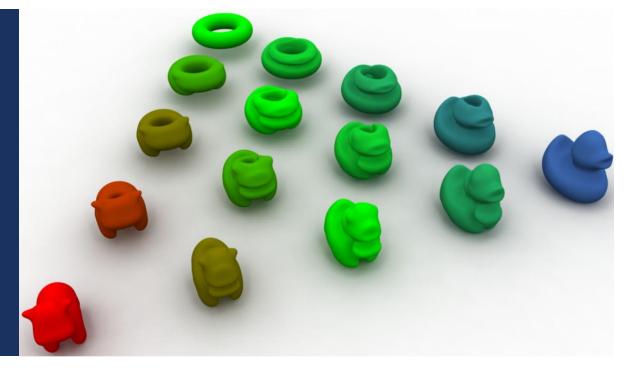
CONVOLUTIONAL WASSERSTEIN DISTANCES: EFFICIENT OPTIMAL TRANSPORTATION ON GEOMETRIC DOMAINS

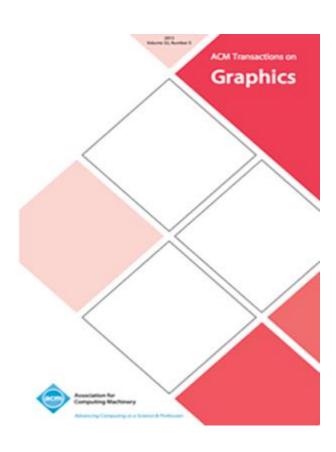
JUSTIN SOLOMON, FERNANDO DE GOES, GABRIEL PEYRE, MARCO CUTURI, ADRIAN BUTSCHER, ANDY NGUYEN, TAO DU, LEONIDAS GUIBAS

Presenter: Zhakshylyk Nurlanov Supervisor: Marvin Eisenberger



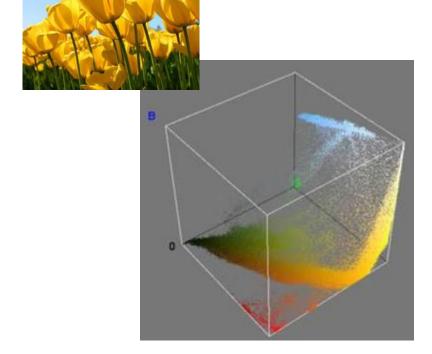
CONVOLUTIONAL WASSERSTEIN DISTANCES

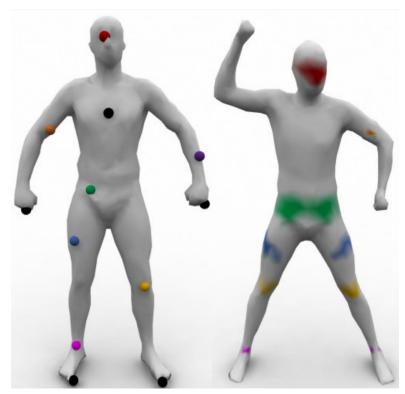
- SIGGRAPH 2015
- ACM Transactions on Graphics (TOG)
- Code available: https://github.com/gpeyre/2015-SIGGRAPH-convolutional-ot
- 239 Citations for May, 2020



- Distance between Probability Distributions
- Approach: Entropy Regularization, Heat Kernel
- Applications
- Conclusion

PROBABILITY DISTRIBUTIONS IN GRAPHICS





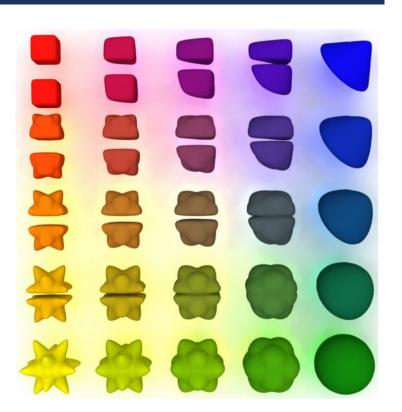


Image histograms

Correspondence maps

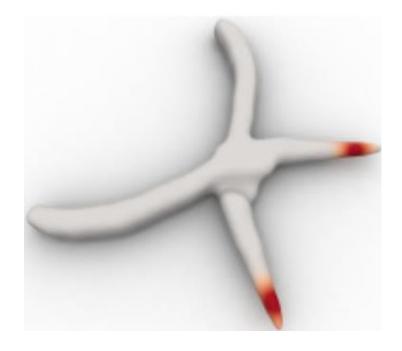
Shapes

PROBABILITY DISTRIBUTIONS IN GRAPHICS

$$p:M \to \mathbb{R}_+$$

$$\int\limits_{M} p(x)dx = 1$$

How is the feature distributed **over** geometric domain *M*?



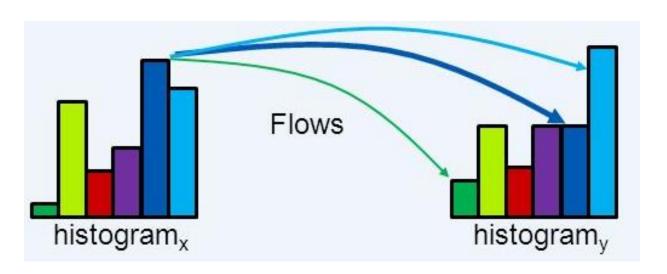
GOAL

To manipulate distributions over geometric domains



$$t = 0$$
 $t = 1/4$ $t = 1/2$ $t = 3/4$ $t = 1$

EARTH MOVER'S DISTANCE (EMD)



Perceptual Metrics for Image Database Navigation, Rubner, 2001

$$\min_{T \ge 0} \sum_{ij} T_{ij} d(x_i, x_j) \qquad \text{mass} \times \text{distance}$$

s. t.
$$\sum_{j} T_{ij} = p_i \sum_{i} T_{ij} = q_j$$

Starts at p Ends at q

- Transform the mass from source distribution to match the target distribution
- Minimum "mass_flow × distance" for transformation

WASSERSTEIN DISTANCE

$$W_2^2(\mu_0, \mu_1) := \inf_{T \in \Pi} \left[\iint_{M \times M} \frac{d(x, y)^2 T(x, y) dx dy}{\sup_{\text{geodesic} \atop \text{distance}} | \text{transportation} \atop \text{plan}} \right]$$

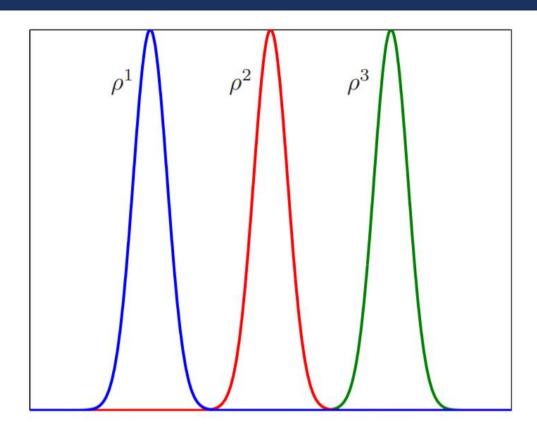
$$\Pi(\mu_0, \mu_1) := \{ T \in Prob(M \times M) : T(\cdot, M) = \mu_0, T(M, \cdot) = \mu_1 \}$$

Continuous analog of EMD



Why do we use Wasserstein distance?

WHICH DISTRIBUTION IS MORE SIMILAR?



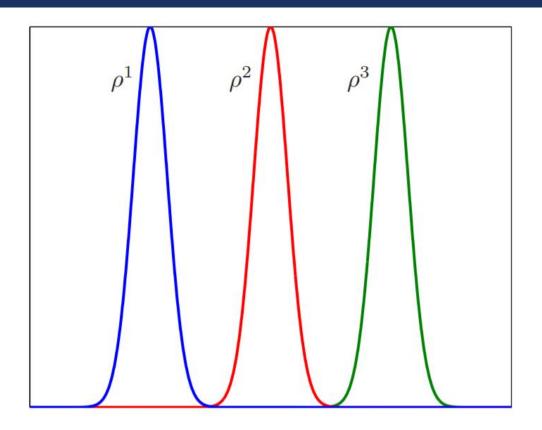
$$L_1(\rho_1, \rho_2) = E[||\rho_1 - \rho_2||_1] = 2$$

 $L_1(\rho_1, \rho_3) = E[||\rho_1 - \rho_3||_1] = 2$

Fig. 4. L^p distance vs. Wasserstein distance.

Sensitivity analysis of the LWR model for traffic forecast on large networks using Wasserstein distance, Briani et al., 2016

WHICH DISTRIBUTION IS MORE SIMILAR?



$$L_1(\rho_1, \rho_2) = \mathbb{E}\left[\left|\left|\rho_1 - \rho_2\right|\right|_1\right] = 2$$

$$L_1(\rho_1, \rho_3) = \mathbb{E}\left[\left|\left|\rho_1 - \rho_3\right|\right|_1\right] = 2$$
but

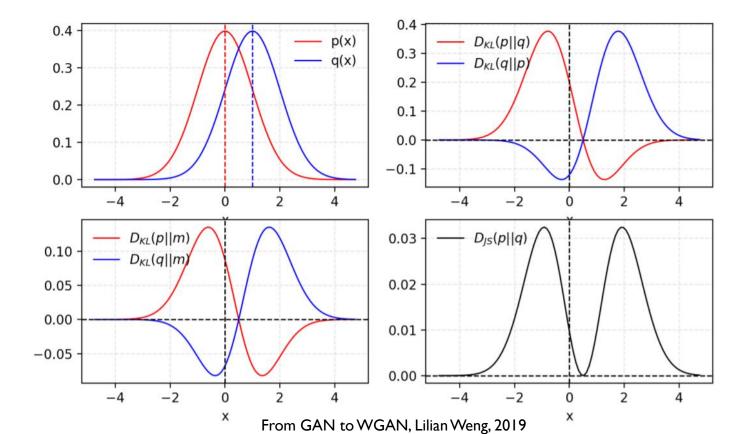
$$W_2(\rho_1, \rho_2) < W_2(\rho_1, \rho_3)$$

Fig. 4. L^p distance vs. Wasserstein distance.

Sensitivity analysis of the LWR model for traffic forecast on large networks using Wasserstein distance, Briani et al., 2016

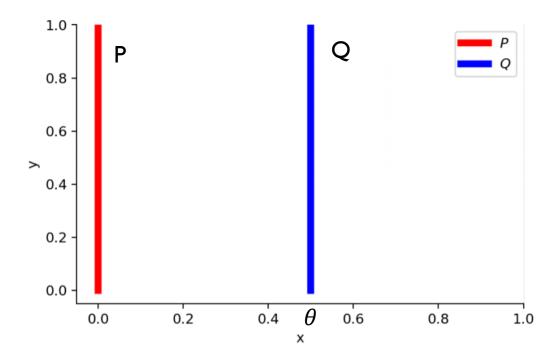
KULLBACK-LEIBLER (KL), JENSEN-SHANNON (JS) DIVERGENCE

$$D_{KL}(p||q) = \int_{x} p(x) \log \frac{p(x)}{q(x)} dx, \quad D_{JS}(p,q) = \frac{1}{2} D_{KL}(p||\frac{p+q}{2}) + \frac{1}{2} D_{KL}(q||\frac{p+q}{2})$$



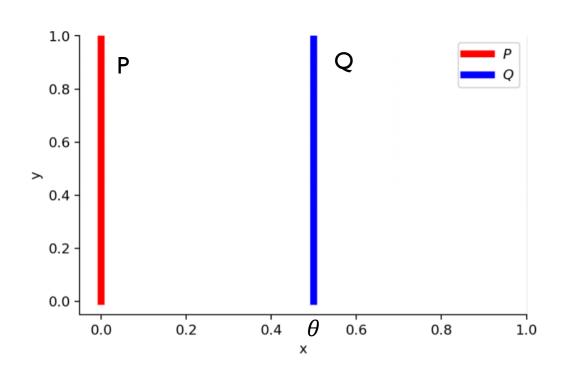
WHY W_2 IS BETTER THAN JS OR KL DIVERGENCE?

$$\forall (x,y) \in P, x = 0 \text{ and } y \sim U(0,1) \forall (x,y) \in Q, x = \theta, 0 \le \theta \le 1 \text{ and } y \sim U(0,1)$$



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When $\theta \neq 0$:

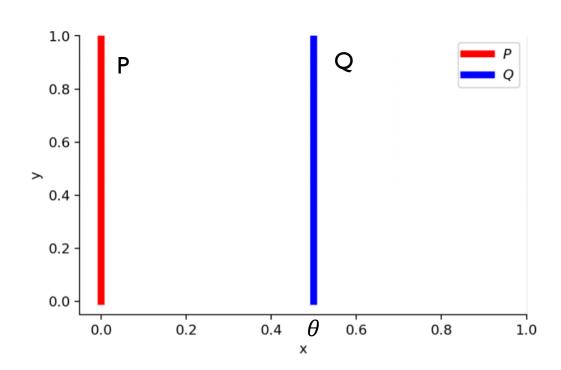
$$D_{KL}(P||Q) = +\infty$$
, $D_{KL}(Q||P) = +\infty$

$$D_{JS}(P,Q) = log2$$

$$W_2(P,Q) = |\theta|$$

WHY W_2 IS BETTER THAN JS OR KL DIVERGENCE?

$$\forall (x,y) \in P, x = 0 \text{ and } y \sim U(0,1) \forall (x,y) \in Q, x = \theta, 0 \le \theta \le 1 \text{ and } y \sim U(0,1)$$



When $\theta \neq 0$:

$$D_{KL}(P||Q) = +\infty$$
, $D_{KL}(Q||P) = +\infty$

$$D_{IS}(P,Q) = log2$$

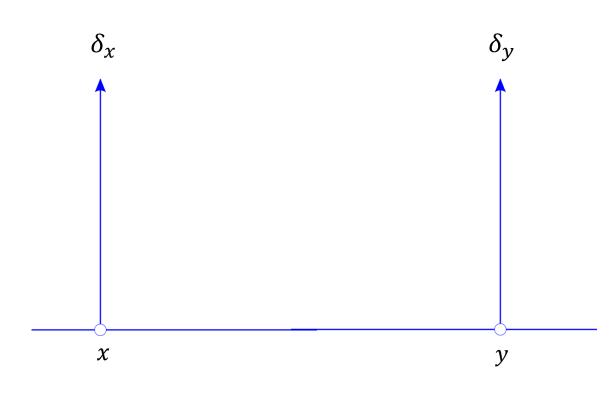
$$W_2(P,Q) = |\theta|$$

But when $\theta = 0$:

$$D_{KL}(P||Q) = D_{KL}(Q||P) = D_{IS}(P,Q) = 0$$

$$W_2(P,Q) = |\theta| = 0$$

AVERAGING DISTRIBUTIONS

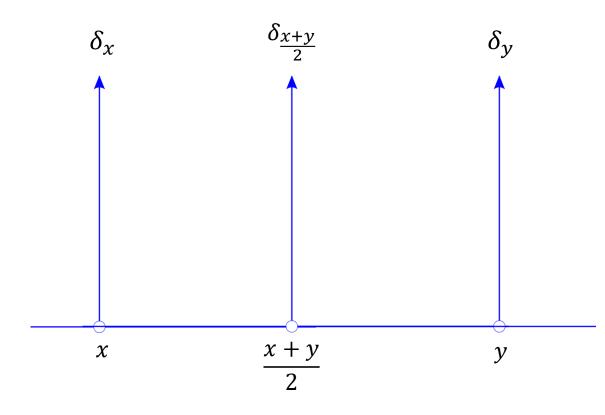


What is between two given distributions?

$$\delta_x$$
 ? δ_y

$$\frac{\delta_x + \delta_y}{2}$$
 is bimodal centered at x and y

AVERAGING DISTRIBUTIONS



What is between two given distributions?

$$\delta_x$$
 ? δ_y

$$\frac{\delta_x + \delta_y}{2}$$
 is bimodal centered at x and y

but

$$f^* = \underset{f}{\operatorname{argmin}}(W_2^2(f, \delta_x) + W_2^2(f, \delta_y))$$

$$f^* = \delta_{\frac{x+y}{2}}$$
 is a Dirac at midpoint

GOAL

 To manipulate distributions over geometric domains using <u>Wasserstein Distance</u>



$$t = 0$$
 $t = \frac{1}{4}$ $t = \frac{1}{2}$ $t = \frac{3}{4}$ $t = 1$

INTERPOLATION

$$\mu_t = \arg\min_{\mu} \left[(1 - t) W_2^2(\mu, \mu_0) + t W_2^2(\mu, \mu_1) \right]$$

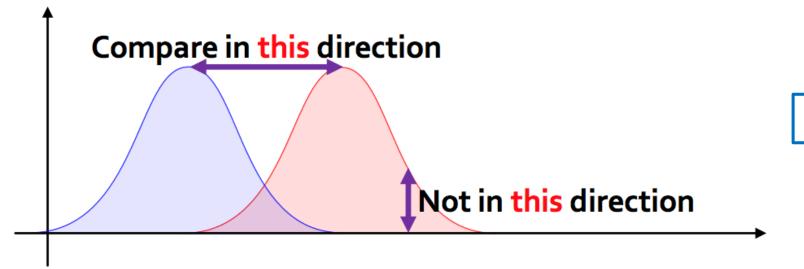


$$t = 0$$
 $t = \frac{1}{4}$ $t = \frac{1}{2}$ $t = \frac{3}{4}$ $t = 1$

How to compute Wasserstein distance?

WASSERSTEIN DISTANCE

$$W_2^2(\mu_0, \mu_1) := \inf_{T \in \Pi} \left[\iint_{M \times M} d(x, y)^2 T(x, y) dx dy \right]$$



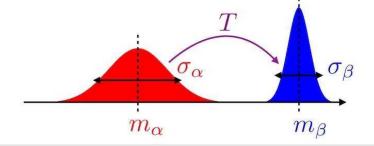
Looks terribly complex!

WASSERSTEIN DISTANCE BETWEEN 2 GAUSSIANS

$$W_2^2(N(m_1, \Sigma_1); N(m_2, \Sigma_2)) = ||m_1 - m_2||_2^2 + Tr(\Sigma_1 + \Sigma_2 - 2(\Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2})^{1/2})$$

One Dimensional case:

$$\frac{\mathrm{d}\alpha}{\mathrm{d}x} = \frac{1}{\sigma_{\alpha}\sqrt{2\pi}}e^{-\frac{(x-m_{\alpha})^2}{2\sigma_{\alpha}^2}}$$

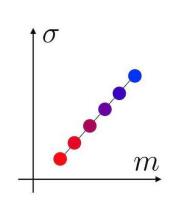


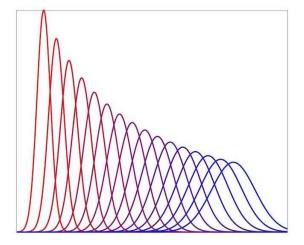
Optimal transport:

$$T(x) = \frac{\sigma_{\beta}}{\sigma_{\alpha}}(x - m_{\alpha}) + m_{\beta}$$

Wasserstein distance: $W_2^2(\alpha, \beta) = (m_{\alpha} - m_{\beta})^2 + (\sigma_{\alpha} - \sigma_{\beta})^2$

Interpolation





Wasserstein geometry of Gaussian measures, Asuka Takatsu, 2010

COMPUTATIONAL ISSUES

$$W_2^2(\mu_0, \mu_1) := \inf_{T \in \Pi} \left[\iint_{M \times M} d(x, y)^2 T(x, y) dx dy \right]$$

- Quadratic number of unknowns
- Needs d(x, y) for all (x, y) to compute

In discrete case:
$$p(x) \sim \vec{p} \in \mathbb{R}^n$$

$$q(x) \sim \vec{q} \in \mathbb{R}^n$$

$$T(x,y) \sim T \in \mathbb{R}^{n \times n}$$

General linear programming is impractical

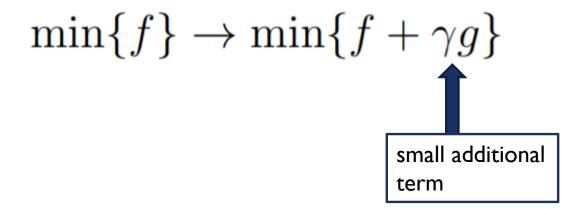
Approach:

- First Approximation: Entropy Regularization
- Second Approximation: Heat Kernel for geodesic distances
- Alternating Projections algorithm: Sinkhorn iterations

FIRST APPROXIMATION: REGULARIZATION

$$\min\{f\} \to \min\{f + \gamma g\}$$

FIRST APPROXIMATION: REGULARIZATION



FIRST APPROXIMATION: REGULARIZATION

$$\min\{f\} \to \min\{f + \gamma g\}$$

$$\max\{f\} = \min\{g\}$$
 small additional term

$$f_{\gamma}^* \xrightarrow{\gamma \to 0} f^*$$

ENTROPY

$$H(T) := -\iint_{M \times M} T(x, y) ln T(x, y) dx dy$$



Small H



Large H

Measure of unsertainty

FIRST APPROXIMATION: ENTROPIC REGULARIZATION

$$W_{2,\gamma}^{2}(\mu_{0},\mu_{1}) := \inf_{T \in \Pi} \left[\iint_{M \times M} d(x,y)^{2} T(x,y) dx dy - \gamma H(T) \right]$$

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Remember KL Divergence?
$$D_{KL}(p||q) = \int_{x} p(x) \log \frac{p(x)}{q(x)} dx,$$

KERNEL REPRESENTATION OF DISTANCE

$$\mathcal{K}_{\gamma}(x,y) = e^{-\frac{d(x,y)^2}{\gamma}}, \quad d(x,y)^2 = -\gamma ln \mathcal{K}_{\gamma}(x,y)$$

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$$\mathcal{K}_{\gamma}(x,y) \geq 0 \quad \forall x,y \in M \times M$$

$$W_{2,\gamma}^{2}(\mu_{0},\mu_{1}) := \gamma \inf_{T \in \Pi} \left[\iint_{M \times M} T(x,y) ln \frac{T(x,y)}{\mathcal{K}_{\gamma}(x,y)} dx dy \right]$$

REGULARIZED PROBLEM: INTERPRETATION, CONVEXITY

$$W_{2,\gamma}^2(\mu_0,\mu_1) := \gamma \inf_{T \in \Pi} KL \left(T || \mathcal{K}_{\gamma} \right) + \gamma \cdot const$$

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The optimal transportation plan T is the projection of the distance-based kernel \mathcal{K}_{γ} onto Π (w.r.t. KL div)

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KL(p,q) is strictly convex in p for fixed q

REGULARIZED PROBLEM

$$W_2^2(\mu_0, \mu_1) := \inf_{T \in \Pi} \left[\iint_{M \times M} d(x, y)^2 T(x, y) dx dy \right]$$



Entropy Regularization

$$W_{2,\gamma}^2(\mu_0,\mu_1) := \gamma \inf_{T \in \Pi} KL \left(T || \mathcal{K}_{\gamma} \right)$$

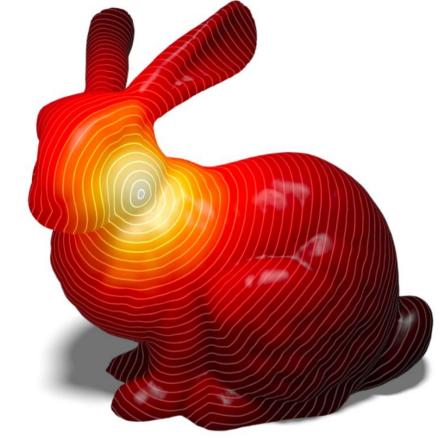
$$d(x,y)^2 = -\gamma ln \mathcal{K}_{\gamma}(x,y)$$

PAIRWISE GEODESIC DISTANCE

$$\mathcal{K}_{\gamma}(x,y) = e^{-\frac{d(x,y)^2}{\gamma}}$$

Problem:

All geodesic distances are to be computed



Geodesics in Heat, Keenan Crane, 2013

INTRODUCING HEAT KERNEL

$$\begin{cases} \frac{\partial f(t,x)}{\partial t} = \Delta f(t,x) \\ f(0,x) = f_0(x) \end{cases} \longrightarrow f(t,x) = \int_M f_0(y) \mathcal{H}_t(x,y) dy$$
Heat equation Heat kernel

$$\mathcal{H}_t(x,y)$$
 determines diffusion between $x,y \in M$ after time t

$$d(x,y)^{2} = \lim_{t \to 0} \left[-2t \cdot \ln \mathcal{H}_{t}(x,y) \right]$$

[Geodesics in Heat, Crane et al. 2013]

the distance d(x, y) can be recovered by transferring the heat from x to y through manifold M over a short time interval t

$$d(x,y)^{2} = \lim_{t \to 0} \left[-2t \cdot \ln \mathcal{H}_{t}(x,y) \right]$$

BROWNIAN MOTION

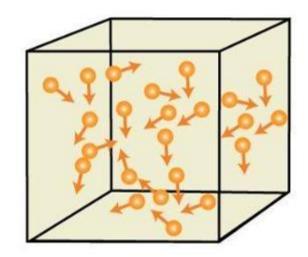








FIGURE 2. Simulations of a the kinetic Brownian motion on the torus over different time intervals.

$$d(x,y)^2 = \lim_{t \to 0} \left[-2t \cdot \ln \mathcal{H}_t(x,y) \right]$$

Reminder: Kernel Representation of Distance

$$\mathcal{K}_{\gamma}(x,y) = e^{-\frac{d(x,y)^2}{\gamma}}, \quad d(x,y)^2 = -\gamma ln \mathcal{K}_{\gamma}(x,y)$$

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SECOND APPROXIMATION: HEAT KERNEL

$$t := \frac{\gamma}{2} \longrightarrow \mathcal{K}_{\gamma}(x, y) \approx \mathcal{H}_{\frac{\gamma}{2}}(x, y)$$

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$$W_2^2 \approx W_{2,\gamma}^2 \approx W_{2,\mathcal{H}_{\frac{\gamma}{2}}}^2$$

DISCRETE SETTING

$$\begin{cases} \frac{\partial f(t,x)}{\partial t} = \Delta f(t,x) \\ f(0,x) = g(x) \end{cases} \longrightarrow f(t,x) = \int_{M} g(y) \mathcal{H}_{t}(x,y) dy$$

Discretization

$$\begin{cases} \vec{f}_{t+1} - \vec{f}_t = L\vec{f}_t \\ \vec{f}_0 = \vec{g} \end{cases} \longrightarrow \vec{f}_t = \mathcal{H}_t(\vec{a} \circ \vec{g})$$

DISCRETE SETTING

$$\begin{cases} \vec{f}_{t+1} - \vec{f}_t = L\vec{f}_t & \longrightarrow \vec{f}_t = \mathcal{H}_t(\vec{a} \circ \vec{g}) \\ \vec{f}_0 = \vec{g} & \end{cases}$$

$$f(t, x) = \int_{M}^{n} g(y) \mathcal{H}_t(x, y) dy$$

$$\mathcal{H}_t \in \mathbb{R}^{n \times n}$$

"area weights" vector

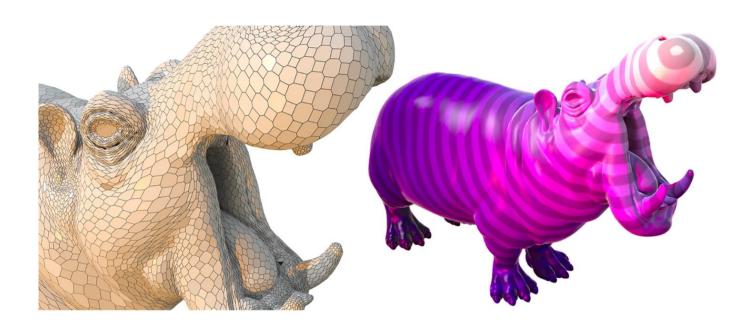
$$\vec{a} \in \mathbb{R}^n_+, \quad \vec{a}^T \vec{1} = 1$$

$$\int_{M} f(x)dx \approx \vec{a}^T \vec{f}$$

COMPUTING HEAT KERNEL: FOR IMAGES, AND MESHES



Gaussian kernel for images



Distance on poly meshes based on heat method

Geodesics in Heat, Crane et al. 2013

CONVOLUTIONAL WASSERSTEIN DISTANCE

$$W_2^2(\mu_0, \mu_1) := \inf_{T \in \Pi} \left[\iint_{M \times M} d(x, y)^2 T(x, y) dx dy \right]$$



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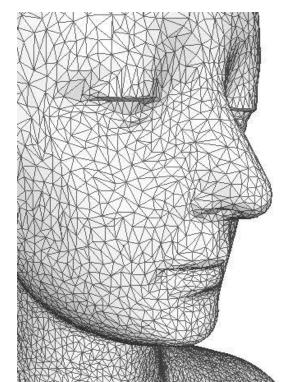
Heat Kernel

$$W_{2,\mathcal{H}_{\frac{\gamma}{2}}}^{2}(\mu_{0},\mu_{1}) := \gamma \inf_{T \in \Pi} KL(T||\mathcal{H}_{\frac{\gamma}{2}})$$

PROBLEM

$$W_{2,\mathcal{H}_{\frac{\gamma}{2}}}^{2}(\mu_{0},\mu_{1}) := \gamma \inf_{T \in \Pi} KL(T||\mathcal{H}_{\frac{\gamma}{2}})$$

Still quadratic number of unknowns



PROPOSITION I: LINEAR NUMBER OF VARIABLES

$$W_{2,\mathcal{H}_{\frac{\gamma}{2}}}^{2}(\mu_{0},\mu_{1}) := \gamma \inf_{T \in \Pi} KL(T||\mathcal{H}_{\frac{\gamma}{2}})$$
(*)

Proposition I:

The transportation plan $T \in \Pi(\mu_0, \mu_1)$ minimizing (*) is of the form:

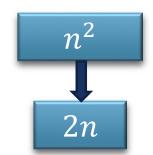
$$T = diag(\vec{v}) \mathcal{H}_t diag(\vec{w}) = D_{\vec{v}} \mathcal{H}_t D_{\vec{w}}$$
 with unique vectors $\vec{v}, \vec{w} \in \mathbb{R}^n$, satisfying:

$$\begin{cases} T\vec{a} = \mu_0 \\ T^T\vec{a} = \mu_1 \end{cases} \longleftrightarrow \begin{cases} D_{\vec{v}}\mathcal{H}_t D_{\vec{w}}\vec{a} = \mu_0 \\ D_{\vec{w}}\mathcal{H}_t D_{\vec{v}}\vec{a} = \mu_1 \end{cases}$$

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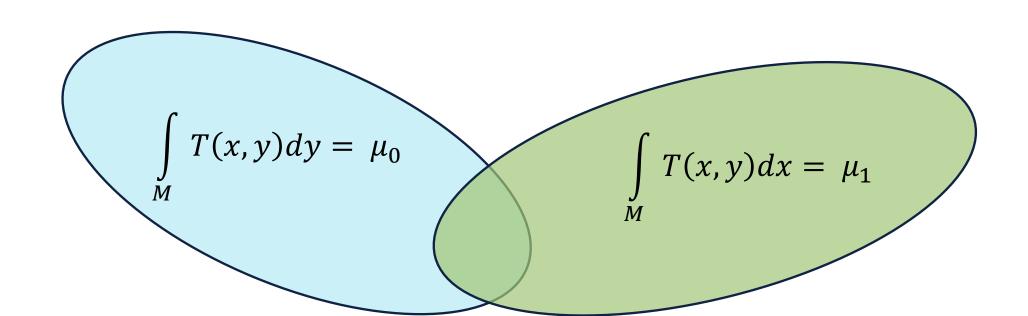


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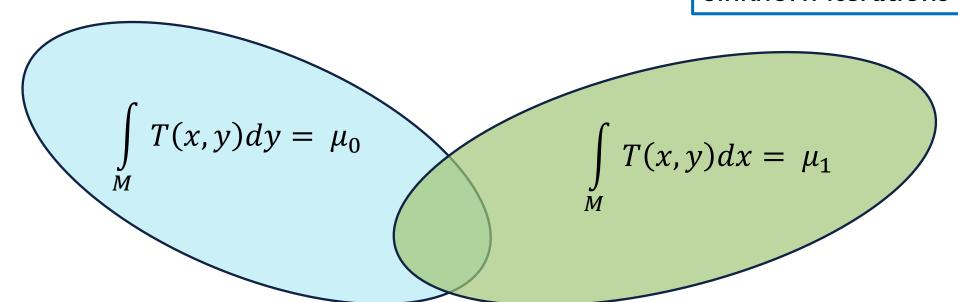
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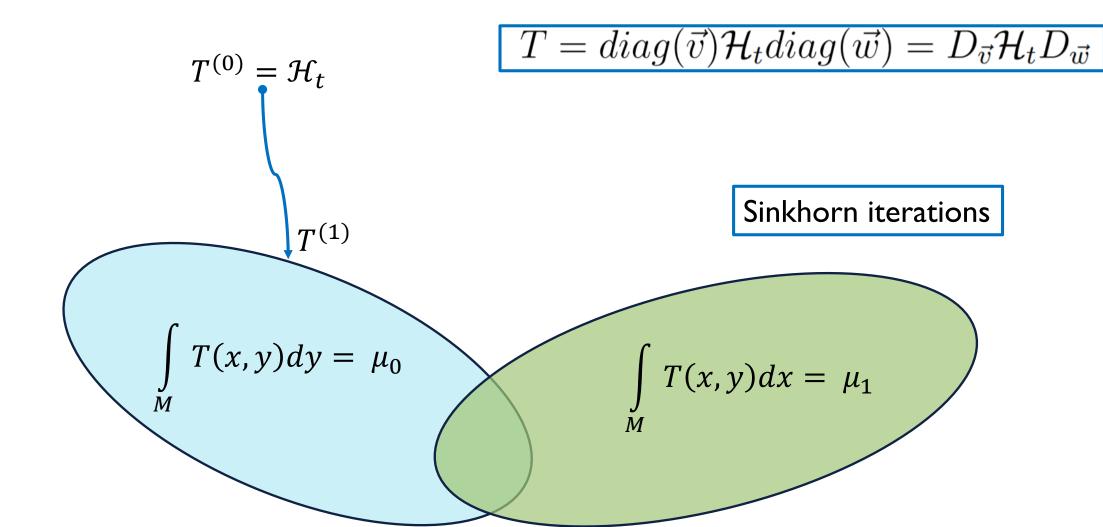


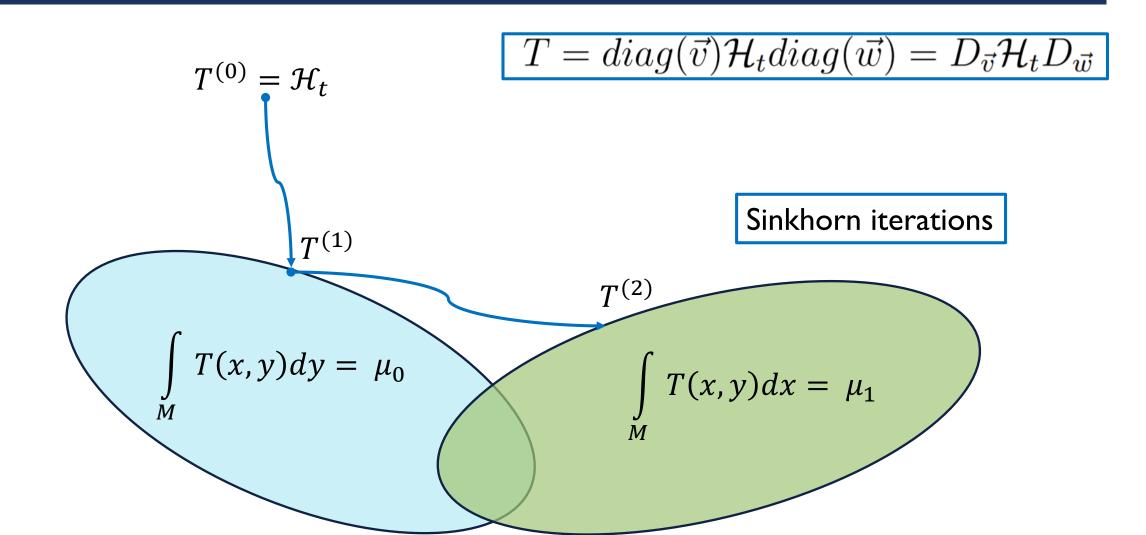
$$T^{(0)} = \mathcal{H}_t$$

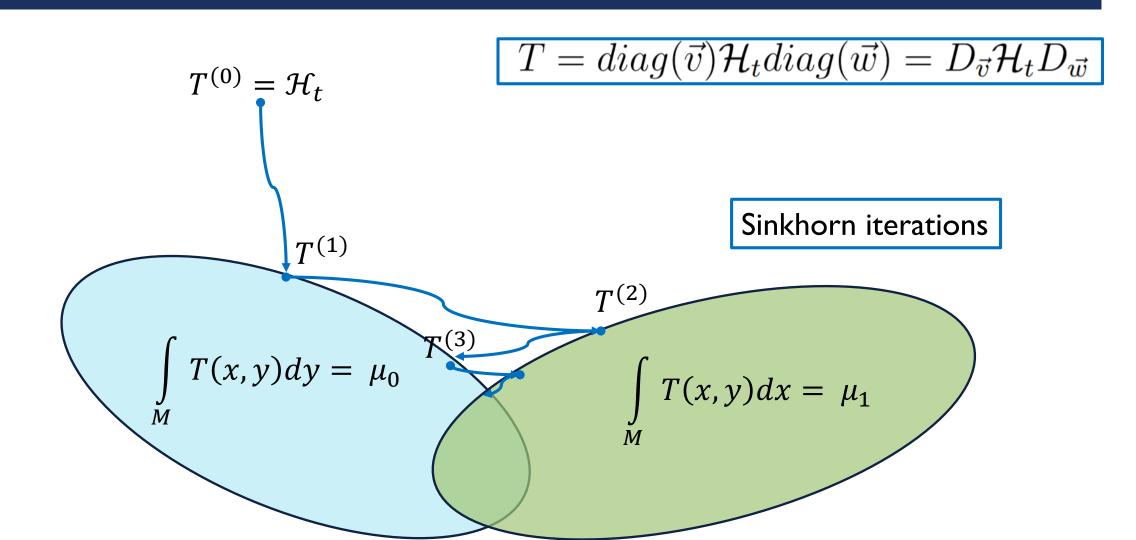
$$T = diag(\vec{v})\mathcal{H}_t diag(\vec{w}) = D_{\vec{v}}\mathcal{H}_t D_{\vec{w}}$$

Sinkhorn iterations









ALTERNATING PROJECTIONS ALGORITHM: SINKHORN ITERATIONS

```
function Convolutional-Wasserstein(\mu_0, \mu_1; \mathbf{H}_t, \mathbf{a})
        // Sinkhorn iterations
         \mathbf{v}, \mathbf{w} \leftarrow \mathbf{1}
        for i = 1, 2, 3, \dots
                 \mathbf{v} \leftarrow \boldsymbol{\mu}_0 \oslash \mathbf{H}_t (\mathbf{a} \otimes \mathbf{w})
                 \mathbf{w} \leftarrow \boldsymbol{\mu}_1 \oslash \mathbf{H}_t(\mathbf{a} \otimes \mathbf{v})
        // KL divergence
        return \gamma \mathbf{a}^{\top} [(\boldsymbol{\mu}_0 \otimes \ln \mathbf{v}) + (\boldsymbol{\mu}_1 \otimes \ln \mathbf{w})]
```

Algorithm 1: Sinkhorn iteration for convolutional Wasserstein distances. \otimes , \otimes denote elementwise multiplication and division, resp.

ALTERNATING PROJECTIONS ALGORITHM: SINKHORN ITERATIONS

```
function Convolutional-Wasserstein(\mu_0, \mu_1; \mathbf{H}_t, \mathbf{a})
        // Sinkhorn iterations
        \mathbf{v}, \mathbf{w} \leftarrow \mathbf{1}
                                                                                   Solve linear
        for i = 1, 2, 3, \dots
                                                                                   equation
                 \mathbf{v} \leftarrow \boldsymbol{\mu}_0 \oslash \mathbf{H}_t (\mathbf{a} \otimes \mathbf{w})
                \mathbf{w} \leftarrow \boldsymbol{\mu}_1 \oslash \mathbf{H}_t (\mathbf{a} \otimes \mathbf{v})
        // KL divergence
        return \gamma \mathbf{a}^{\top} [(\boldsymbol{\mu}_0 \otimes \ln \mathbf{v}) + (\boldsymbol{\mu}_1 \otimes \ln \mathbf{w})]
```

Algorithm 1: Sinkhorn iteration for convolutional Wasserstein distances. \otimes , \otimes denote elementwise multiplication and division, resp.

- Results:
 - Timing comparison
 - Applications

RESULTS

V	T	PD	LP	[Cuturi 2013]	PF	$oldsymbol{\mathcal{W}}_{2,\mathbf{H}_t}^2$
693	1382	0.10	9.703	0.625	0.00	1.564
1150	2296	0.28	36.524	1.284	0.00	0.571
1911	3818	0.79	*	2.725	0.02	1.010
3176	6348	2.15	*	5.435	0.03	1.553
5278	10552	6.47	*	10.490	0.06	2.477
8774	17544	18.55	*	23.326	0.10	4.516
14584	29164	53.41	*	*	0.17	8.152

Table 1: Timing (in sec.) for approximating W_2 between random distributions on triangle meshes, averaged over 10 trials. An asterisk * denotes time-out after one minute. Pairwise distance (PD) computation is needed for the linear program (LP) and [Cuturi 2013]; timing for this step is written separately. Cholesky pre-factorization (PF) is needed for convolutional distance and is similarly separated.

INTERPOLATION

$$\mu_t = \arg\min_{\mu} \left[(1 - t) W_2^2(\mu, \mu_0) + t W_2^2(\mu, \mu_1) \right]$$



$$t = 0$$
 $t = \frac{1}{4}$ $t = \frac{1}{2}$ $t = \frac{3}{4}$ $t = 1$

INTERPOLATION

$$\mu_t = \arg\min_{\mu} \left[(1 - t) W_2^2(\mu, \mu_0) + t W_2^2(\mu, \mu_1) \right]$$



BARYCENTER

$$\mu^* = arg \min_{\mu} \sum_{i=1}^{N} \alpha_i W_2^2(\mu, \mu_i)$$

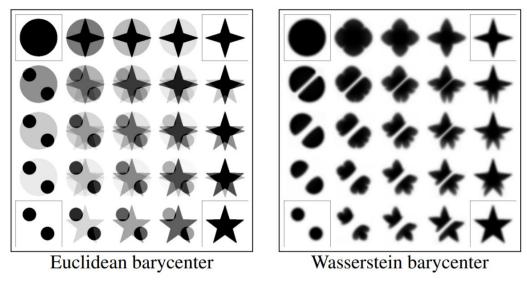
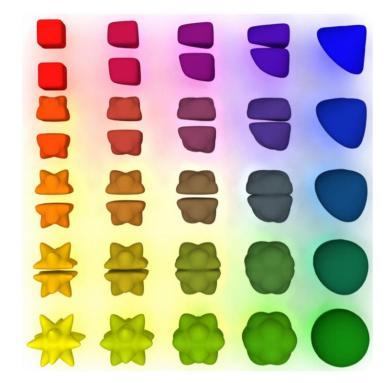
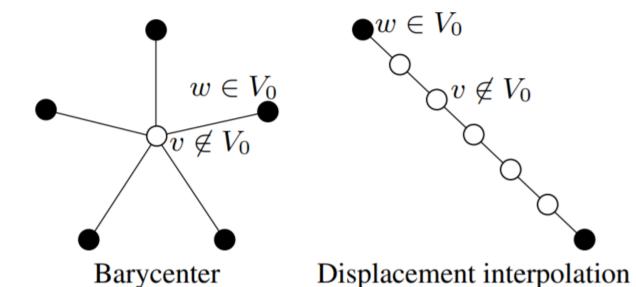


Figure 12: Interpolating indicators using linear combinations (left) is ineffective for shape interpolation, but convolutional Wasserstein barycenters (right) move features by matching mass of the underlying distributions.



PROPAGATION

$$\{\mu_v\} = \arg\min_{\mu_v, v \notin V_0} \sum_{(v,w) \in E} \alpha_{(v,w)} W_2^2(\mu_v, \mu_w)$$
$$s.t.\mu_v \quad fixed \quad \forall v \in V_0$$



PROPAGATION

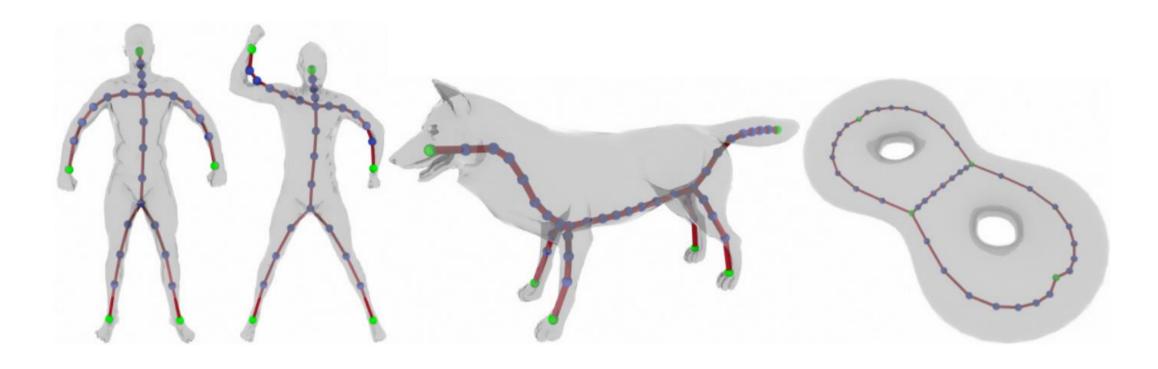
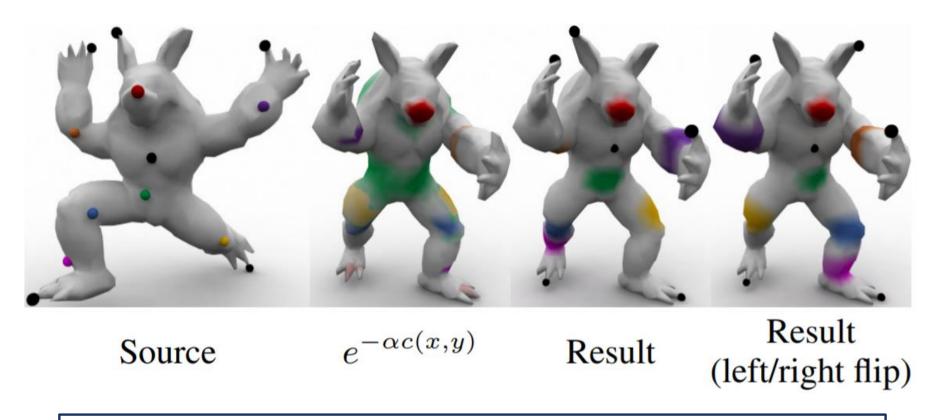


Figure 9: Embeddings of skeletons computed using Wasserstein propagation; the positions of the blue vertices are computed automatically using the fixed green vertices and topology of the graph.

PROPAGATION



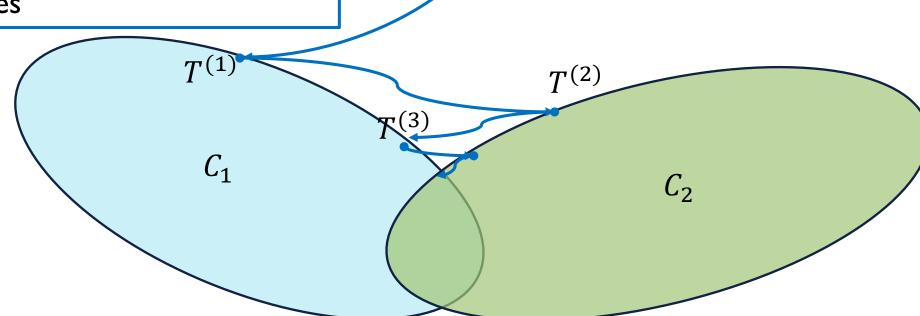
Soft maps: Colored points on the source are mapped to the colored distributions on the target, where black points are fixed input correspondences.

COMMONALITY OF ALGORITHMS

for i = 1,2,3,...

Projections onto C_1 and C_2

- Convolutions against Heat Kernel
- Element-wise operations
- Compute final values



 $T^{(0)}$

Conclusion:

- Main contribution of the work
- Drawbacks
- Questions

- First Approximation: Entropy Regularization
- Second Approximation: Heat Kernel
- Alternating Projections algorithm

- First Approximation: Entropy Regularization Convexity, Projection wrt KL
- Second Approximation: Heat Kernel
- Alternating Projections algorithm

- First Approximation: Entropy Regularization Convexity, Projection wrt KL
- Second Approximation: Heat Kernel Geodesic distances by linear equation
- Alternating Projections algorithm

- First Approximation: Entropy Regularization Convexity, Projection wrt KL
- Second Approximation: Heat Kernel Geodesic distances by linear equation
- Alternating Projections algorithm
 Linear number of unknowns, the result by Iterations of element-wise operations and linear equation solutions

DRAWBACKS

• Solution is unstable when $\gamma \to 0$

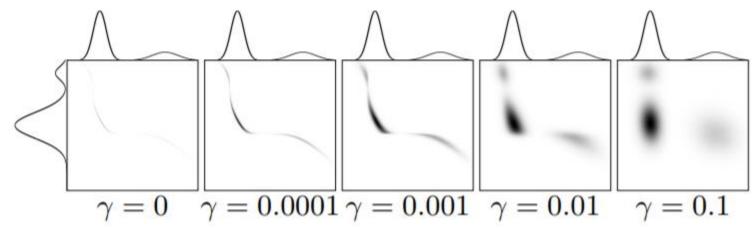


Figure 2: Transportation plans with different values of γ , with 1D quadratic costs; $\mu_0, \mu_1 \in \text{Prob}([0, 1])$ are shown on the axes.

CONVOLUTIONAL WASSERSTEIN DISTANCES: EFFICIENT OPTIMAL TRANSPORTATION ON GEOMETRIC DOMAINS

JUSTIN SOLOMON, FERNANDO DE GOES, GABRIEL PEYRE, MARCO CUTURI, ADRIAN BUTSCHER, ANDY NGUYEN, TAO DU, LEONIDAS GUIBAS

Questions?

Presenter: Zhakshylyk Nurlanov Supervisor: Marvin Eisenberger

