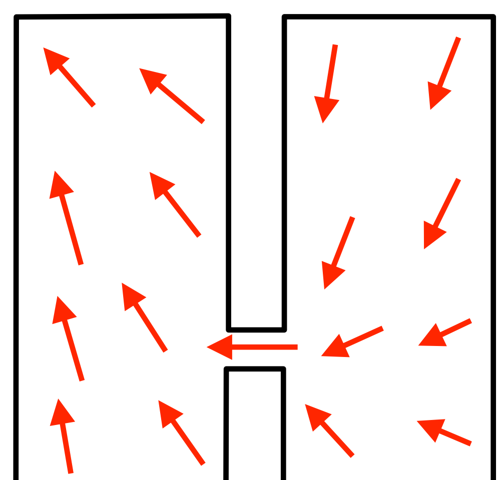


∇w



Evolution μ_t



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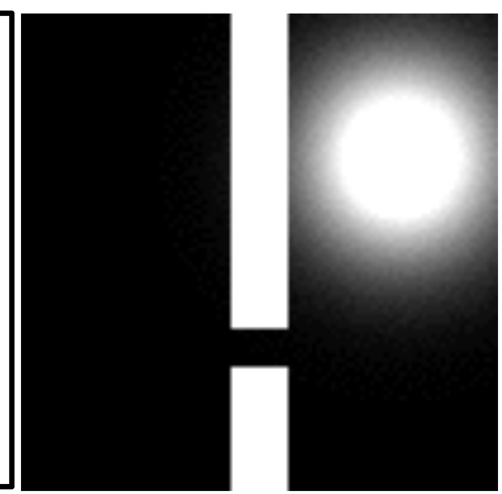

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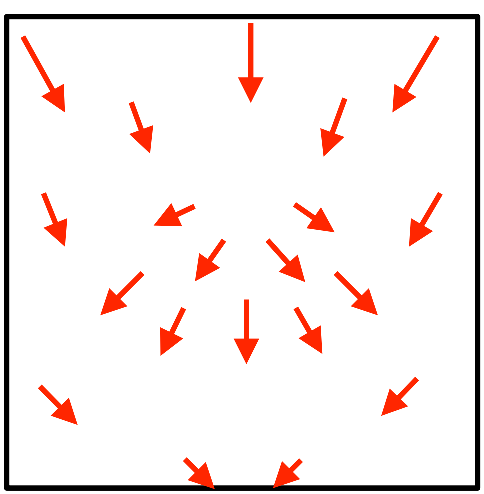
$f(\mu) = \frac{1}{m-1} \int (\frac{\mathrm{d}\mu}{\mathrm{d}x})^{m-1}\mathrm{d}\mu \longrightarrow \partial_t \mu = \Delta \mu^m$ (non-linear diffusion)



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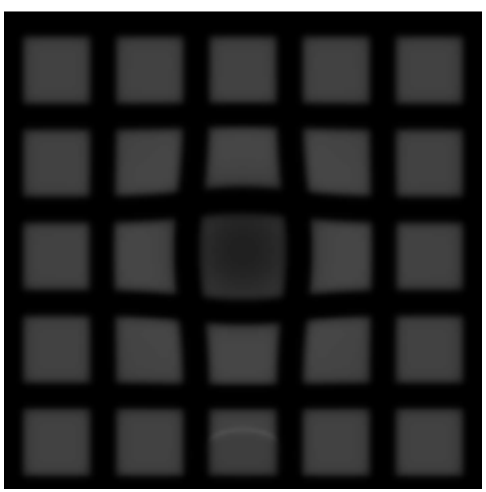

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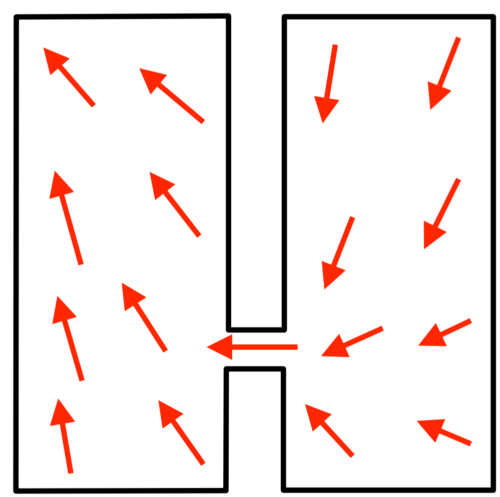

∇w

Evolution μ_t

Overview

- Transportation-like Problems
- **Regularized Transport**
- Optimal Transport Barycenters
- Heat Kernel Approximation

Transportation-like Problems

$$\min_{\pi \in \mathcal{M}_+(X \times X)} \mathcal{E}(\pi) \stackrel{\text{def.}}{=} \langle c,\, \pi \rangle + f_1(P_{1\sharp}\pi) + f_2(P_{2\sharp}\pi)$$

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Regularization: $\min_\pi \mathcal{E}(\pi) + \varepsilon \mathrm{KL}(\pi|\pi_0)$

$\varepsilon \mathrm{KL}(\pi|\pi_0)$ Regularization and positivity barrier.

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$\varepsilon \mathrm{KL}(\pi|\pi_0)$ → Discretization grid (prescribed support).

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$\varepsilon \mathrm{KL}(\pi|\pi_0)$ →
- Regularization and positivity barrier.
- Discretization grid (prescribed support).
- Implicit KL stepping.

π_0

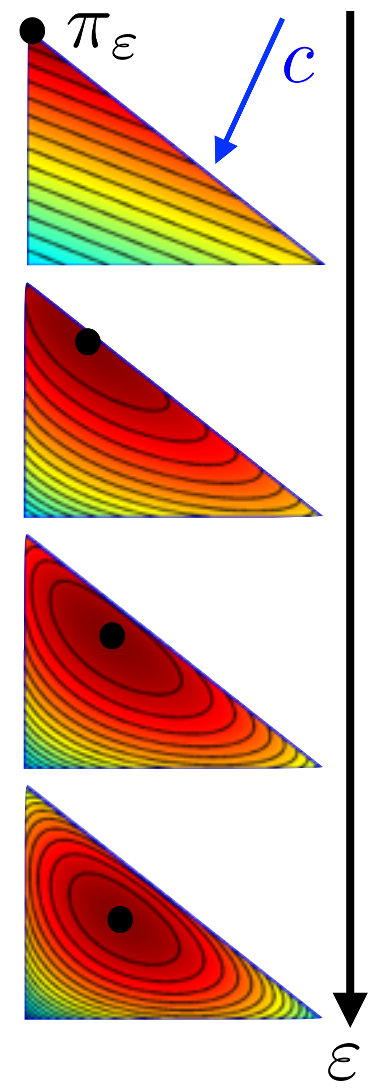
$\pi_1 = \mathrm{Prox}_{\frac{1}{\varepsilon}\mathcal{E}}(\pi_0)$

$\pi_2 = \mathrm{Prox}_{\frac{1}{\varepsilon}\mathcal{E}}(\pi_1)$

$\mathrm{argmin}\, \mathcal{E}(\pi)$

Entropy Regularized Transport

$$\pi_\varepsilon \stackrel{\text{def.}}{=} \underset{\pi}{\operatorname{argmin}} \; \{\langle c, \pi\rangle + \varepsilon \mathrm{KL}(\pi|\pi_0) \; ; \; \pi \in \Pi(\mu,\nu)\}$$



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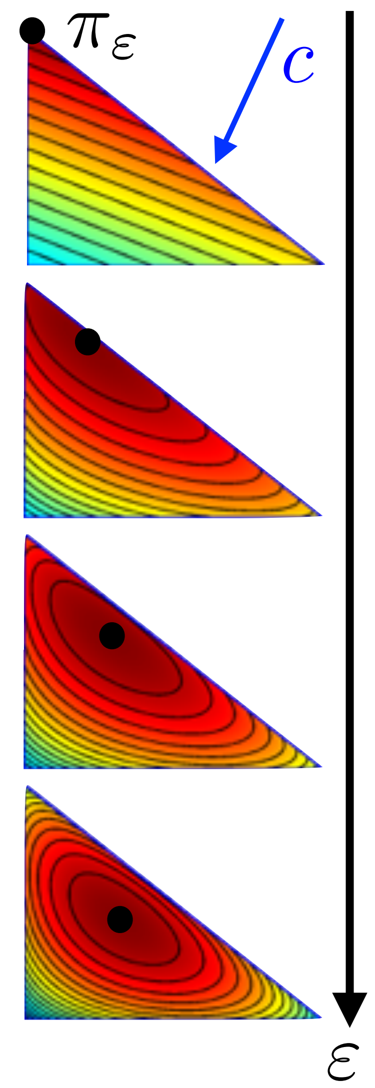
Schrödinger's problem: $\pi_\varepsilon = \underset{\pi \in \Pi(\mu,\nu)}{\text{argmin}} \ \text{KL}(\pi|K)$

Gibbs kernel: $K(x,y) \overset{\text{def.}}{=} e^{-\frac{c(x,y)}{\varepsilon}} \pi_0(x,y)$

Landmark computational paper: [Cuturi 2013].



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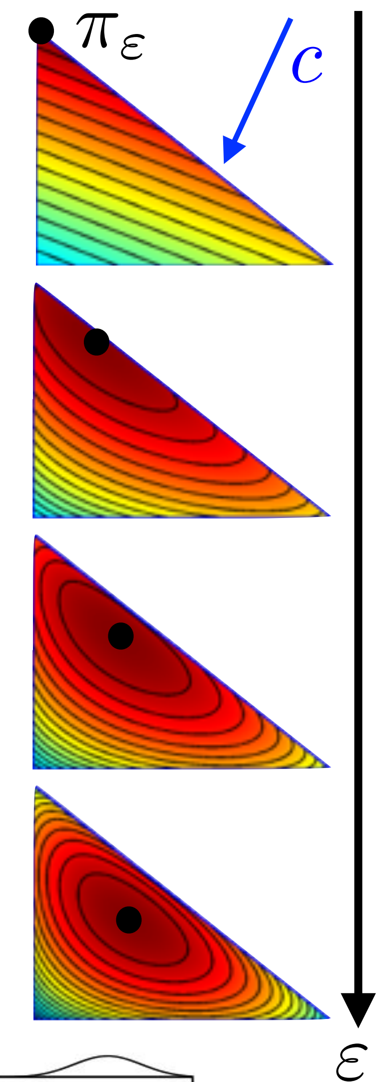

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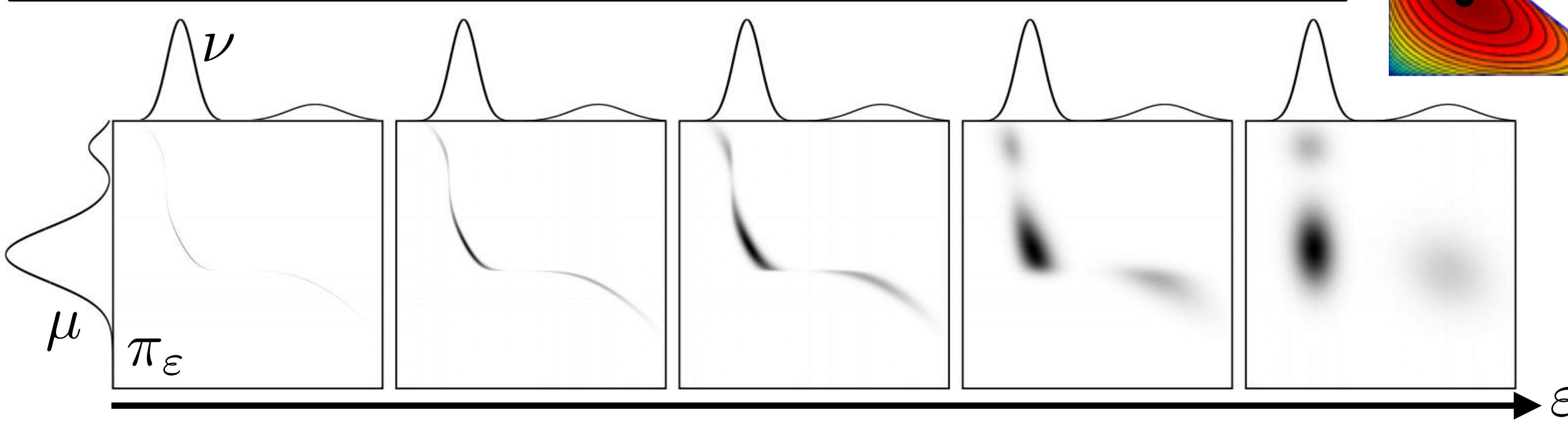
Proposition: [Carlier, Duval, Peyré, Schmitzer 2015]

$$\pi_\varepsilon \xrightarrow{\varepsilon \to 0} \underset{\pi \in \Pi(\mu,\nu)}{\operatorname{argmin}} \; \langle c,\, \pi\rangle \qquad \pi_\varepsilon \xrightarrow{\varepsilon \to +\infty} \mu(x)\nu(y)$$



Dykstra-like Iterations

$$\textit{Primal:}\ \min_{\pi}\ \langle c,\, \pi\rangle + f_1(P_{1\sharp}\pi) + f_2(P_{2\sharp}\pi) + \varepsilon \mathrm{KL}(\pi|\pi_0)$$

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Primal: $\min_{\pi} \langle c,\, \pi\rangle + f_1(P_{1\sharp}\pi) + f_2(P_{2\sharp}\pi) + \varepsilon \mathrm{KL}(\pi|\pi_0)$

Dual: $\max_{u,v} \; - f_1^*(u) - f_2^*(u) - \varepsilon\langle e^{\frac{u}{\varepsilon}},\, K e^{-\frac{v}{\varepsilon}}\rangle$

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Block coordinates relaxation: $\max_{u} - f_1^*(u) - \varepsilon \langle e^{\frac{u}{\varepsilon}}, K e^{-\frac{v}{\varepsilon}} \rangle \qquad (\mathcal{I}_u)$

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Proposition: the solutions of $(\mathcal{I}_u)$ and $(\mathcal{I}_v)$ read:

$$a = \frac{\mathrm{Prox}^{\mathrm{KL}}_{f_1/\varepsilon}(Kb)}{Kb} \qquad b = \frac{\mathrm{Prox}^{\mathrm{KL}}_{f_2/\varepsilon}(K^*a)}{K^*a}$$

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→ Only matrix-vector multiplications. → Highly parallelizable.

→ On regular grids: only convolutions! Linear time iterations.

Sinkhorn's Algorithm

Optimal transport problem:

$$f_1 = \iota_\mu \longrightarrow \mathrm{Prox}^{\mathrm{KL}}_{f_1/\varepsilon}(\tilde{\mu}) = \mu$$

$$f_2 = \iota_\nu \longrightarrow \mathrm{Prox}^{\mathrm{KL}}_{f_2/\varepsilon}(\tilde{\nu}) = \nu$$

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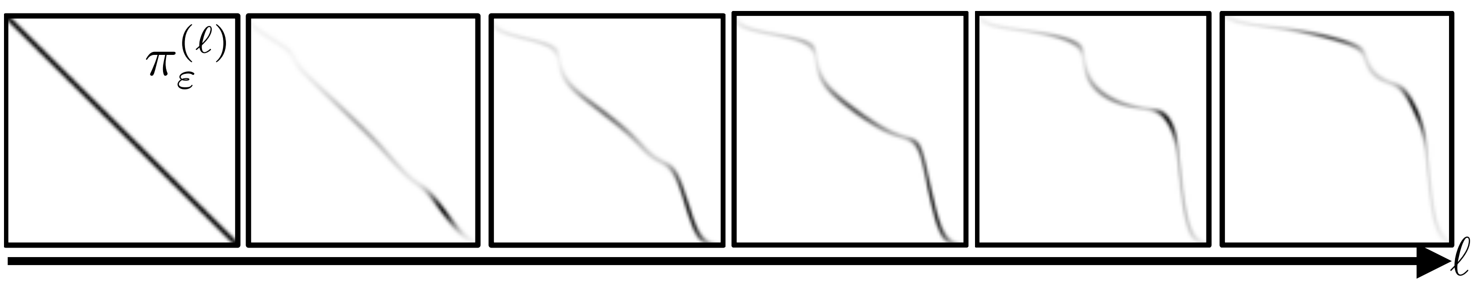
Sinkhorn/IPFP algorithm: [Sinkhorn 1967][Deming,Stephan 1940]

$$a^{(\ell+1)} \overset{\text{def.}}{=} \frac{\mu}{K b^{(\ell)}} \quad \text{and} \quad b^{(\ell+1)} \overset{\text{def.}}{=} \frac{\nu}{K^* a^{(\ell+1)}}$$



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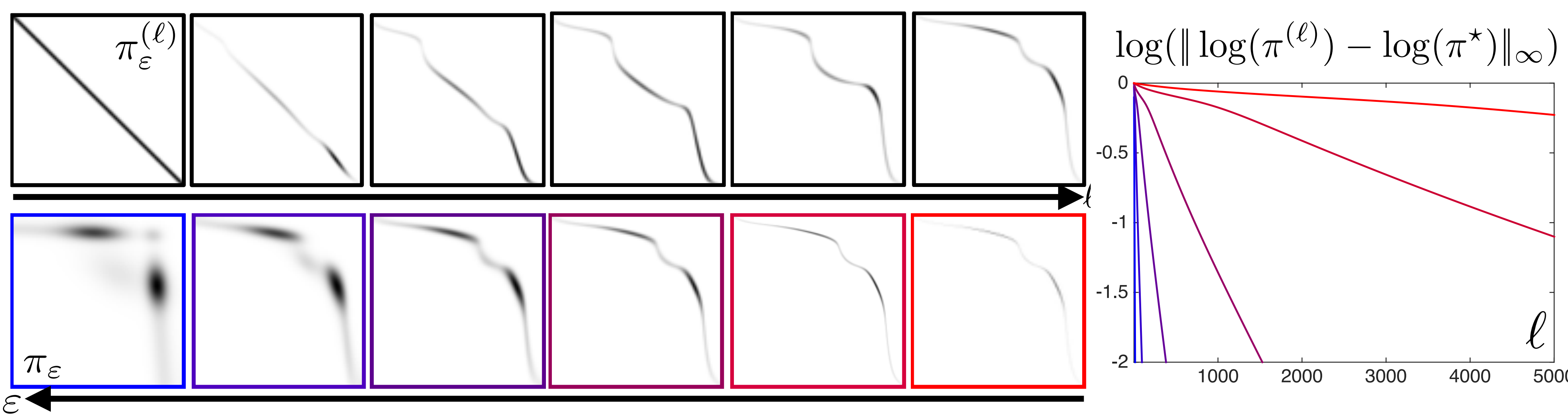
Proposition: $\| \log(\pi^{(\ell)}) - \log(\pi^\star) \|_\infty = O(1-\delta)^\ell, \quad \delta \sim \kappa_c^{-1/\varepsilon}$

$$\pi^{(\ell)} \overset{\text{def.}}{=} \mathrm{diag}(a^{(\ell)}) K \, \mathrm{diag}(b^{(\ell)})$$

[Franklin,Lorenz 1989]
Local rate: [Knight 2008]



Gradient Flows: Crowd Motion

$$\mu_{t+1} \overset{\text{def.}}{=} \operatorname{argmin}_{\mu} W_\alpha^\alpha(\mu_t, \mu) + \tau f(\mu)$$

Congestion-inducing function:

$$f(\mu) = \iota_{[0,\kappa]}(\mu) + \langle w,\, \mu \rangle$$

[Maury, Roudneff-Chupin, Santambrogio 2010]

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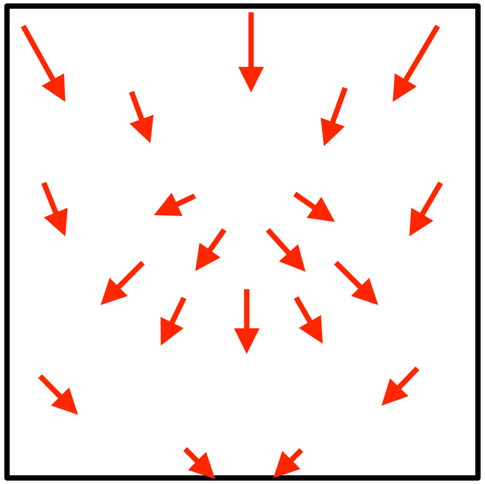
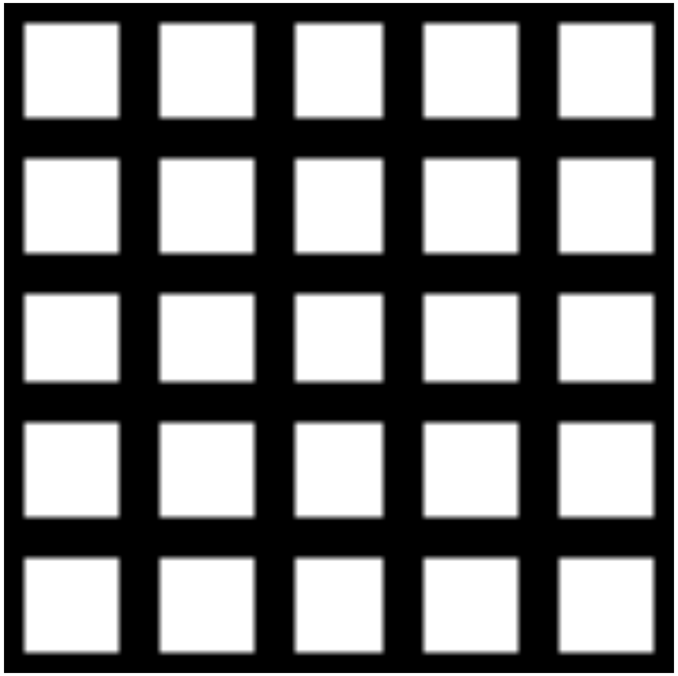
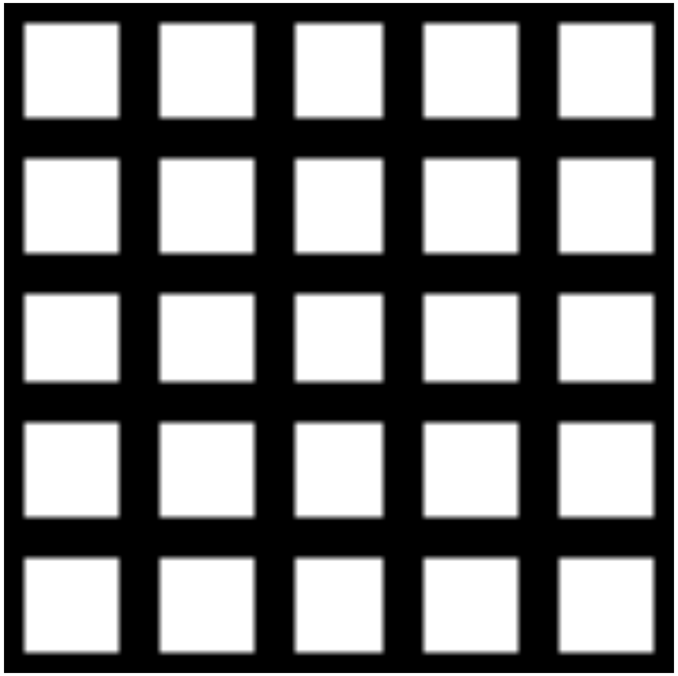


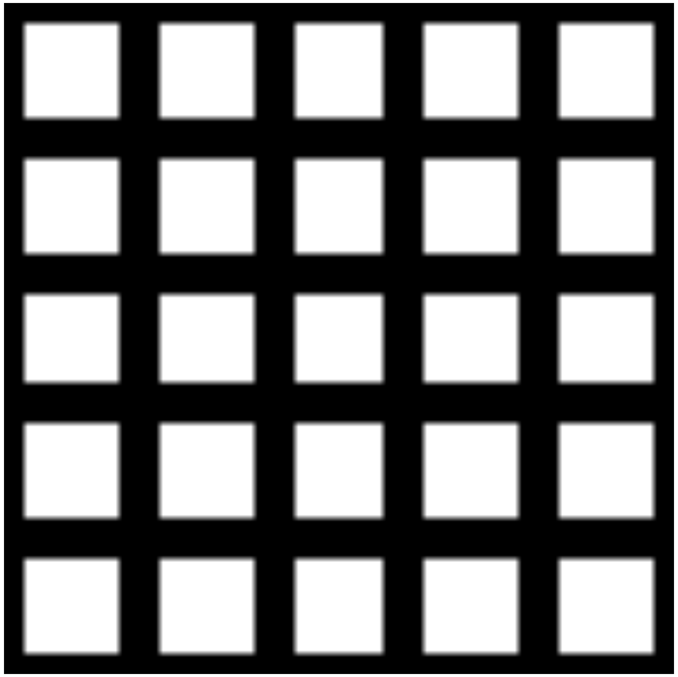
∇w



$\kappa = \|\mu_{t=0}\|_\infty$



$\kappa = 2\|\mu_{t=0}\|_\infty$



$\kappa = 4\|\mu_{t=0}\|_\infty$

Multiple-Density Gradient Flows

$$(\mu_{1,t+1}, \mu_{2,t+1}) \overset{\text{def.}}{=} \underset{(\mu_1,\mu_2)}{\operatorname{argmin}}\, W_\alpha^\alpha(\mu_{1,t}, \mu_1) + W_\alpha^\alpha(\mu_{2,t}, \mu_2) + \tau f(\mu_1, \mu_2)$$

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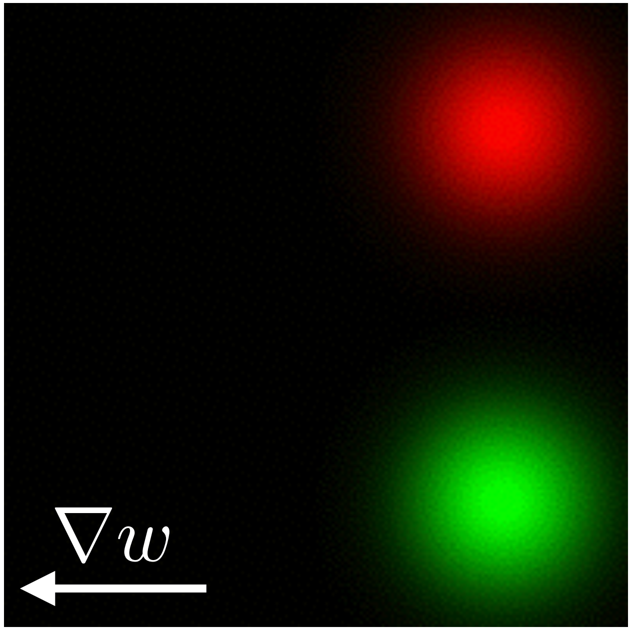
Wasserstein attraction:

$$f(\mu_1, \mu_2) = W_\alpha^\alpha(\mu_1, \mu_2) + h_1(\mu_1) + h_2(\mu_2)$$



Example: $h_i(\mu) = \langle w,\, \mu \rangle.$

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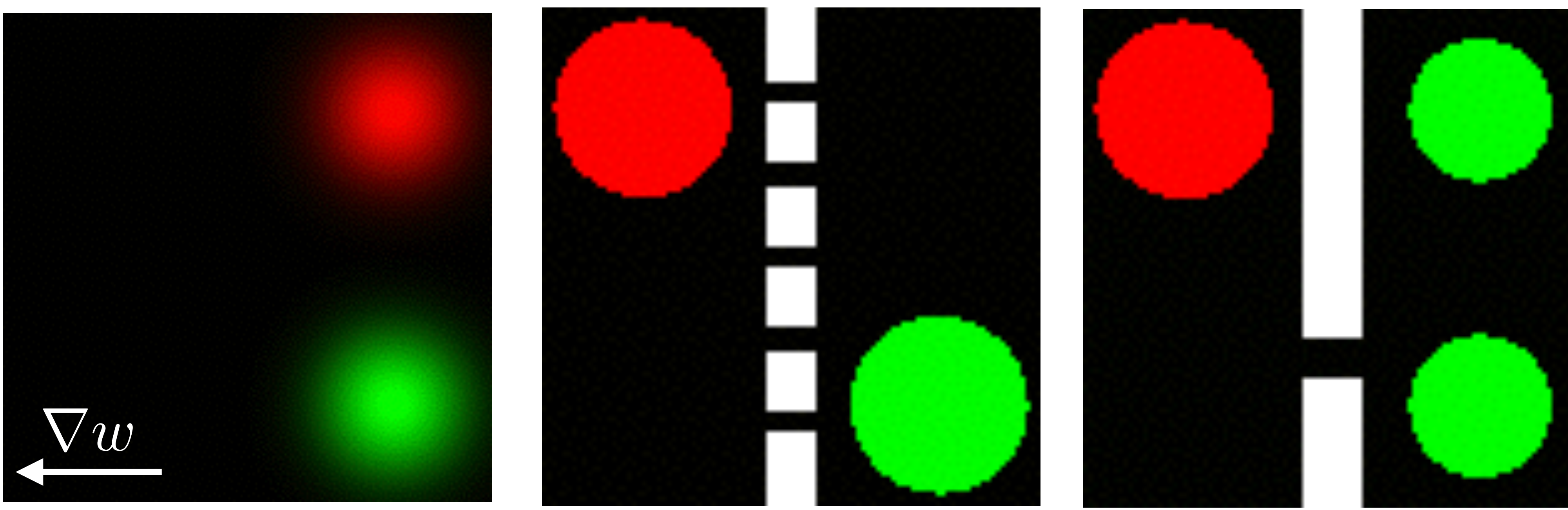

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Overview

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- Heat Kernel Approximation

Wasserstein Barycenters

Barycenters of measures $(\mu_k)_k$: $\quad \sum_k \lambda_k = 1$

$$\mu^\star \in \underset{\mu}{\operatorname{argmin}} \sum_k \lambda_k W_\alpha^\alpha(\mu_k, \mu)$$

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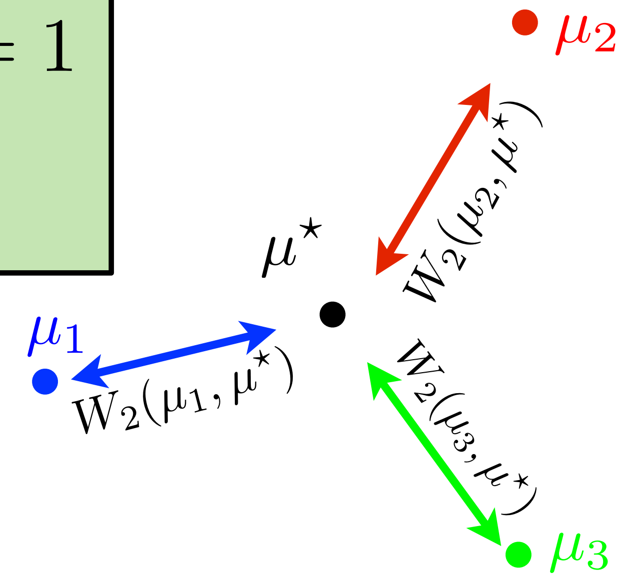

Generalizes Euclidean barycenter:

If $\mu_k = \delta_{x_k}$ then $\mu^\star = \delta_{\sum_k \lambda_k x_k}$

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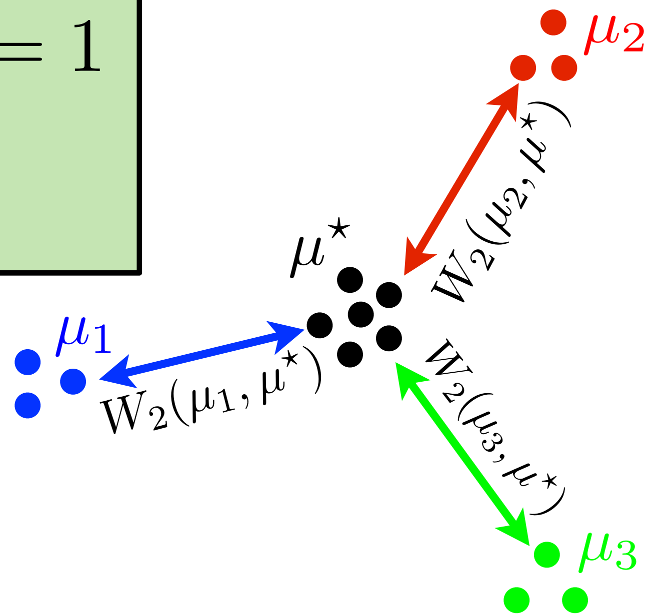

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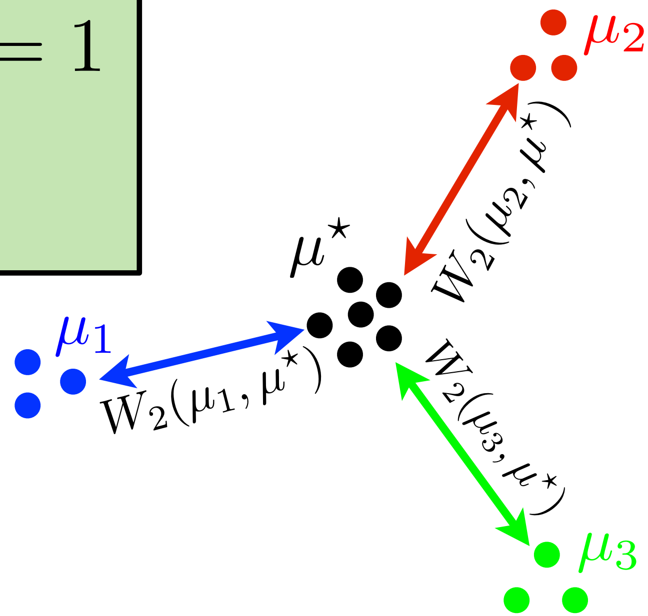

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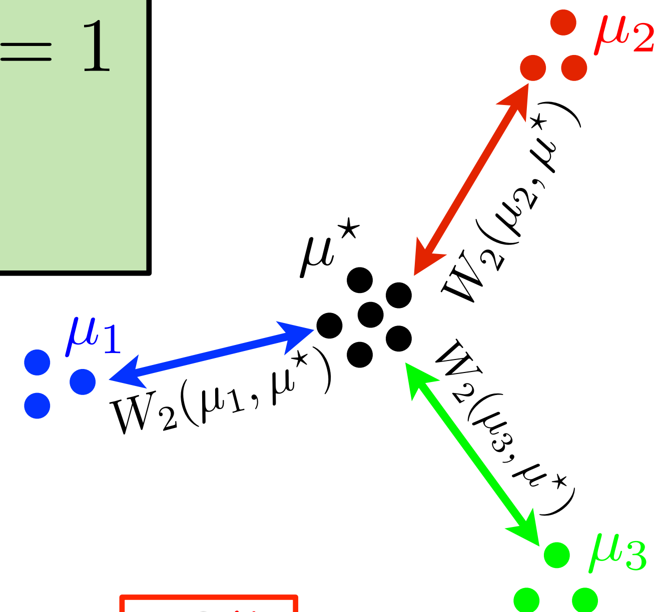

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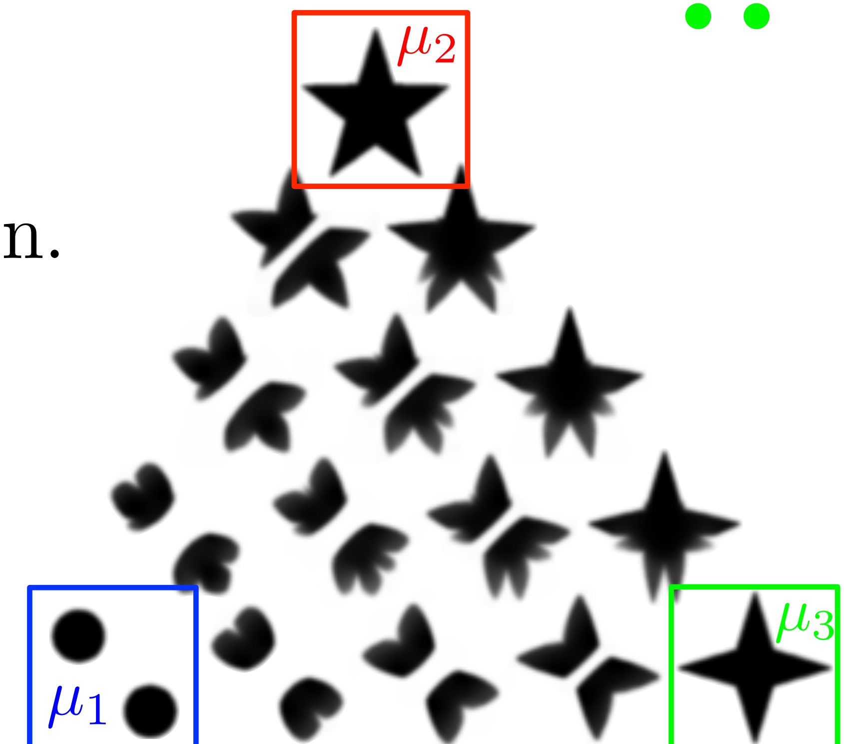

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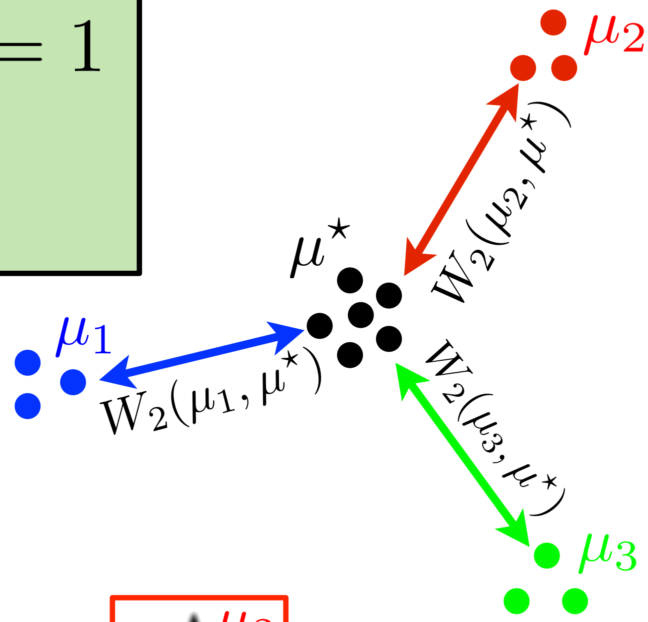

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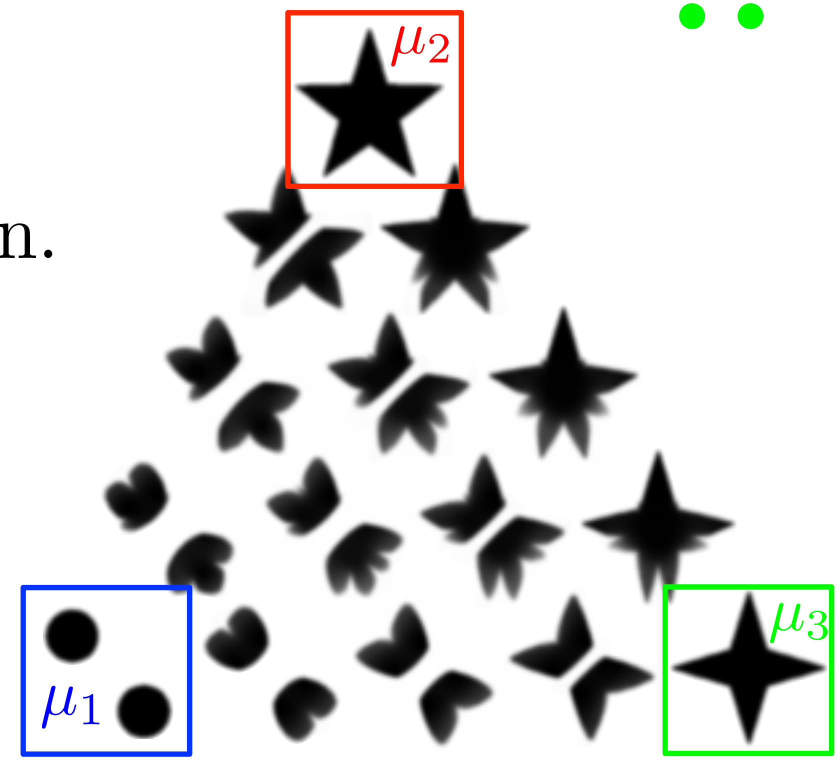

Theorem: [Agueh, Carlier, 2010]

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

if μ_1 does not vanish on small sets, $\mu^\star$ exists and is unique.

Regularized Barycenters

$$\min_{(\pi_k)_k,\mu} \left\{ \sum_k \lambda_k \left(\langle c,\, \pi_k \rangle + \varepsilon \mathrm{KL}(\pi_k | \pi_{0,k}) \right) \ ; \ \forall k, \pi_k \in \Pi(\mu_k, \mu) \right\}$$

Regularized Barycenters

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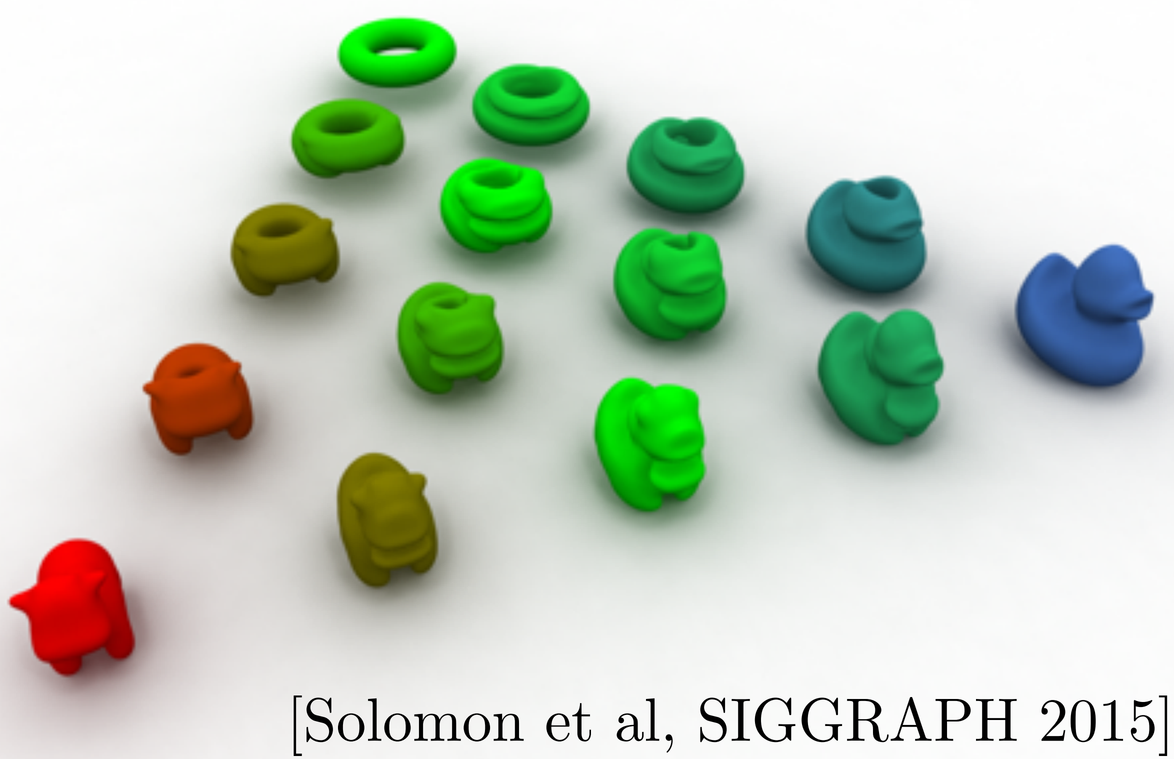
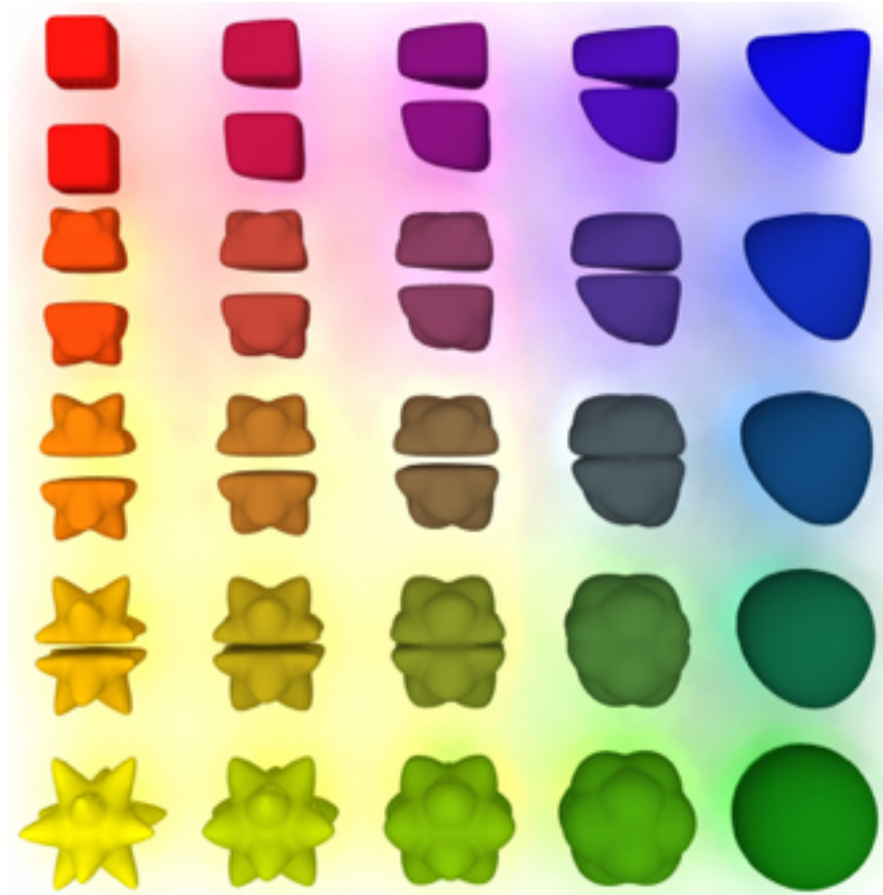


[Solomon et al, SIGGRAPH 2015]

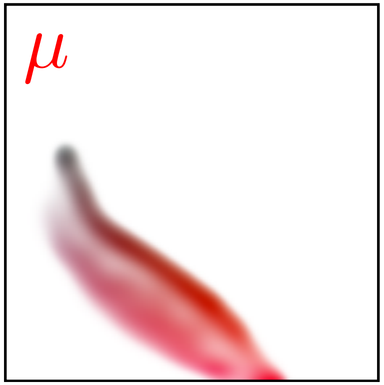


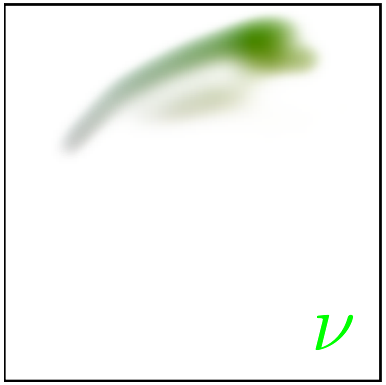
Color Transfer

Input images: (f, g) (chrominance components)

Input measures: $\mu(A) = \mathcal{U}(f^{-1}(A)), \nu(A) = \mathcal{U}(g^{-1}(A))$

f





g

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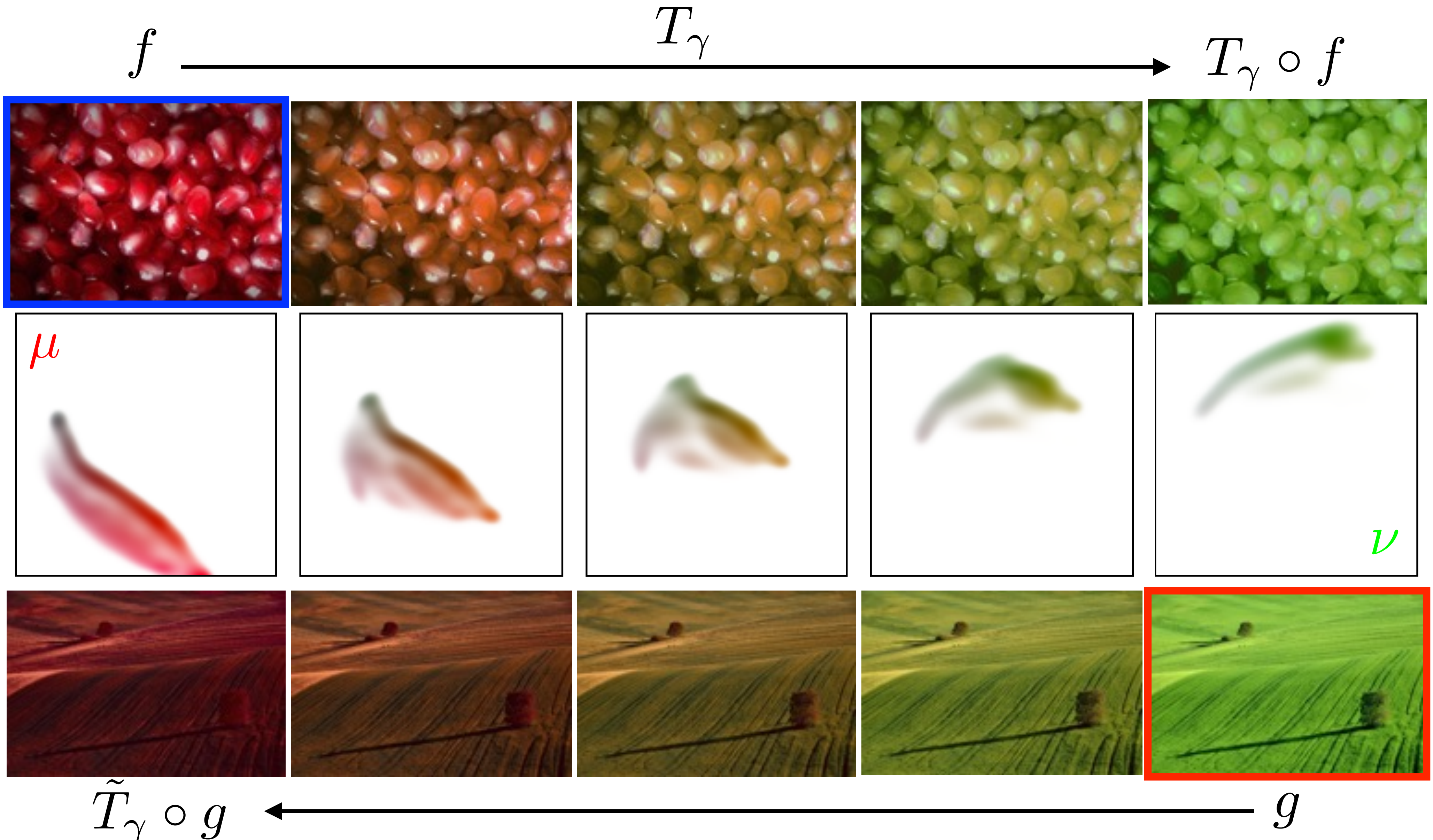


Color Harmonization

Raw image sequence

↓

Color Harmonization

Raw image sequence

↓

Compute Wasserstein barycenter

↓

Project on the barycenter

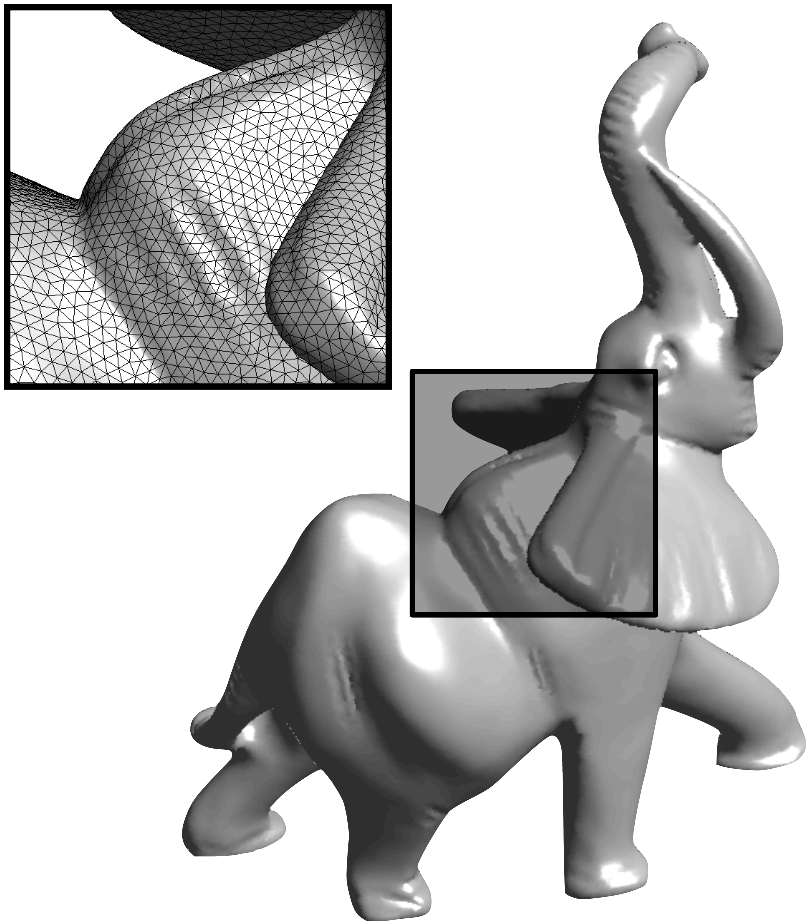
Overview

- Transportation-like Problems
- Regularized Transport
- Optimal Transport Barycenters
- **Heat Kernel Approximation**

Optimal Transport on Surfaces

Triangulated mesh M.

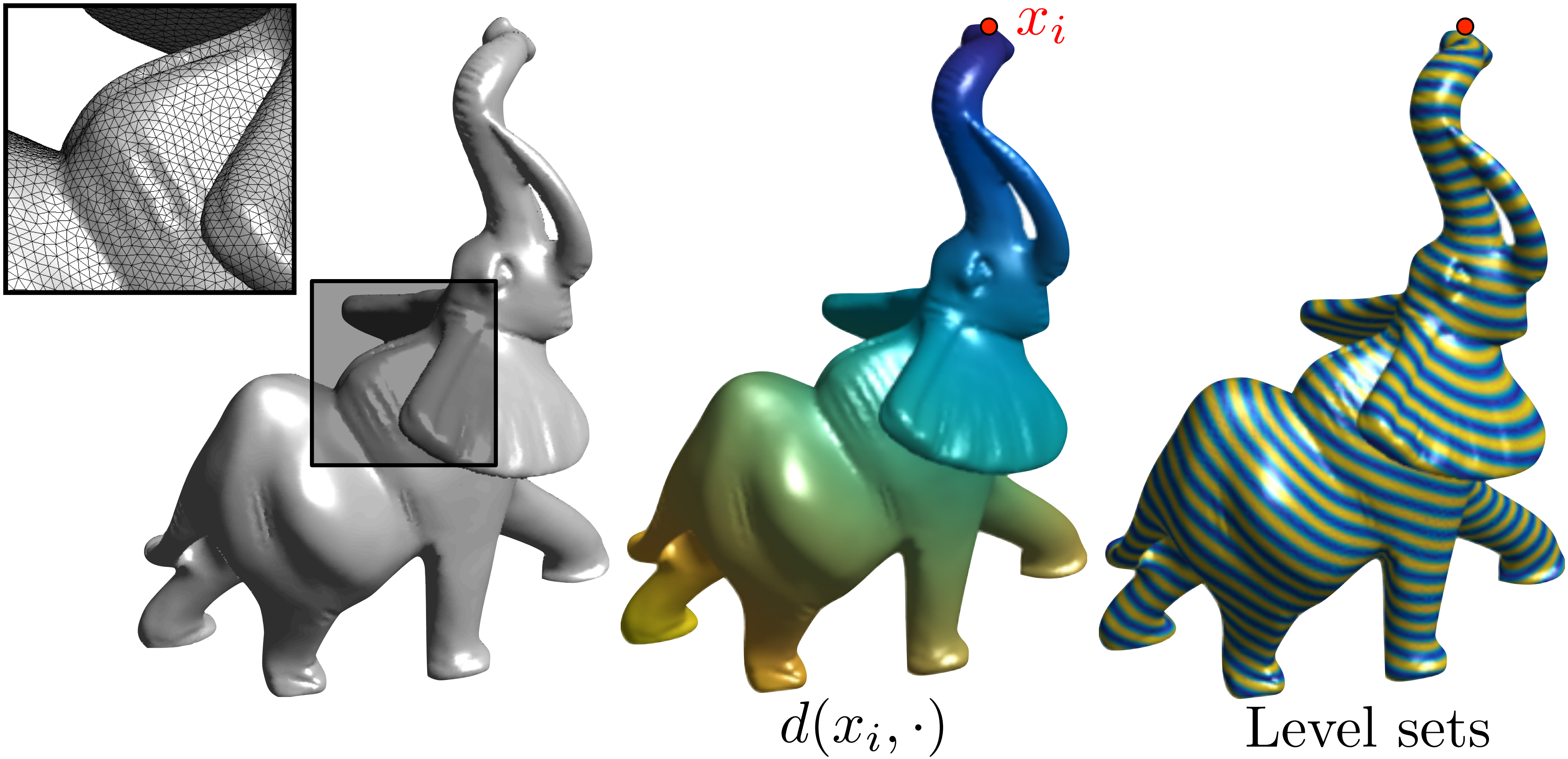
Geodesic distance d_M.



Optimal Transport on Surfaces

Triangulated mesh M. Geodesic distance d_M.

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



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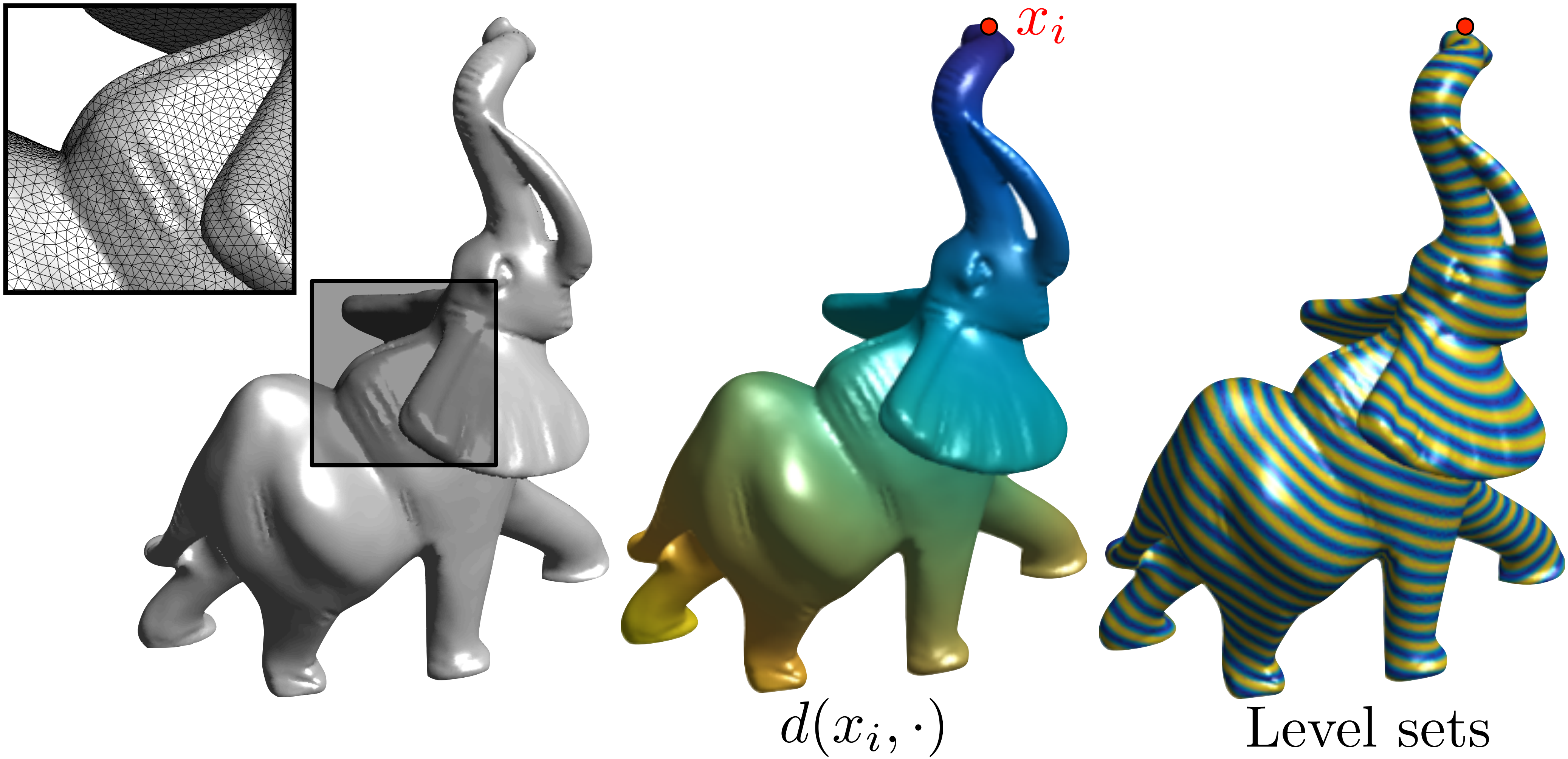
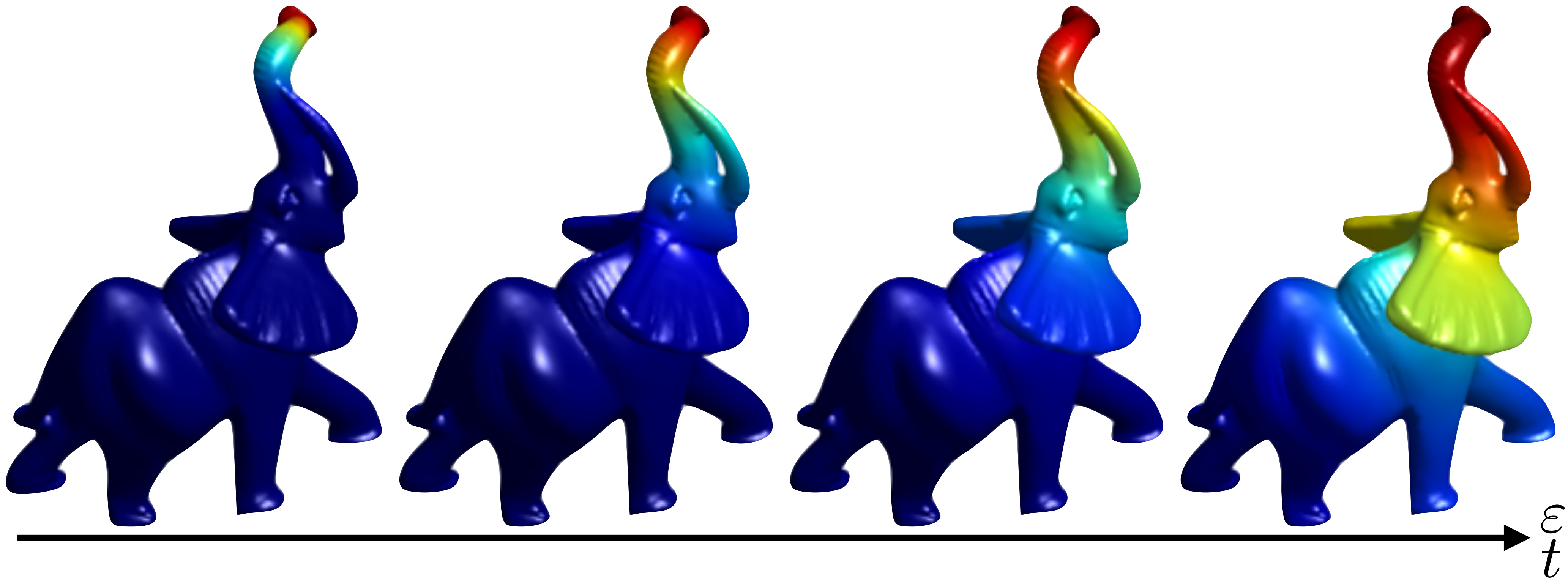


Computing c (Fast-Marching): $N^2 \log(N) \to$ too costly.

Entropic Transport on Surfaces

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



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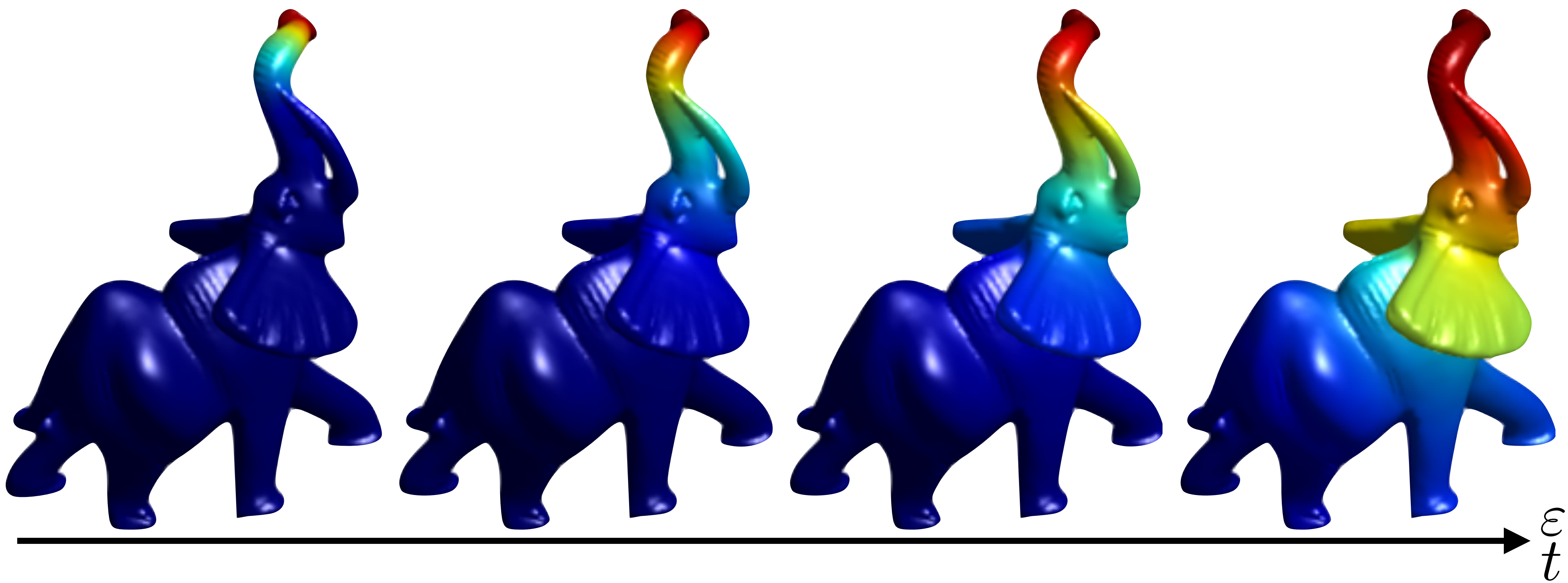
Theorem: [Varadhan] $\quad -\varepsilon \log(u_\varepsilon) \xrightarrow{\varepsilon\to 0} d_M^2$



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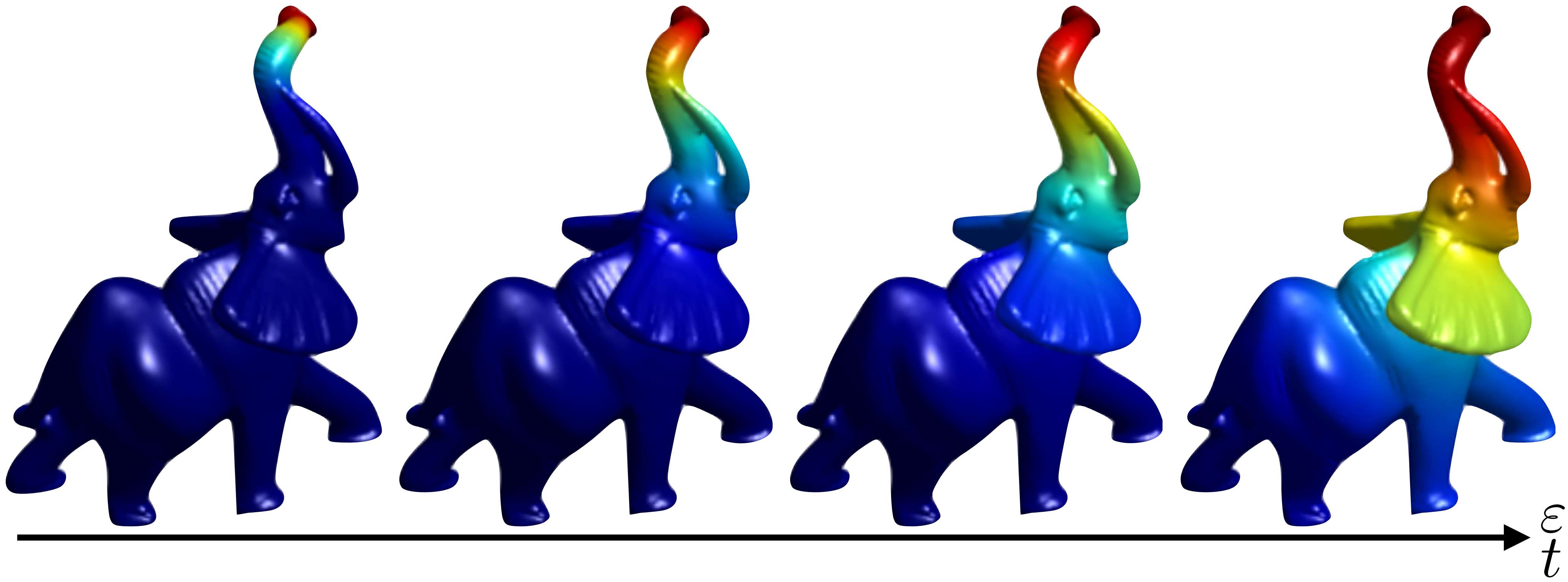
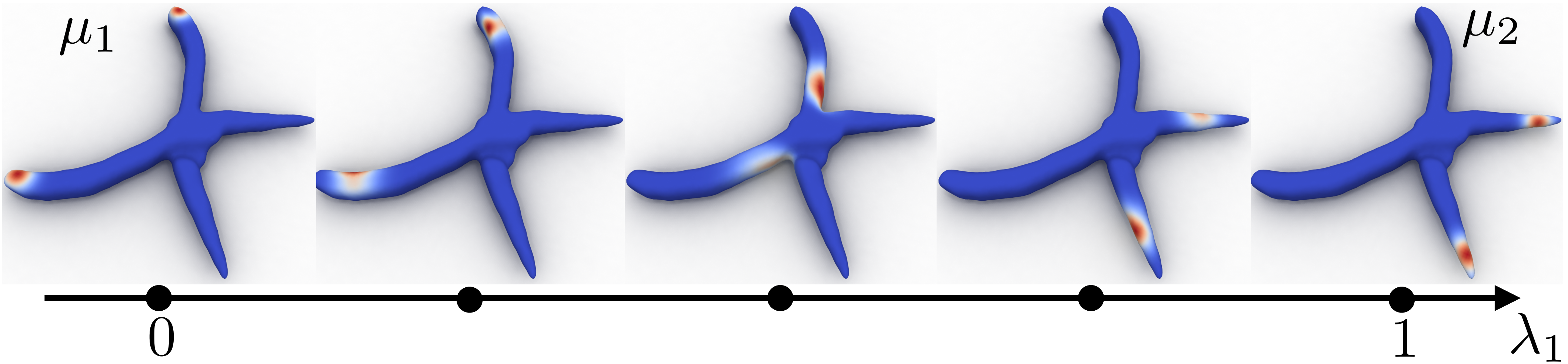
Sinkhorn kernel: $\quad K \overset{\text{def.}}{=} e^{-\frac{d_M^2}{\varepsilon}} \approx u_\varepsilon \approx \left(\mathrm{Id} - \frac{\varepsilon}{\ell}\Delta_M\right)^{-\ell}$



Barycenter on a Surface



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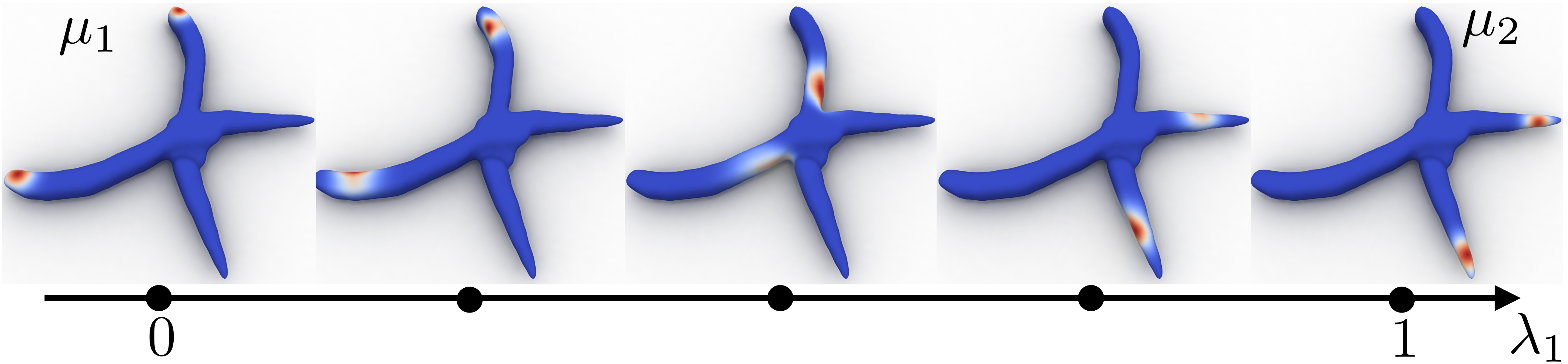

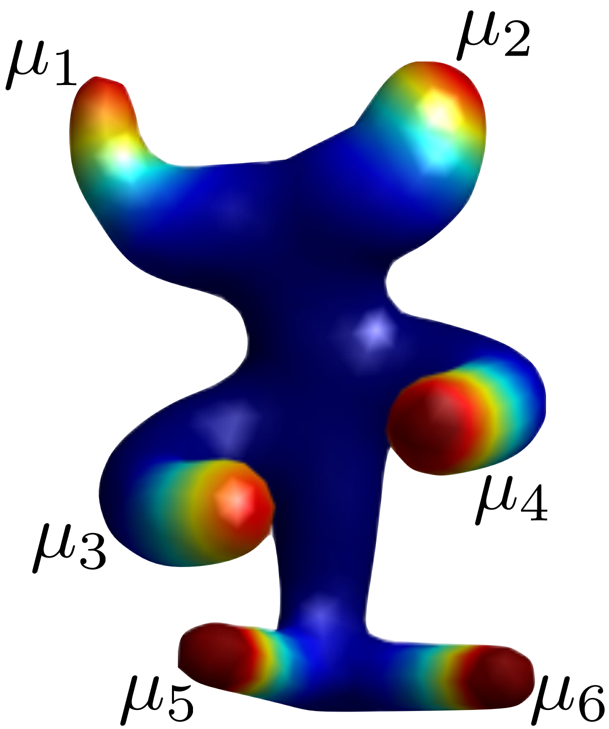

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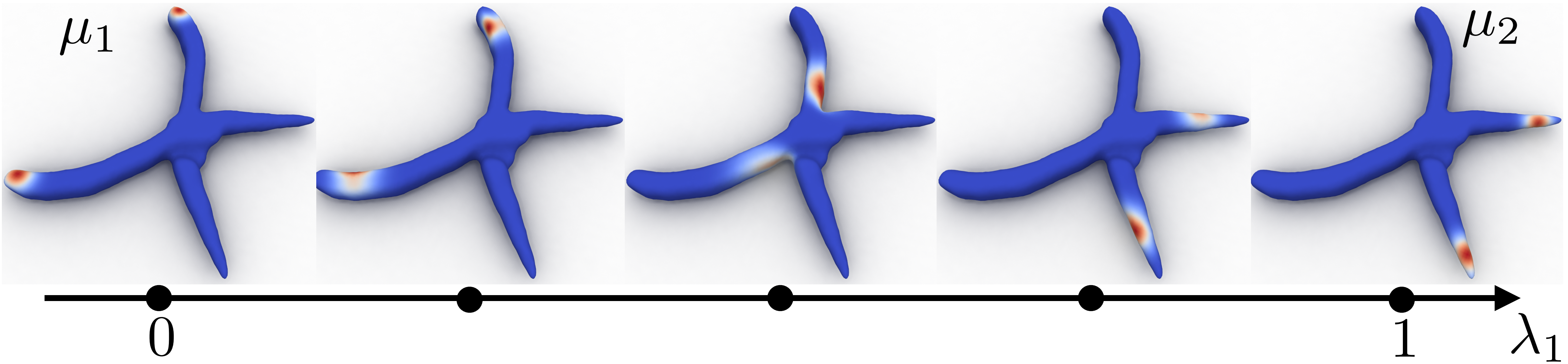
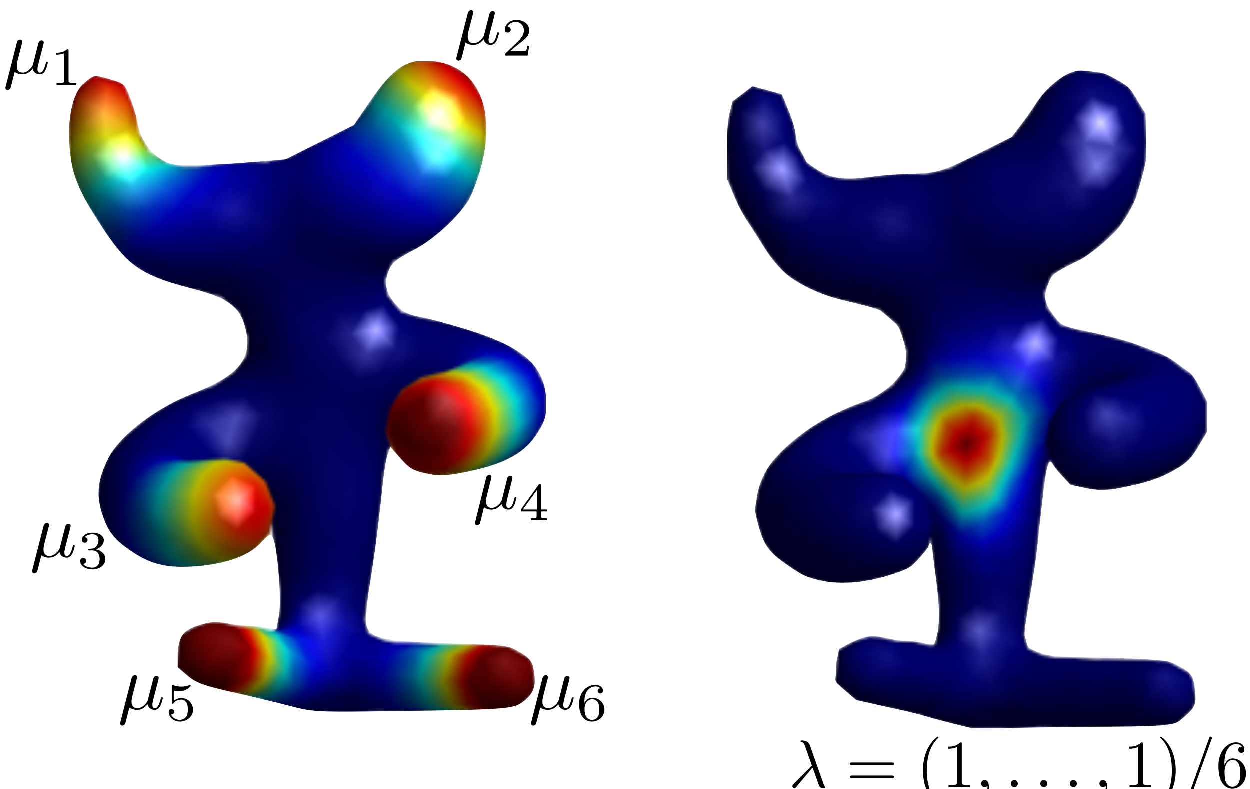
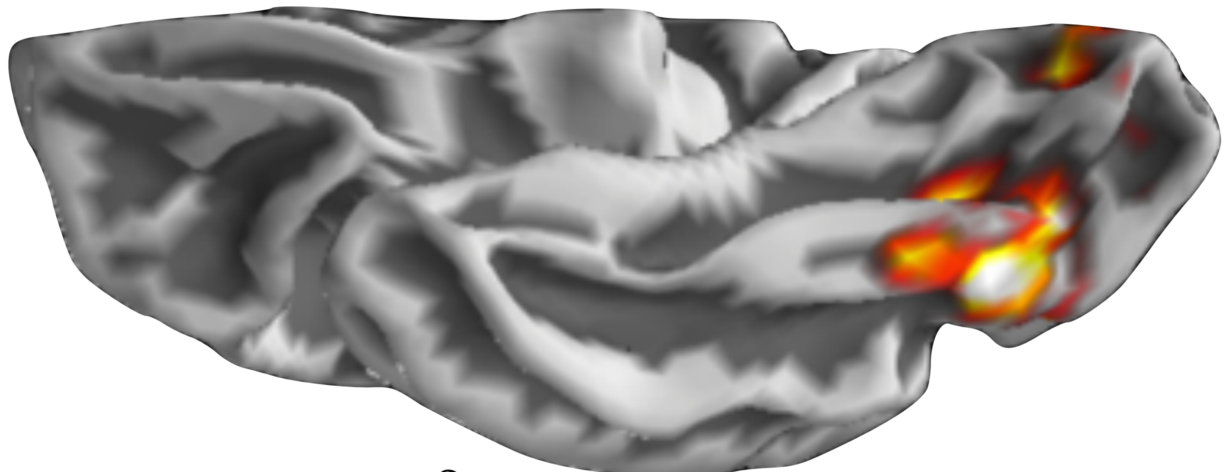


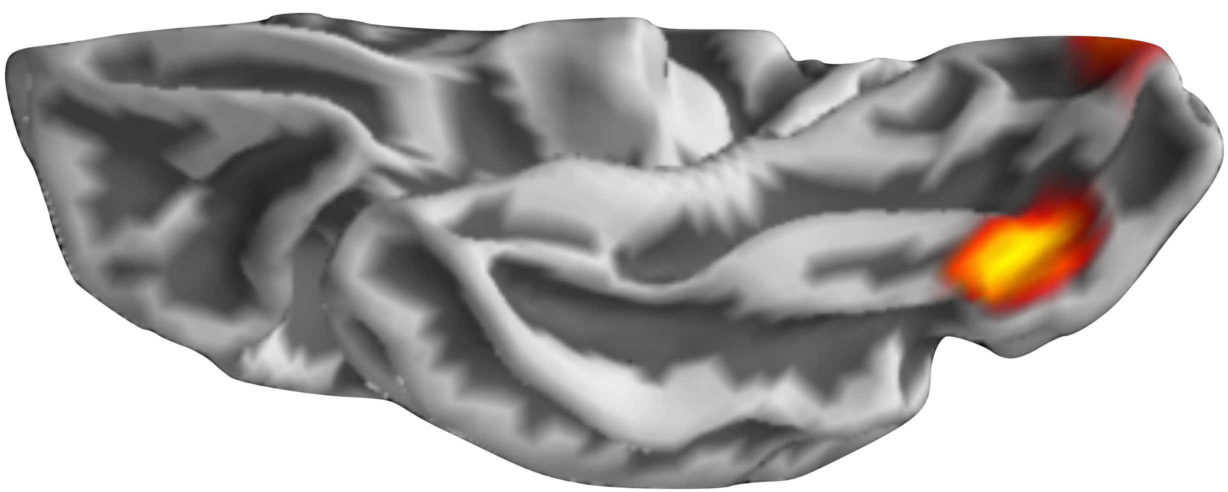


MRI Data Procesing [with A. Gramfort]

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



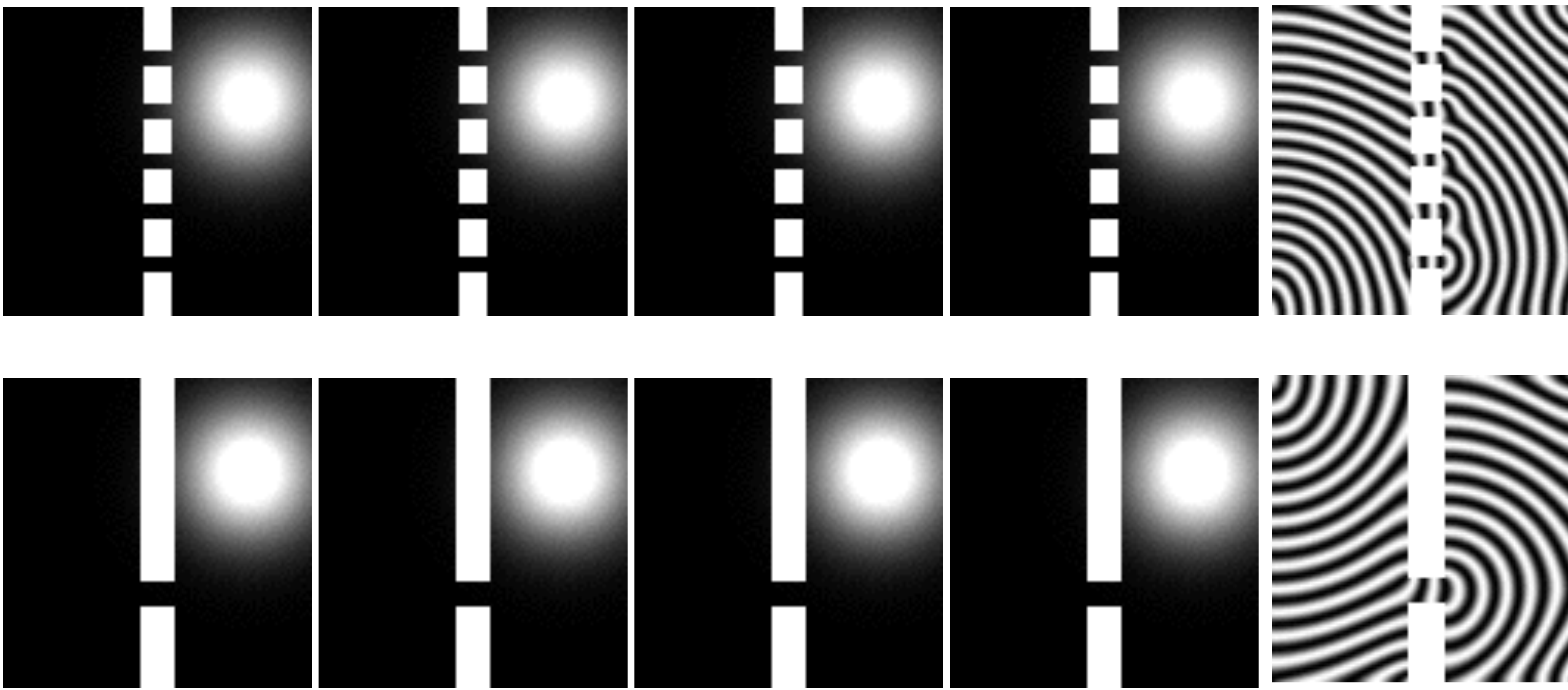
L^2 barycenter



W_2^2 barycenter

Gradient Flows: Crowd Motion with Obstacles

$$M = \text{sub-domain of } \mathbb{R}^2.$$



$\kappa = \|\mu_{t=0}\|_\infty$ $\kappa = 2\|\mu_{t=0}\|_\infty$ $\kappa = 4\|\mu_{t=0}\|_\infty$ $\kappa = 6\|\mu_{t=0}\|_\infty$ Potential $\cos(w)$

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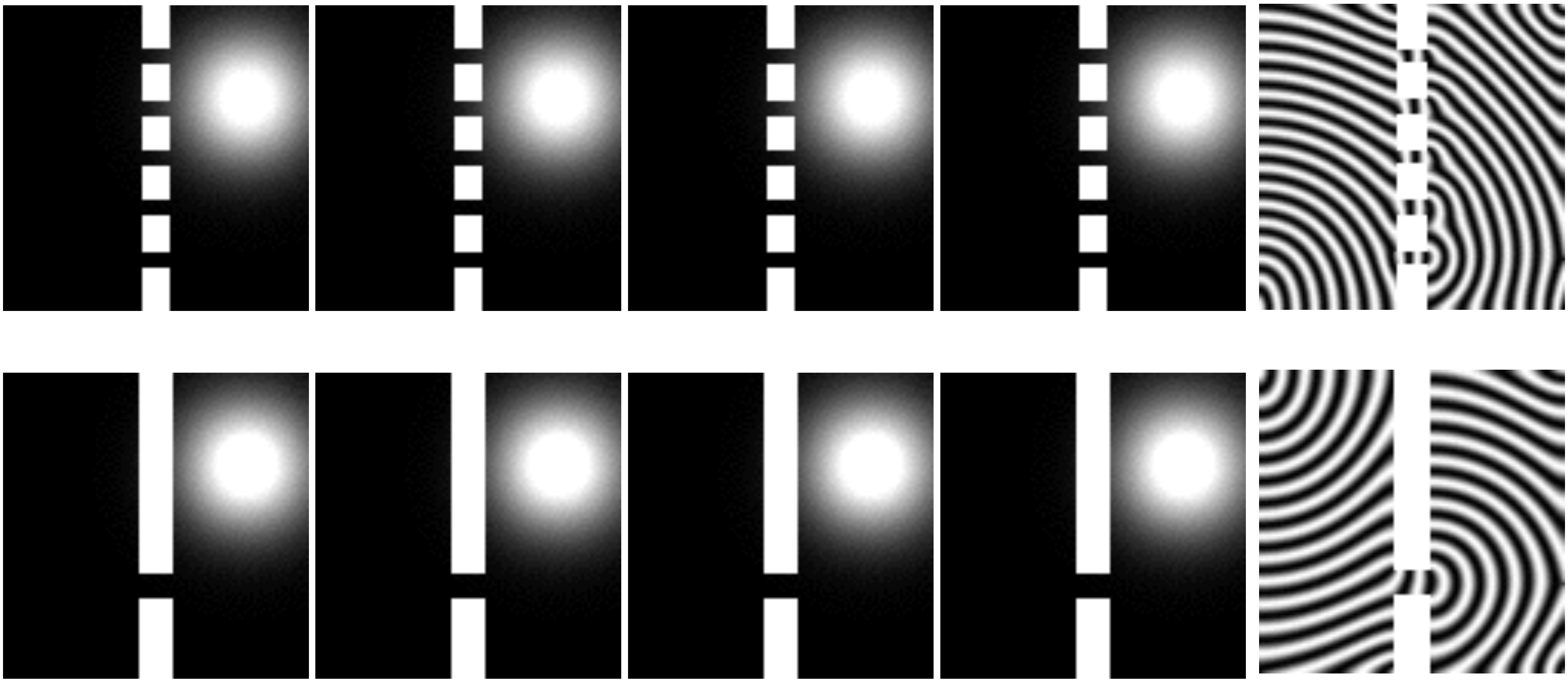

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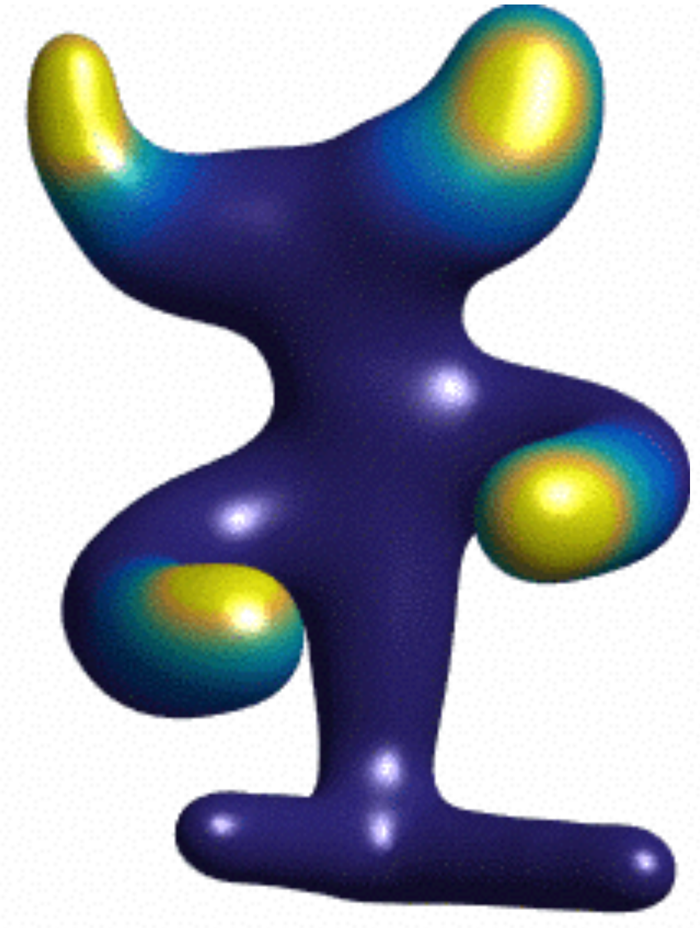

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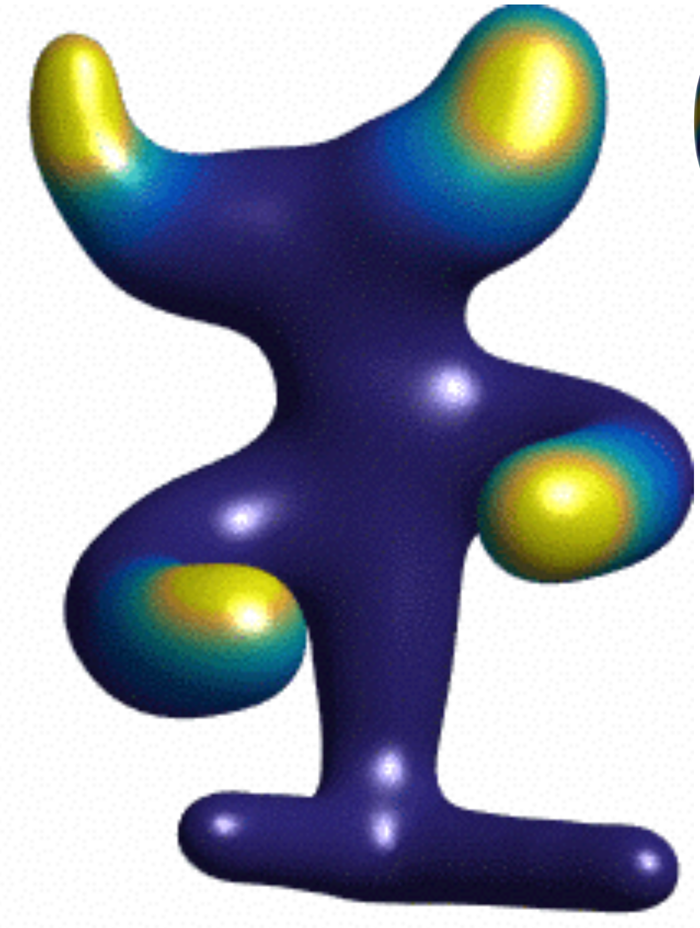

$\kappa = 6\|\mu_{t=0}\|_\infty$

Potential $\cos(w)$

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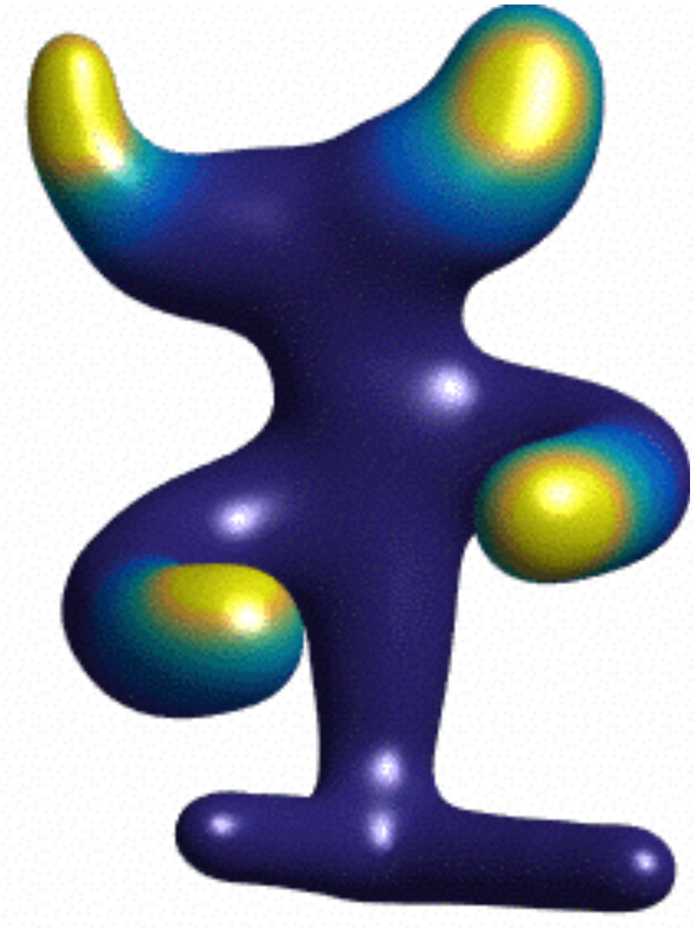

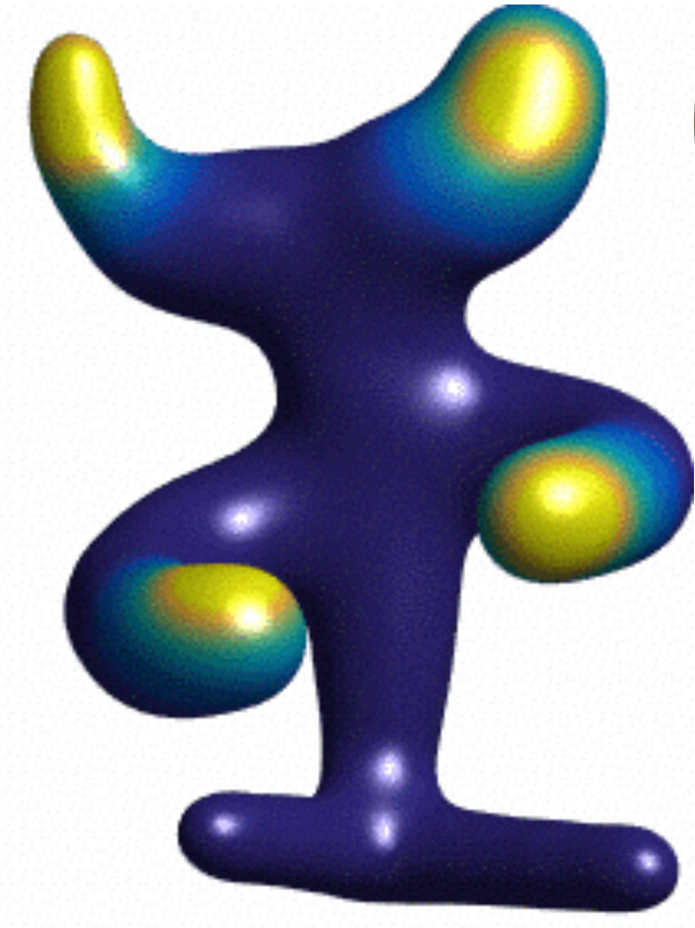

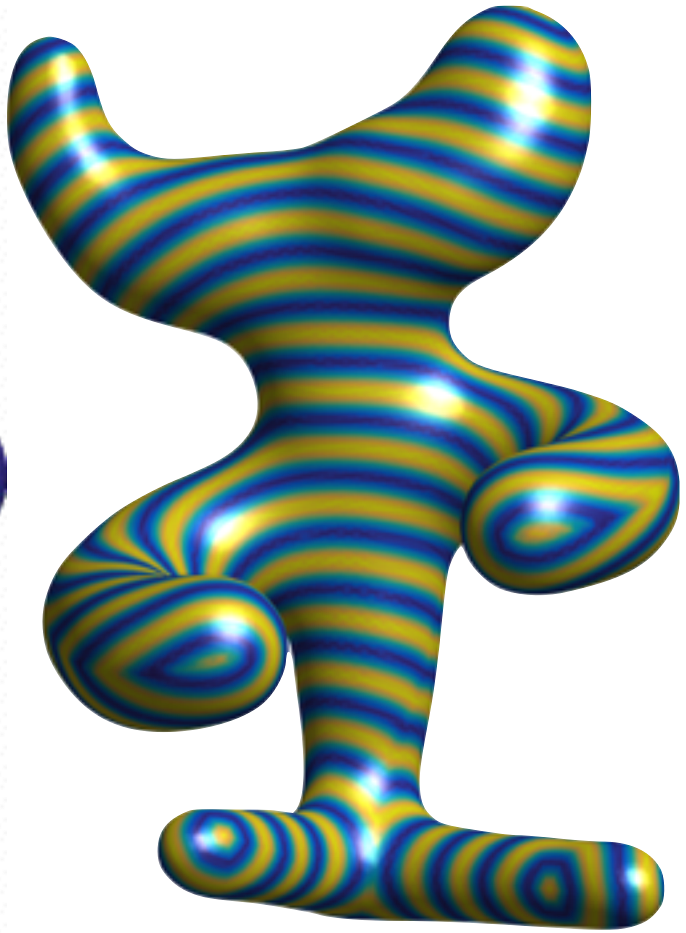

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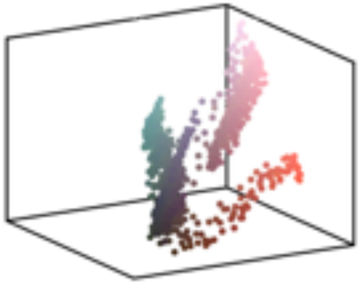
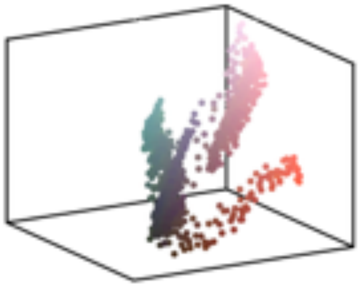
Conclusion

Histogram features in imaging and machine learning.

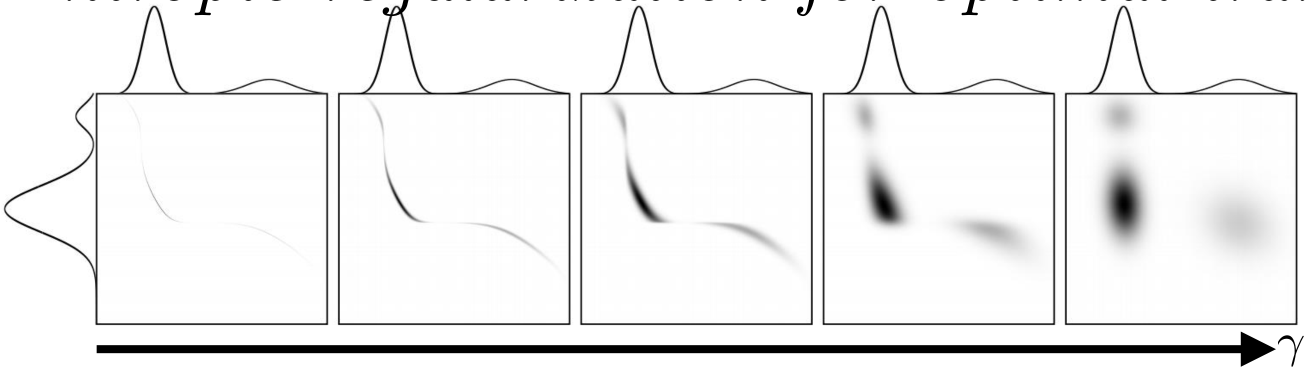


Conclusion



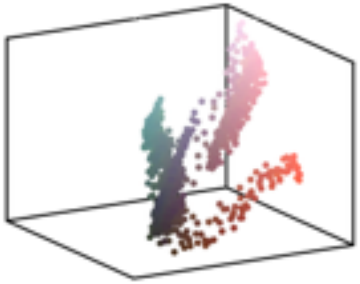
Histogram features in imaging and machine learning.

Entropic regularization for optimal transport.



Conclusion

Histogram features in imaging and machine learning.



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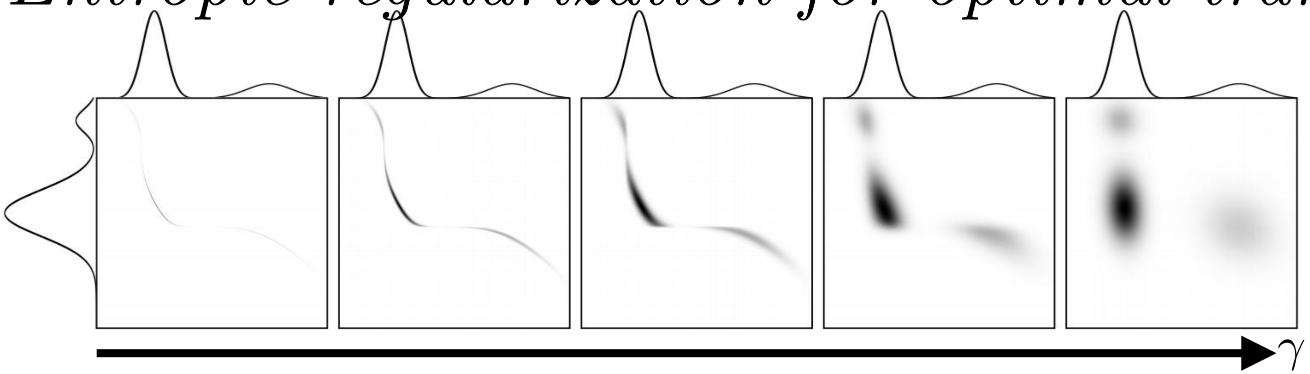

Barycenters, unbalanced OT, gradient flows, . . .