Robust shape matching with Optimal Transport

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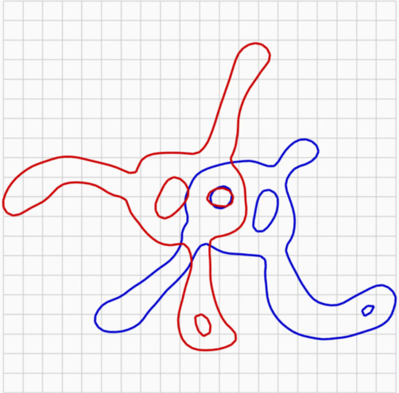
GTTI, ENS Cachan – 13th February, 2019

Écoles Normales Supérieures de Paris et Paris-Saclay
Collaboration with B. Charlier, J. Glaunès (KeOps library);
S.-i. Amari, G. Peyré, T. Séjourné, A. Trouvé, F.-X. Vialard (OT theory)

What is shape matching?

Source A, target B,



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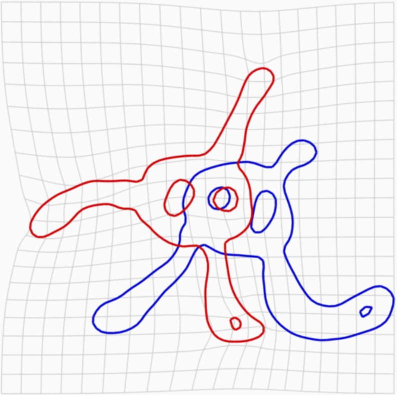
Source A, target B, mapping φ



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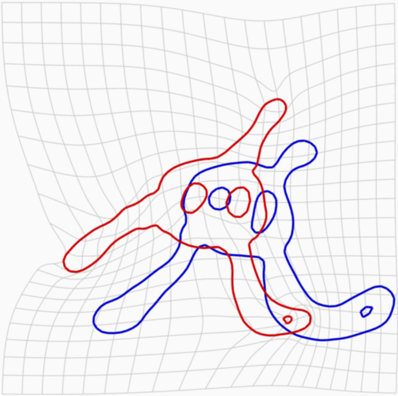

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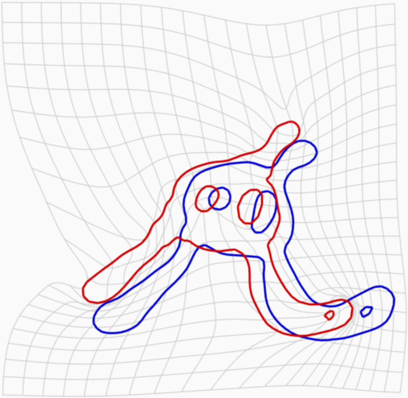
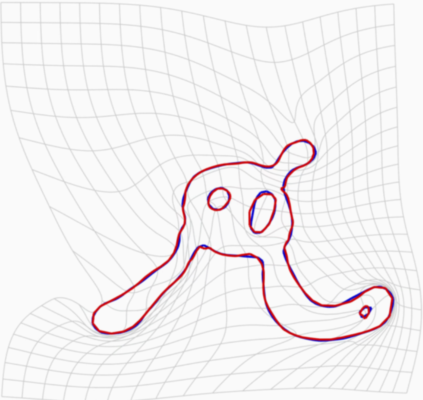


What is shape matching?

Source A, target B, mapping φ

$$A \xrightarrow[\text{Model}]{\varphi} \varphi(A) = A' \underset{\textbf{Loss}}{\rightleftarrows} B$$



A good Loss function is a guarantee of robustness

Iterative Matching Algorithm

1: $A' \leftarrow A$
2: **repeat**
3: $\quad L\,,\, v \leftarrow \text{Loss}(A', B)\,,\; -\partial_{A'}\text{Loss}(A', B)$
4: $\quad A' \leftarrow A' + \text{Model}(v)$
5: **until** $L < \text{tol}$

Output : deformed shape $A' = \varphi(A)$.

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"Model" encodes the **prior knowledge** on admissible deformations:

- *smoothing* convolution
- LDDMM/SVF *backprop* + regularization + *shooting*
- *trained* neural network

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"Model" encodes the **prior knowledge** on admissible deformations:

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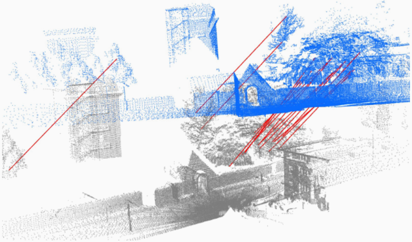
$\Rightarrow$ The *raw* Loss gradient v is what **drives** the registration

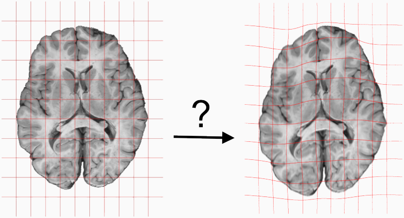
First setting: processing of point clouds



From the documentation of the Point Cloud Library.

- φ is **rigid** or affine
- Occlusions
- Outliers

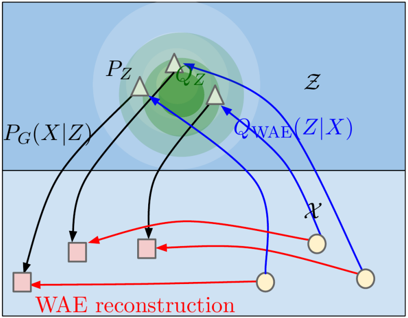
Second setting: medical imaging



From Marc Niethammer's Quicksilver slides.

- φ is a spline or a **diffeomorphism**
- Ill-posed problem
- Some occlusions

Third setting: training a generative model



Wasserstein Auto-Encoders,
Tolstikhin et al., 2018.

- φ is a **neural network**
- Very weak regularization
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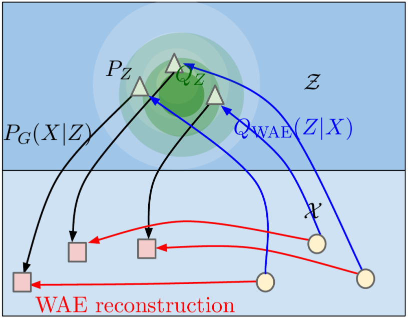

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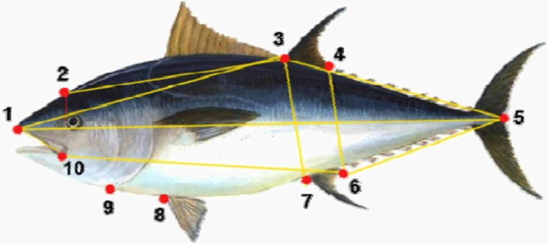
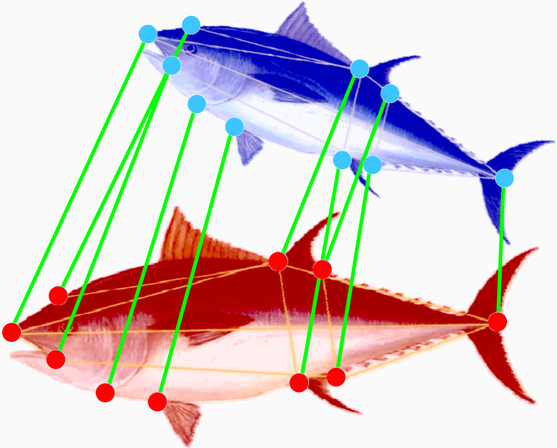
Which **Loss** function should we use?

On labeled shapes, use a spring energy



Anatomical landmarks from *A morphometric approach for the analysis of body shape in bluefin tuna*, Addis et al., 2009.

On labeled shapes, use a spring energy



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Encoding unlabeled shapes as measures

Let's enforce sampling invariance:

$$A \longrightarrow \alpha = \sum_{i=1}^{N} \alpha_i \delta_{x_i}, \qquad B \longrightarrow \beta = \sum_{j=1}^{M} \beta_j \delta_{y_j}.$$

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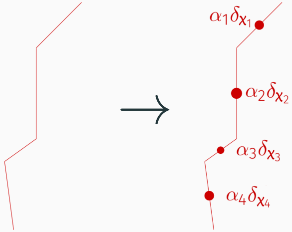

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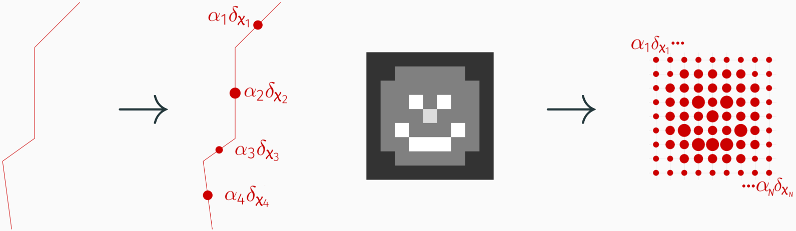
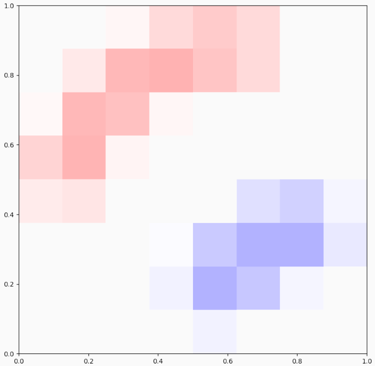


A baseline setting: density registration



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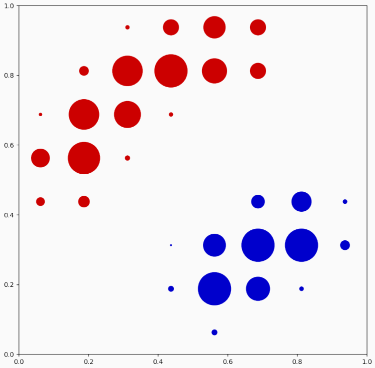

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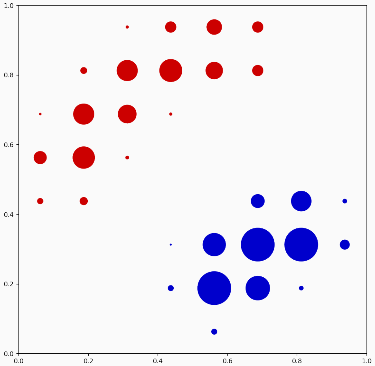

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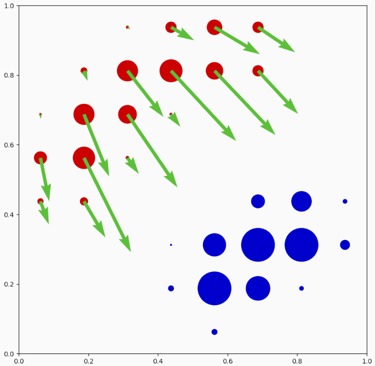

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Display $v \;=\; -\nabla_{x_i} \text{Loss}(\alpha, \beta)$.

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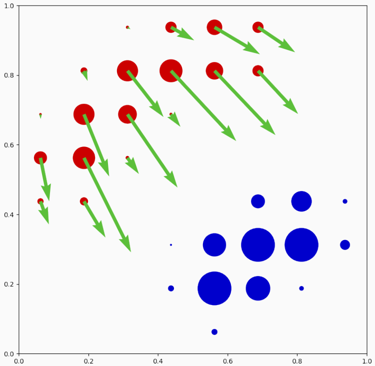

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Seamless extensions to:

- $\sum_i \alpha_i \neq \sum_j \beta_j$, outliers [Chizat et al., 2018],
- curves and surfaces [Kaltenmark et al., 2017],
- variable weights α_i.

Overview

Computing fidelities between **measures**:

1. **Computer graphics:** weighted Hausdorff distance
2. **Statistics:** kernel distances
3. **Optimal Transport**: Wasserstein distance
   $\simeq$ Robust Point Matching

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Computing fidelities between **measures**:

1. **Computer graphics:** weighted Hausdorff distance
2. **Statistics:** kernel distances
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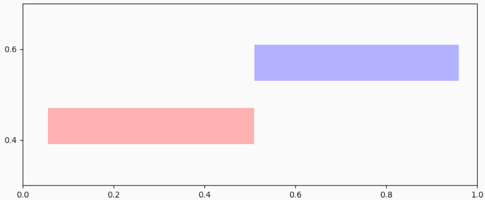
   $\simeq$ Robust Point Matching
4. What's **new**, in 2019?

The weighted Hausdorff distance: Iterative Closest Point algorithm

The weighted Hausdorff distance



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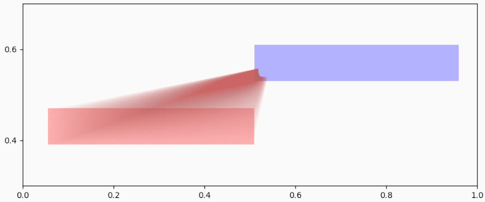

p-Hausdorff distance:

$$\text{Loss}(\alpha, \beta) \;=\; \tfrac{1}{2} \sum_i \alpha_i \cdot \min_j \|x_i - y_j\|^p$$

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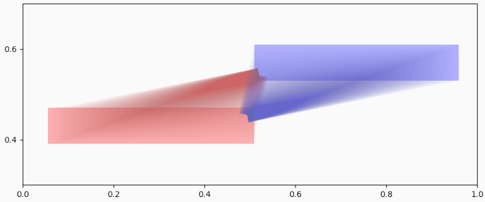

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$$\text{Loss}(\alpha, \beta) \;=\; \tfrac{1}{2}\sum_i \alpha_i \cdot \min_j \|x_i - y_j\|^p \quad + \quad \tfrac{1}{2}\sum_j \beta_j \cdot \min_i \|x_i - y_j\|^p$$

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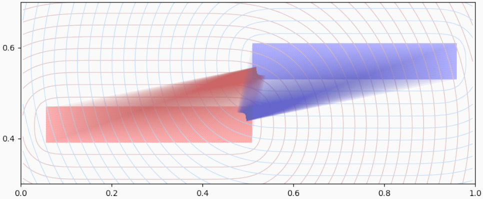

p-Hausdorff distance:

$$\begin{aligned}\text{Loss}(\alpha,\beta) &= \tfrac{1}{2}\textstyle\sum_i \alpha_i \cdot \min_j \|x_i - y_j\|^p &+& \tfrac{1}{2}\textstyle\sum_j \beta_j \cdot \min_i \|x_i - y_j\|^p \\ &= \tfrac{1}{2}\langle\, \alpha\,,\, b\,\rangle &+& \tfrac{1}{2}\langle\, \beta\,,\, a\,\rangle\end{aligned}$$

with
$$\begin{aligned} a(x) &= \mathrm{d}(\,x\,,\,\mathrm{supp}(\alpha))^p \\ b(x) &= \mathrm{d}(\,x\,,\,\mathrm{supp}(\beta))^p \end{aligned}$$

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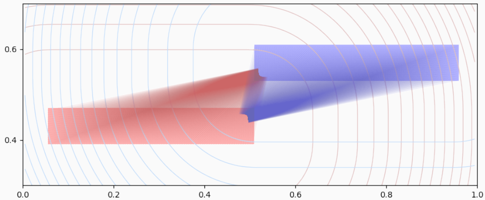

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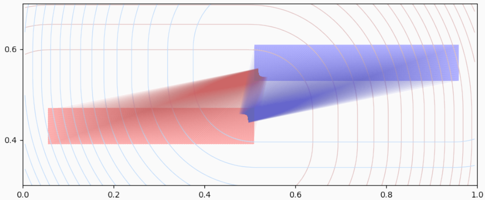

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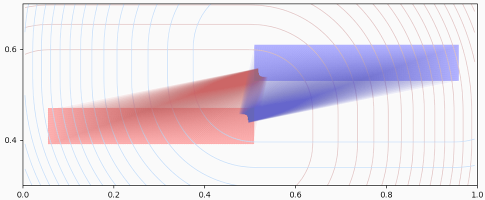

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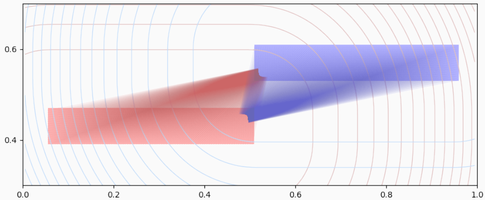

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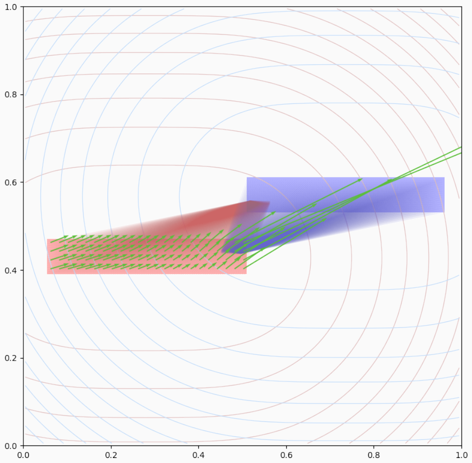
$$
\text{with}\quad \left.\begin{aligned}
a(x) &= \text{d}(\,x\,,\, \text{supp}(\alpha))^p &\simeq&\; -\log(k \star \alpha) \\
b(x) &= \text{d}(\,x\,,\, \text{supp}(\beta))^p &\simeq&\; -\log(k \star \beta)
\end{aligned}\right\}\ \text{GMM log-likelihoods}
$$

Naive projections in Hausdorff cause imbalance

$$\text{Loss}(\alpha, \beta) \quad = \quad \tfrac{1}{2}\langle\, \alpha,\ b - a\,\rangle \ + \ \tfrac{1}{2}\langle\, \beta,\ a - b\,\rangle$$



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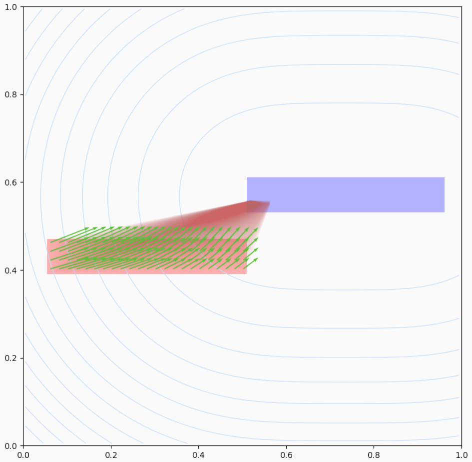

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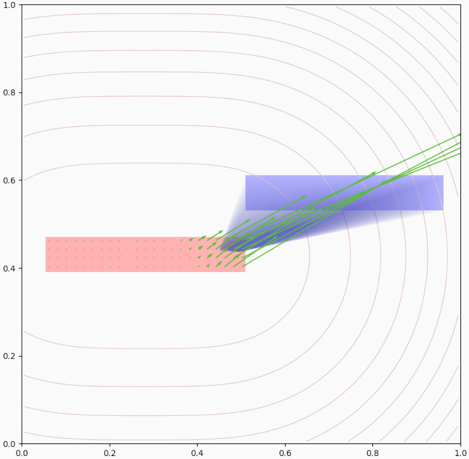

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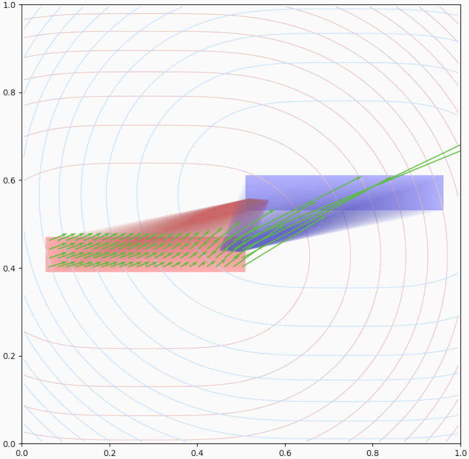
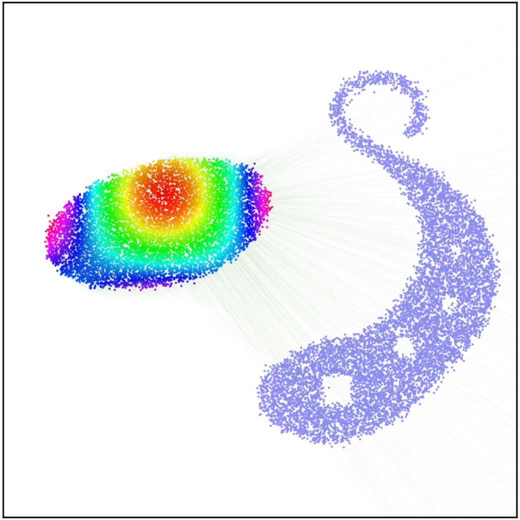


Gradient flow as a toy registration problem



$t = .00$

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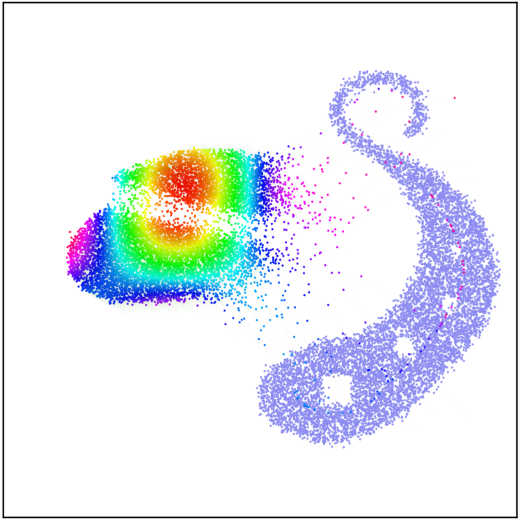
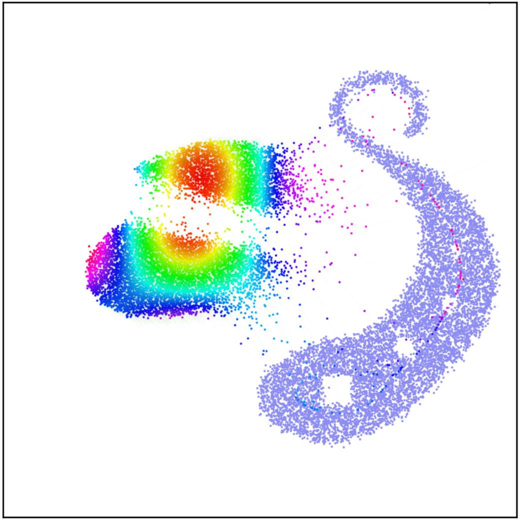


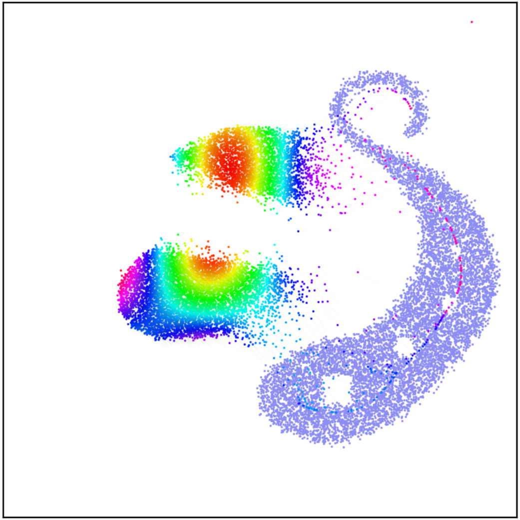
$t = .25$

Gradient flow as a toy registration problem



$t = .50$

Gradient flow as a toy registration problem



$t = 1.00$

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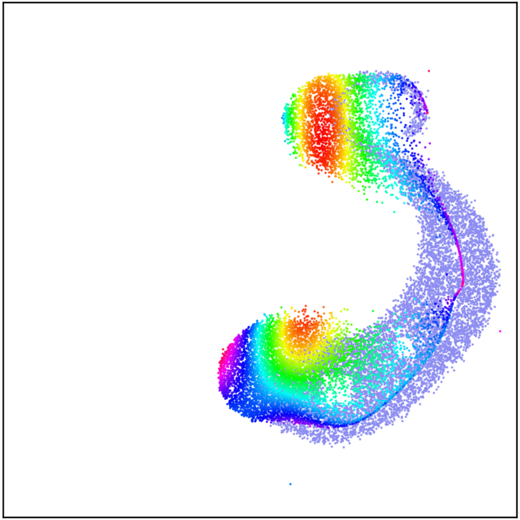

$t = 5.00$

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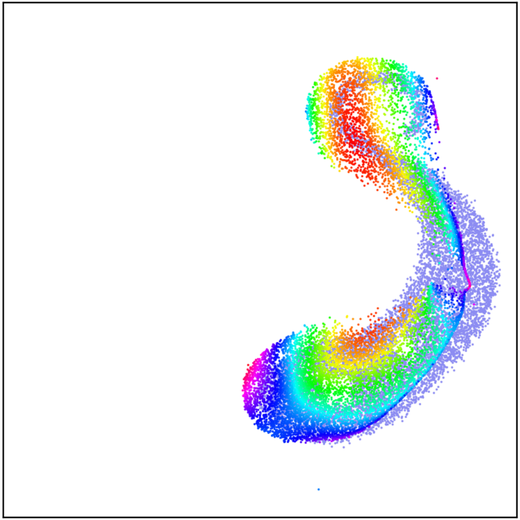
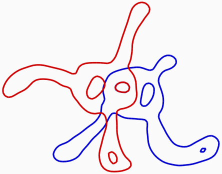


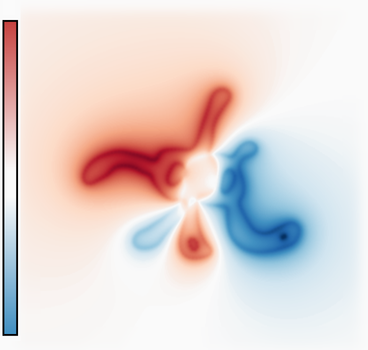
$t = 10.00$

An idea from statistics:
Kernel distances



Raw signal ($\alpha - \beta$).

Kernel fidelities: the simplest formula for $d(\alpha, \beta)$



Blurred signal $g \star (\alpha - \beta)$.

Choose a symmetric blurring function g, a **kernel** $k = g \star g$:

$$\mathrm{d}_k(\alpha, \beta) = \| g \star \alpha - g \star \beta \|_{L^2}^2$$

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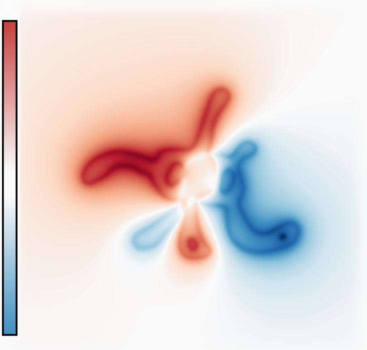

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$$\begin{aligned} \mathrm{d}_k(\alpha, \beta) &= \| \, g \star \alpha - g \star \beta \, \|_{L^2}^2 \\ &= \langle \, \alpha - \beta \, | \, k \star (\alpha - \beta) \, \rangle \end{aligned}$$

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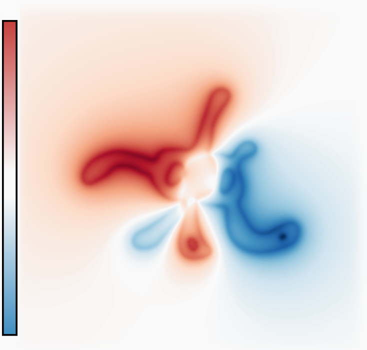

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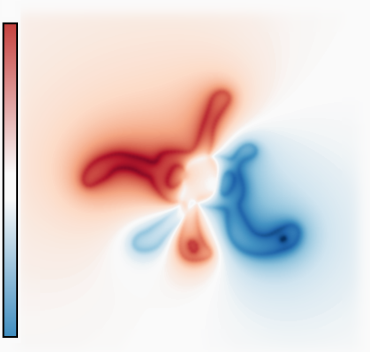
$$
\begin{aligned}
\mathrm{d}_k(\alpha, \beta) &= \| \, g \star \alpha - g \star \beta \, \|_{L^2}^2 \\
&= \langle \, \alpha - \beta \, | \, k \star (\alpha - \beta) \, \rangle \\
&= -2 \sum_{i,j} k(x_i, y_j) \, \alpha_i \, \beta_j + \cdots
\end{aligned}
$$

Kernel fidelities: the simplest formula for $d(\alpha, \beta)$



Blurred signal $g \star (\alpha - \beta)$.

Choose a symmetric blurring function g, a **kernel** $k = g \star g$:

$$\begin{aligned} \mathrm{d}_k(\alpha, \beta) &= \| \, g \star \alpha - g \star \beta \, \|_{L^2}^2 \\ &= \langle \, \alpha - \beta \, | \, k \star (\alpha - \beta) \, \rangle \\ &= -2 \sum_{i,j} k(x_i, y_j) \, \alpha_i \, \beta_j + \cdots \\ &= \langle \, \alpha - \beta \, | \, b^k - a^k \, \rangle \end{aligned}$$

with $a^k = -k \star \alpha$, $b^k = -k \star \beta$.

Kernel distances: distance fields computed through convolutions

Kernel distances, aka. **blurred** SSDs:

$$\text{choose} \qquad a(x) \;=\; -(k \star \alpha)(x) \;=\; -\sum_i \alpha_i \, k(x, x_i)$$

$$\text{and use} \qquad \tfrac{1}{2}\langle\, \alpha - \beta \,,\, b - a \,\rangle \;=\; \tfrac{1}{2}\langle\, \alpha - \beta \,,\, k \star (\alpha - \beta) \,\rangle.$$

Kernel distances: distance fields computed through convolutions

Kernel distances, aka. **blurred** SSDs:

$$\text{choose} \qquad a(x) = -(k \star \alpha)(x) = -\sum_i \alpha_i \, k(x, x_i)$$

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The **Energy Distance:** an underrated kernel, $k(x, y) = -\|x - y\|$.

$$a(x) = \sum_i \alpha_i \, \|x - x_i\| \qquad \text{instead of} \qquad a(x) = \min_i \|x - x_i\|$$

$$b(x) = \sum_j \beta_j \, \|x - y_j\| \qquad \text{instead of} \qquad b(x) = \min_j \|x - y_j\|.$$

Kernel distances: distance fields computed through convolutions

Kernel distances, aka. **blurred** SSDs:

$$\text{choose} \qquad a(x) \;=\; -(k\star\alpha)(x) \;=\; -\sum_i \alpha_i\, k(x, x_i)$$

$$\text{and use} \qquad \tfrac{1}{2}\langle\, \alpha-\beta\,,\; b-a\,\rangle \;=\; \tfrac{1}{2}\langle\, \alpha-\beta\,,\; k\star(\alpha-\beta)\,\rangle.$$

The **Energy Distance:** an underrated kernel, $k(x,y) \;=\; -\|x-y\|$.

$$a(x) \;=\; \sum_i \alpha_i\,\|x-x_i\| \qquad \text{instead of} \quad a(x) \;=\; \min_i \|x-x_i\|$$

$$b(x) \;=\; \sum_j \beta_j\,\|x-y_j\| \qquad \text{instead of} \quad b(x) \;=\; \min_j \|x-y_j\|.$$

$$\text{Loss}(\alpha,\beta) \;=\; \sum_i\sum_j \alpha_i\beta_j\,\|x_i-y_j\| \;-\; \tfrac{1}{2}\sum_i\sum_j \alpha_i\alpha_j\,\|x_i-x_j\| \;-\; \tfrac{1}{2}\sum_i\sum_j \beta_i\beta_j\,\|y_i-y_j\|$$

Kernel distances: distance fields computed through convolutions

Kernel distances, aka. **blurred** SSDs:

$$\text{choose} \qquad a(x) \;=\; -(k \star \alpha)(x) \;=\; -\sum_i \alpha_i\, k(x, x_i)$$

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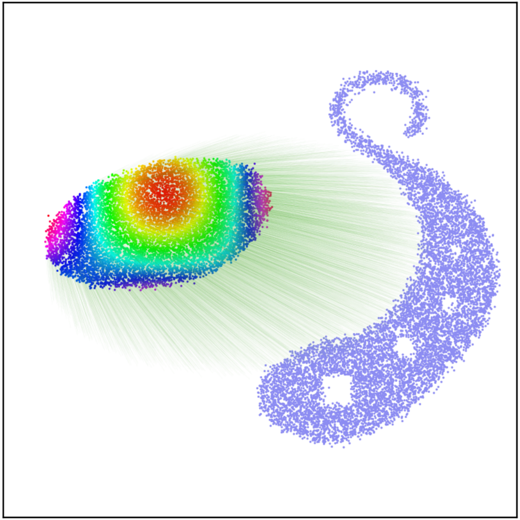
$$\text{Loss}(\alpha, \beta) \;=\; \sum_i \sum_j \alpha_i \beta_j\, \|x_i - y_j\| \;\simeq\; \textbf{Electrostatic Energy}$$

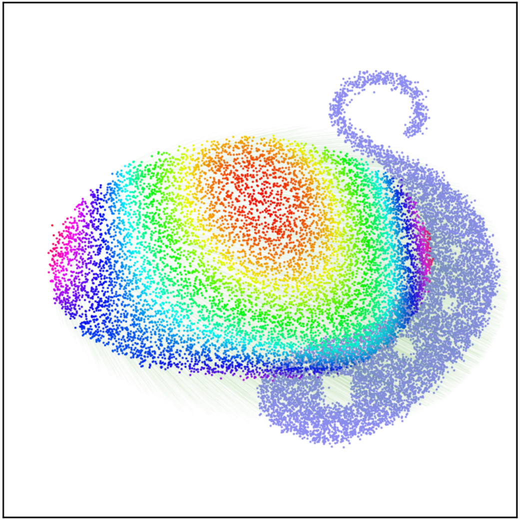
$$-\; \tfrac{1}{2} \sum_i \sum_j \alpha_i \alpha_j\, \|x_i - x_j\| \;-\; \tfrac{1}{2} \sum_i \sum_j \beta_i \beta_j\, \|y_i - y_j\|$$

Gradient flow as a toy registration problem



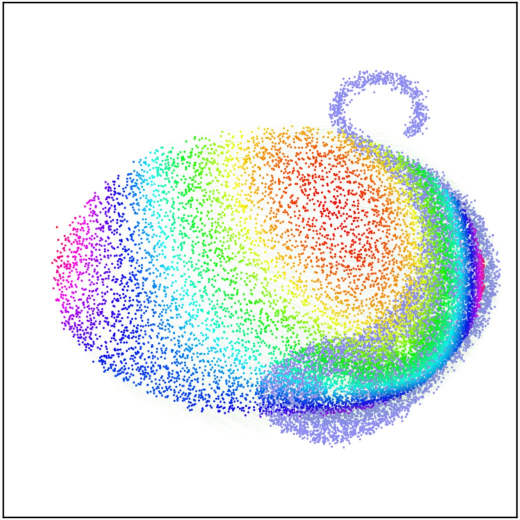
$t = .00$

Gradient flow as a toy registration problem



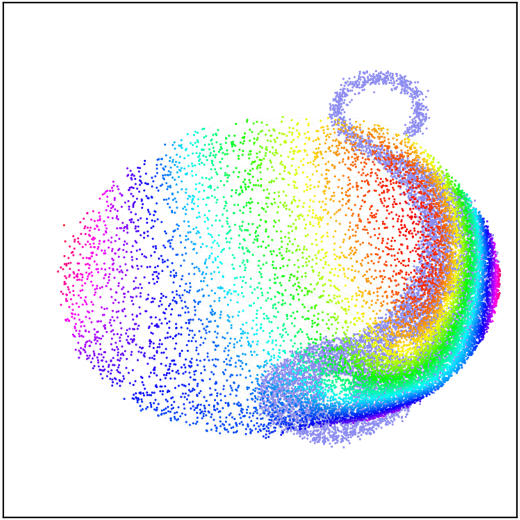
$t = .25$

Gradient flow as a toy registration problem



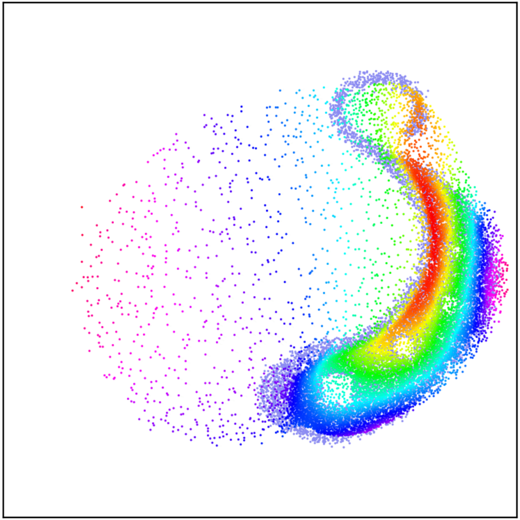
$t = .50$

Gradient flow as a toy registration problem



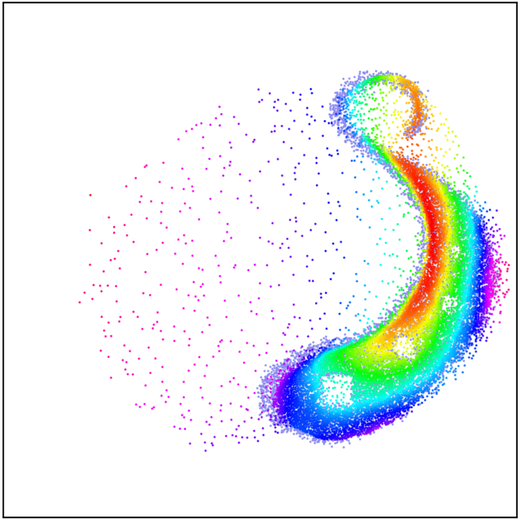
$t = 1.00$

Gradient flow as a toy registration problem



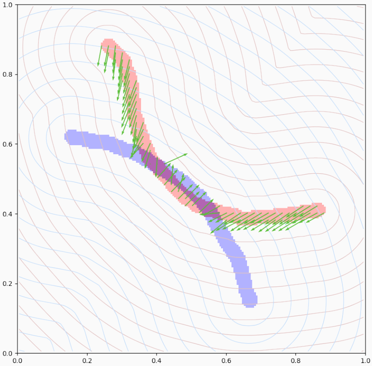
$t = 5.00$

Gradient flow as a toy registration problem

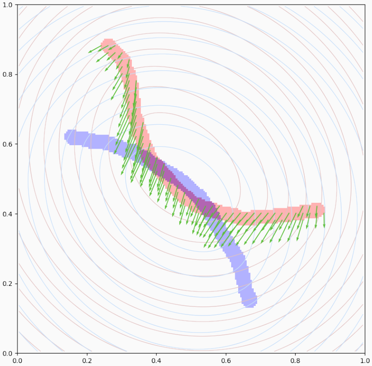


$t = 10.00$

The Hausdorff distance is local, the Energy Distance is global

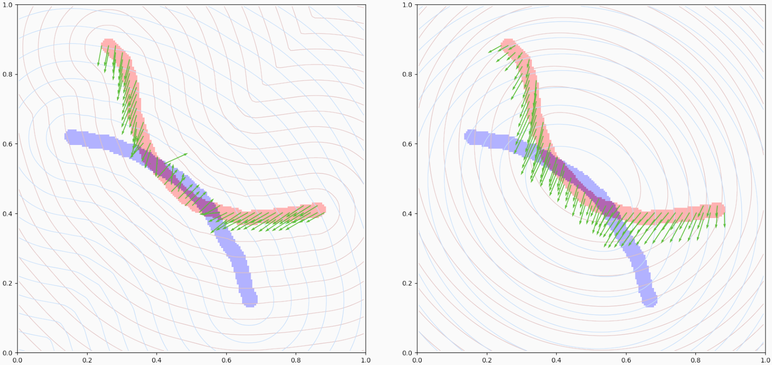


Hausdorff, min



Kernel, $\sum$

The Hausdorff distance is local, the Energy Distance is global

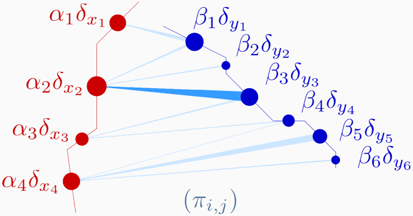


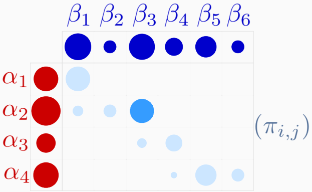
Hausdorff, min   Kernel, $\sum$

$\Longrightarrow$ Can we get the best of both worlds?

An idea from Optimal Transport theory: The SoftAssign algorithm

Introducing the Optimal Transport problem





Minimize over N-by-M matrices (transport plans) π :

$$\mathrm{OT}(\alpha, \beta) \;=\; \min_{\pi} \underbrace{\sum_{i,j} \pi_{i,j} \cdot |x_i - y_j|^2}_{\text{transport cost}}$$

subject to $\quad \pi_{i,j} \;\geqslant\; 0,$

$$\sum_j \pi_{i,j} \;=\; \alpha_i, \quad \sum_i \pi_{i,j} \;=\; \beta_j.$$

Kantorovitch's dual formulation

With $C(x_i, y_j) = \|x_i - y_j\|^p$,

$$\mathrm{OT}(\alpha, \beta) = \min_{\pi} \langle \pi , C \rangle \qquad \longrightarrow \text{Assignment}$$

$$\text{s.t. } \pi \geqslant 0, \qquad \pi \mathbf{1} = \alpha, \qquad \pi^\top \mathbf{1} = \beta$$

Kantorovitch's dual formulation

With $\mathrm{C}(x_i, y_j) = \|x_i - y_j\|^p$,

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$$\text{s.t. } \pi \geqslant 0, \qquad \pi \mathbf{1} = \alpha, \qquad \pi^\top \mathbf{1} = \beta$$

$$= \max_{f,g} \langle \alpha , f \rangle + \langle \beta , g \rangle \qquad \longrightarrow \text{FedEx}$$

$$\text{s.t. } \qquad f(x_i) + g(y_j) \leqslant \mathrm{C}(x_i, y_j),$$

Kantorovitch's dual formulation

With $C(x_i, y_j) = \|x_i - y_j\|^p$,

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$\Longrightarrow$ **Combinatorial** problem on the simplex

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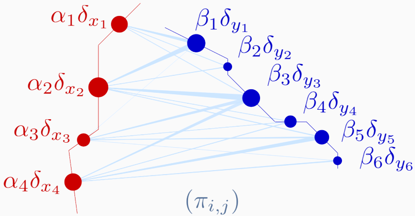
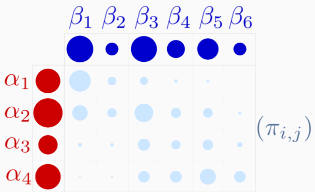
$$\text{s.t. } \qquad f(x_i) + g(y_j) \leqslant C(x_i, y_j),$$

$\Longrightarrow$ **Combinatorial** problem on the simplex

$\Longrightarrow$ Hungarian method in $\mathbf{O(N^3)}$.

Entropic regularization: introducing Schrödinger's problem





For $\varepsilon > 0$:

$$\text{OT}_\varepsilon(\alpha, \beta) = \min_\pi \underbrace{\sum_{i,j} \pi_{i,j} \cdot |x_i - y_j|^2}_{\text{transport cost}}$$

$$+ \; \varepsilon \underbrace{\sum_{i,j} \pi_{i,j} \cdot \log \frac{\pi_{i,j}}{\alpha_i \, \beta_j}}_{\text{entropic barrier}}$$

subject to

$$\sum_j \pi_{i,j} = \alpha_i, \quad \sum_i \pi_{i,j} = \beta_j.$$

Fenchel-Rockafellar to the rescue

$$\mathrm{OT}_\varepsilon(\alpha, \beta) \;=\; \min_{\pi} \,\langle\, \pi \,,\, \mathrm{C} \,\rangle \;+\; \varepsilon\, \mathrm{KL}(\, \pi \,,\, \alpha \otimes \beta \,) \quad \longrightarrow \text{Fuzzy assignment}$$

$$\text{s.t.} \qquad \pi\, \mathbf{1} \;=\; \alpha, \qquad \pi^{\intercal} \mathbf{1} \;=\; \beta$$

Fenchel-Rockafellar to the rescue

$$\mathrm{OT}_\varepsilon(\alpha,\beta) = \min_{\pi} \langle \pi , \mathrm{C} \rangle + \varepsilon \, \mathrm{KL}(\pi , \alpha \otimes \beta) \quad \longrightarrow \text{ Fuzzy assignment}$$

$$\text{s.t.} \quad \pi \mathbf{1} = \alpha, \qquad \pi^\intercal \mathbf{1} = \beta$$

$$= \max_{f,g} \langle \alpha , f \rangle + \langle \beta , g \rangle \quad \longrightarrow \text{ Cheeky FedEx}$$

$$- \underbrace{\varepsilon \langle \alpha \otimes \beta , e^{(f \oplus g - \mathrm{C})/\varepsilon} - 1 \rangle}_{\text{soft constraint } f \oplus g \leqslant \mathrm{C}}$$

Fenchel-Rockafellar to the rescue

$$\mathrm{OT}_\varepsilon(\alpha, \beta) = \min_{\pi} \langle \pi , \mathrm{C} \rangle + \varepsilon \, \mathrm{KL}(\pi , \alpha \otimes \beta) \longrightarrow \text{Fuzzy assignment}$$

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$\Longrightarrow$ **Strictly convex** problem on the simplex

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$$= \max_{f,g} \langle \alpha , f \rangle \;+\; \langle \beta , g \rangle \quad \longrightarrow \text{Cheeky FedEx}$$

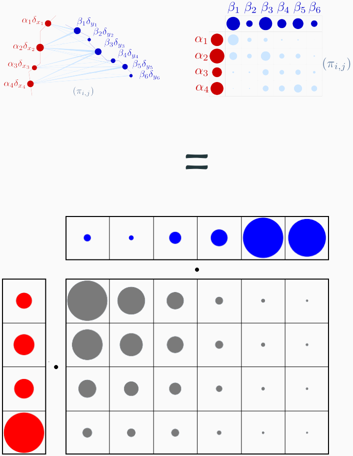
$$- \underbrace{\varepsilon \langle \alpha\otimes\beta , e^{(f\oplus g - \mathrm{C})/\varepsilon} - 1 \rangle}_{\text{soft constraint } f\oplus g \leqslant \mathrm{C}}$$

$\Longrightarrow$ **Strictly convex** problem on the simplex

$$\text{At the optimum,} \quad \pi \;=\; e^{(f\oplus g - \mathrm{C})/\varepsilon} \cdot \alpha\otimes\beta$$

$$\text{i.e.} \qquad \pi_{i,j} \;=\; \alpha_i\, e^{f_i/\varepsilon}\, e^{-\mathrm{C}(x_i,y_j)/\varepsilon}\, e^{g_j/\varepsilon}\, \beta_j.$$

Textbook interpretation: balancing of a kernel matrix



$$\pi_{i,j} \;=\; \Delta(U\alpha) \cdot \mathrm{K}_{x,y} \cdot \Delta(V\beta)$$

with

- a kernel function k

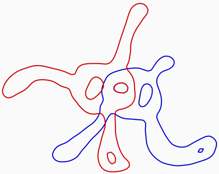
$$k(x_i - y_j) \;=\; e^{-\mathrm{C}(x_i,y_j)/\varepsilon}.$$

- $U = e^{f/\varepsilon}$ and $V = e^{g/\varepsilon}$, positive weights on $\{x_i\}$ and $\{y_j\}$.

$\rightarrow$ Enforce the **constraints**

$$\pi\,\mathbf{1} \;=\; \alpha, \qquad \pi^{\mathsf{T}}\mathbf{1} \;=\; \beta$$

Enforcing $\pi 1 = \alpha$ and $\pi^T 1 = \beta$ alternatively



Source and target.

Sinkhorn Iterative Algorithm

Input : source $\alpha = \sum_i \alpha_i \delta_{x_i}$

target $\beta = \sum_j \beta_j \delta_{y_j}$

Parameter : $k : x \mapsto e^{-|x|^2/\varepsilon}$

1: $U \leftarrow ones(size(\alpha))$

2: $V \leftarrow ones(size(\beta))$

3: **while** updates > tol **do**

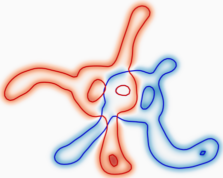
4: $U \leftarrow 1 \;./\; K \cdot (V\beta)$

5: $V \leftarrow 1 \;./\; K^T \cdot (U\alpha)$

6: **return** $\varepsilon \left(\langle \alpha, \log(U) \rangle + \langle \beta, \log(V) \rangle \right)$

Output : fidelity $\mathrm{OT}_\varepsilon(\alpha, \beta)$

Enforcing $\pi 1 = \alpha$ and $\pi^\top 1 = \beta$ alternatively



Seen by the kernel k.

Sinkhorn Iterative Algorithm

Input : source $\alpha = \sum_i \alpha_i \delta_{x_i}$

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Parameter : $k : x \mapsto e^{-|x|^2/\varepsilon}$

$U \leftarrow ones(size(\alpha))$

$V \leftarrow ones(size(\beta))$

while updates $>$ tol **do**

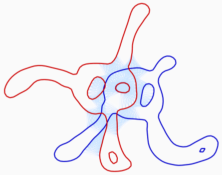
$\quad U \leftarrow 1 \;./\; \mathrm{K} \cdot (V\beta)$

$\quad V \leftarrow 1 \;./\; \mathrm{K}^\top \cdot (U\alpha)$

return $\varepsilon \left(\langle \alpha, \log(U) \rangle + \langle \beta, \log(V) \rangle \right)$

Output : fidelity $\mathrm{OT}_\varepsilon(\alpha, \beta)$

Enforcing $\pi 1 = \alpha$ and $\pi^{\top} 1 = \beta$ alternatively



Starting estimate.

Sinkhorn Iterative Algorithm

Input : source $\alpha = \sum_i \alpha_i \delta_{x_i}$

target $\beta = \sum_j \beta_j \delta_{y_j}$

Parameter : $k : x \mapsto e^{-|x|^2/\varepsilon}$

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2: $V \leftarrow ones(size(\beta))$

3: **while** updates > tol **do**

4: $U \leftarrow 1 \; ./ \; K \cdot (V\beta)$

5: $V \leftarrow 1 \; ./ \; K^{\top} \cdot (U\alpha)$

6: **return** $\varepsilon \left(\langle \alpha, \log(U) \rangle + \langle \beta, \log(V) \rangle \right)$

Output : fidelity $\mathrm{OT}_\varepsilon(\alpha, \beta)$

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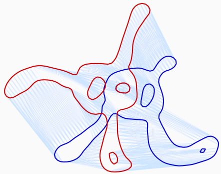

Sinkhorn Iteration 250

Computing the OT plan.

Sinkhorn Iterative Algorithm

Input : source $\alpha = \sum_i \alpha_i \delta_{x_i}$

target $\beta = \sum_j \beta_j \delta_{y_j}$

Parameter : $k : x \mapsto e^{-|x|^2/\varepsilon}$

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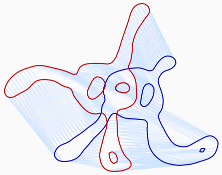
6: **return** $\varepsilon\,(\langle \alpha, \log(U) \rangle + \langle \beta, \log(V) \rangle)$

Output : fidelity $\mathrm{OT}_\varepsilon(\alpha, \beta)$

Enforcing $\pi \mathbb{1} = \alpha$ and $\pi^\top \mathbb{1} = \beta$ alternatively



Sinkhorn Iteration 250

Computing the OT plan.

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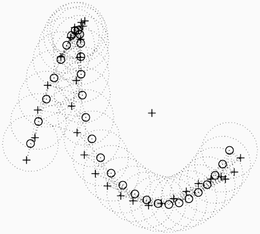
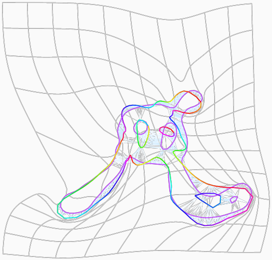
Output : fidelity $\mathrm{OT}_\varepsilon(\alpha, \beta)$

Robust Point Matching, 1998-2017



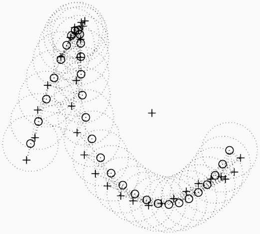
$\simeq$



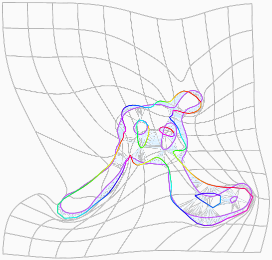
TPS-RPM algorithm,
Chui and Rangarajan, CVPR **2000**

Optimal Transport for diffeomorphic registration, Feydy et al., MICCAI **2017**

Robust Point Matching, 1998-2017



$\simeq$



TPS-RPM algorithm,
Chui and Rangarajan, CVPR **2000**

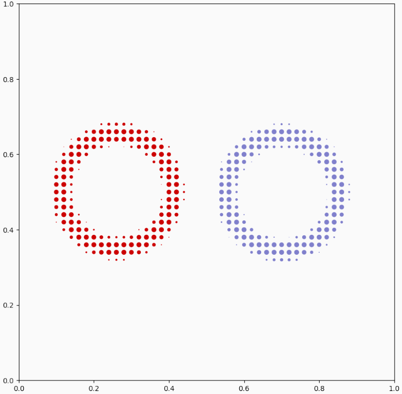
Optimal Transport for diffeomorphic registration, Feydy et al., MICCAI **2017**

$\Longrightarrow$ We've added weights, orientations, convergence analysis...
But shouldn't we go a bit **further**?

It's 2019 now:
What's new?

Fact 1 : if $\varepsilon > 0$, OT_ε is *not* a valid divergence

Registrating circles, $C(x, y) = \|x - y\|^2$, $\sqrt{\varepsilon} = 0.1$:



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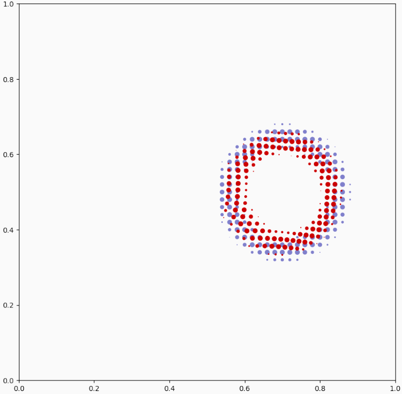

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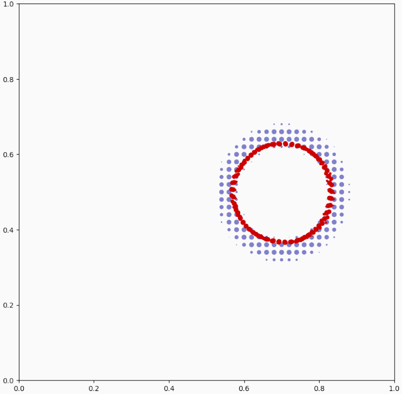
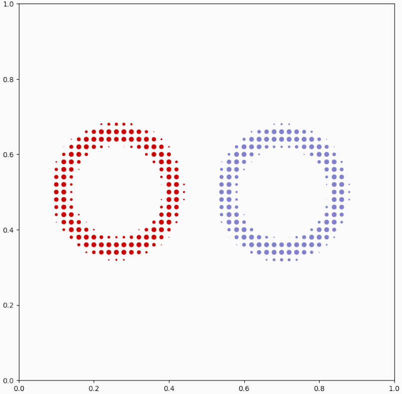


Fact 1 : if $\varepsilon > 0$, OT_ε is *not* a valid divergence

Registrating circles, $C(x, y) = \|x - y\|^2$, $\sqrt{\varepsilon} = 0.2$:



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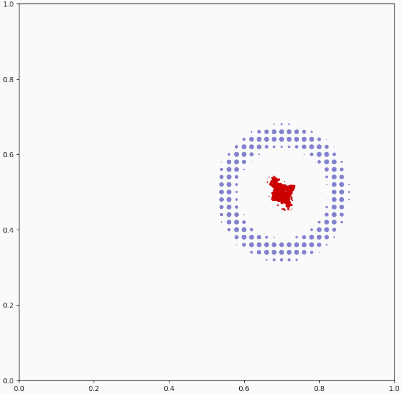

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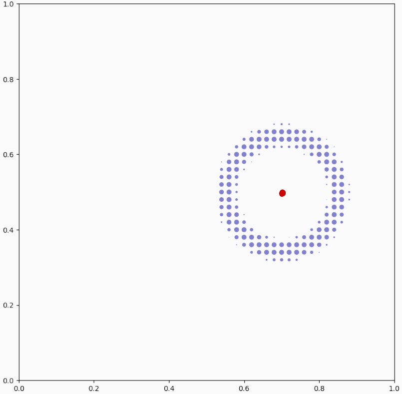

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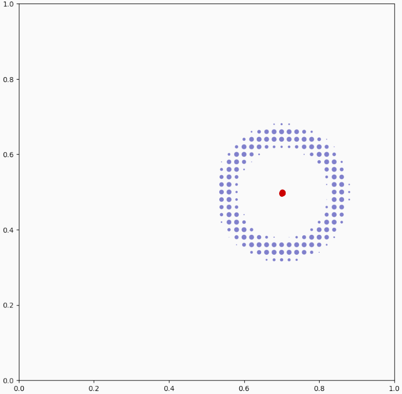
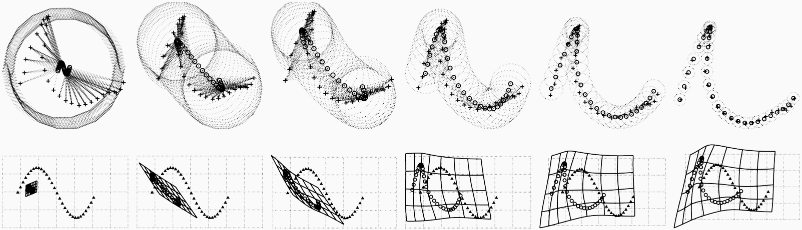


Bad news: for $0 < \varepsilon \leqslant +\infty$, we converge towards α such that

$$\mathrm{OT}_\varepsilon(\alpha, \beta) \ < \ \mathrm{OT}_\varepsilon(\beta, \beta).$$

Standard solution: use an annealing scheme in the descent



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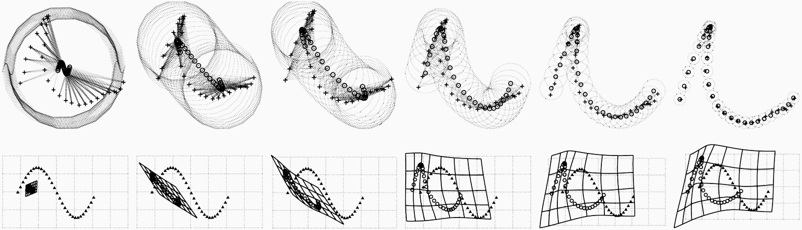

TPS-RPM algorithm, Chui and Rangarajan, CVPR 2000

$\Longrightarrow$ **Cumbersome** and brittle workaround,
with parameters to tune.

A new idea in 2017 : un-biased Sinkhorn divergences

$$\mathrm{OT}_\varepsilon(\alpha, \beta) \;=\; \min_{\pi} \,\langle\, \pi \,,\, \mathrm{C} \,\rangle \;+\; \varepsilon\,\mathrm{KL}(\, \pi \,,\, \alpha \otimes \beta \,) \quad \longrightarrow \text{Fuzzy assignment}$$

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Define the **Sinkhorn divergence** [Ramdas et al., 2017]:

$$\mathrm{S}_\varepsilon(\alpha, \beta) = \mathrm{OT}_\varepsilon(\alpha, \beta) - \tfrac{1}{2}\mathrm{OT}_\varepsilon(\alpha, \alpha) - \tfrac{1}{2}\mathrm{OT}_\varepsilon(\beta, \beta)$$

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In practice, S_ε is “good enough” for ML applications [Genevay et al., 2018, Salimans et al., 2018, Sanjabi et al., 2018].

In our paper: theoretical guarantees

Theorem (F., Séjourné, Vialard, Amari, Trouvé, Peyré; 2018)

For all probability measures α, β *and regularization* $\varepsilon > 0$ *:*

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Loss = OT_ε Loss = S_ε

Fact 2 : Sinkhorn is best implemented in the log-domain

Unfortunately,

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$$\begin{aligned}\mathrm{OT}_\varepsilon(\alpha,\beta) \;=\; \max_{f,g}\, \langle\, \alpha\,,\, f \rangle \,+\, \langle\, \beta\,,\, g\,\rangle \qquad\qquad & \longrightarrow \text{ Cheeky FedEx} \\ -\; \underbrace{\varepsilon\,\langle\, \alpha\otimes\beta\,,\, e^{(f\oplus g - \mathrm{C})/\varepsilon} - 1\,\rangle}_{\text{soft constraint } f\oplus g \,\leqslant\, \mathrm{C}} &\end{aligned}$$

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$$- \underbrace{\varepsilon \langle \alpha \otimes \beta , e^{(f \oplus g - \mathrm{C})/\varepsilon} - 1 \rangle}_{\text{soft constraint } f \oplus g \leqslant \mathrm{C}}$$

Equivalent to the constraints on π, the optimality conditions read:

$$f(x_i) = -\varepsilon \log \sum_j \beta_j \exp \tfrac{1}{\varepsilon}(g(y_j) - \mathrm{C}(x_i, y_j)),$$

$$g(y_j) = -\varepsilon \log \sum_i \alpha_i \exp \tfrac{1}{\varepsilon}(f(x_i) - \mathrm{C}(x_i, y_j)).$$

The SoftMin interpolates between a minimum and a sum

$$\log\left(e^{c} + e^{d}\right) = \max(c,d) + \log\big(\underbrace{e^{c-\max(c,d)} + e^{d-\max(c,d)}}_{\in[1,2]}\big)$$

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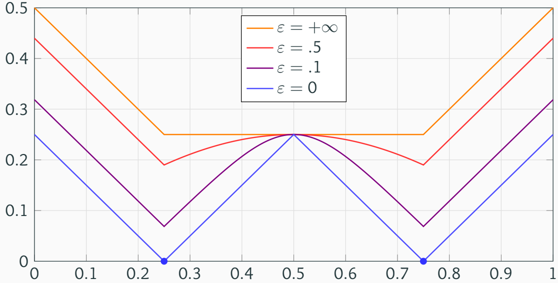
Building on this, for a regularization parameter $\varepsilon > 0$, we define

$$b^\varepsilon(x) = \min_{y\sim\beta}{}_\varepsilon \; \|x-y\| = -\varepsilon \log \sum_{j=1}^{M} \beta_j \exp\left(-\tfrac{1}{\varepsilon}\|x-y_j\|\right)$$



$b^\varepsilon(x)$, with $\beta = \frac{1}{2}\delta_{.25} + \frac{1}{2}\delta_{.75}$

Optimal Transport = Hausdorff + mass spreading constraint

The optimality conditions read:

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Final cost:

$$\begin{aligned} \mathrm{OT}_\varepsilon(\alpha,\beta) &= \langle\, \alpha \,,\, f \,\rangle + \langle\, \beta \,,\, g \,\rangle = \langle\, \alpha \,,\, b \,\rangle + \langle\, \beta \,,\, a \,\rangle, \\ \mathrm{S}_\varepsilon(\alpha,\beta) &= \langle\, \alpha \,,\, b^{\beta\to\alpha} - a^{\alpha\leftrightarrow\alpha} \,\rangle + \langle\, \beta \,,\, a^{\alpha\to\beta} - b^{\beta\leftrightarrow\beta} \,\rangle. \end{aligned}$$

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$$\mathrm{S}_\varepsilon(\alpha,\beta) \;=\; \langle\, \alpha \,,\, b^{\beta\rightarrow\alpha} \;-\; a^{\alpha\leftrightarrow\alpha} \,\rangle \;+\; \langle\, \beta \,,\, a^{\alpha\rightarrow\beta} \;-\; b^{\beta\leftrightarrow\beta} \,\rangle.$$

Discrete, computational OT [Cuturi, 2013, Peyré and Cuturi, 2018]:

Start from an ε-smoothed **Hausdorff** distance, but let the influence fields a and b **interact** with each other.

Enforce a **mass spreading** constraint on the spring system: all of α should be linked to all of β.

Fact 3: You should use a *multiscale* strategy [Schmitzer, 2016]

Iteration 0

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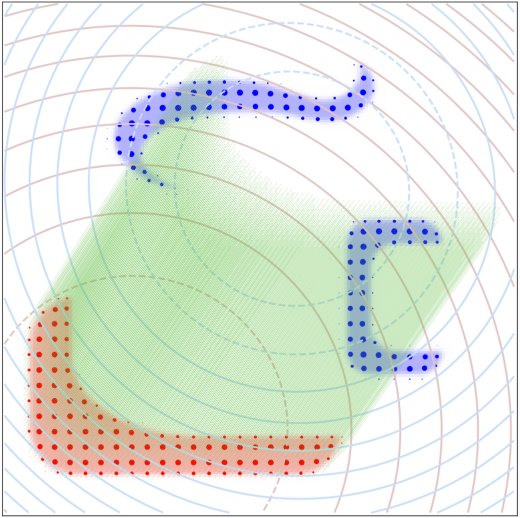

Iteration 1

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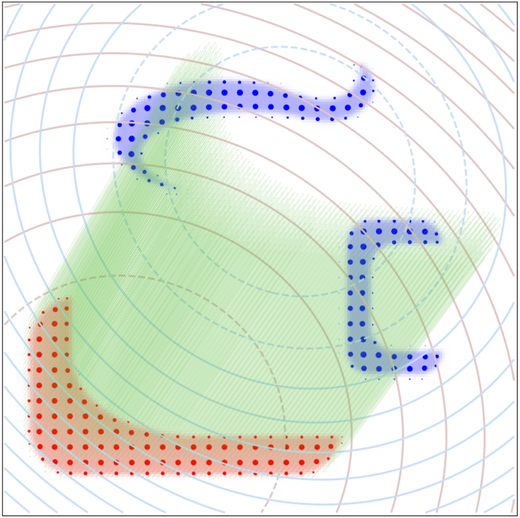

Iteration 2

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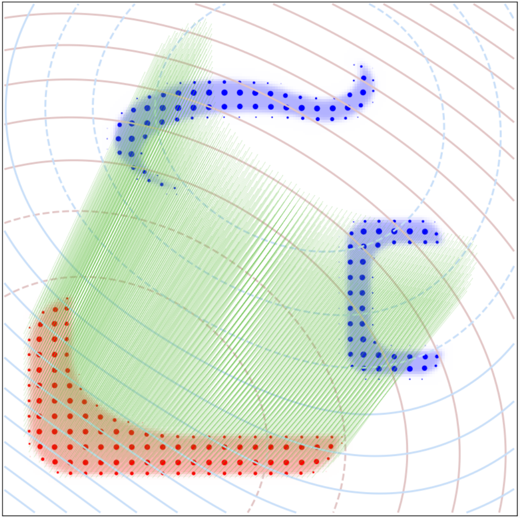

Iteration 3

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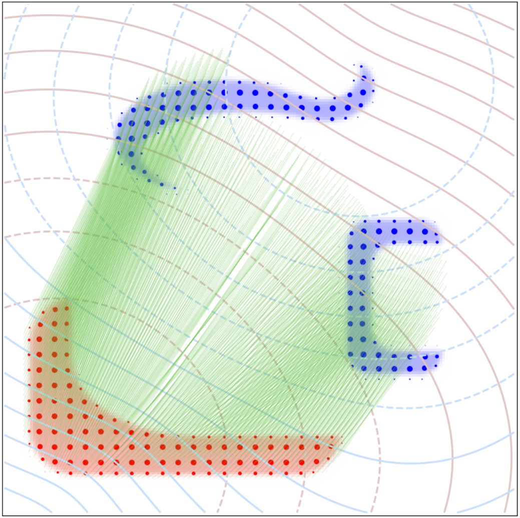

Iteration 4

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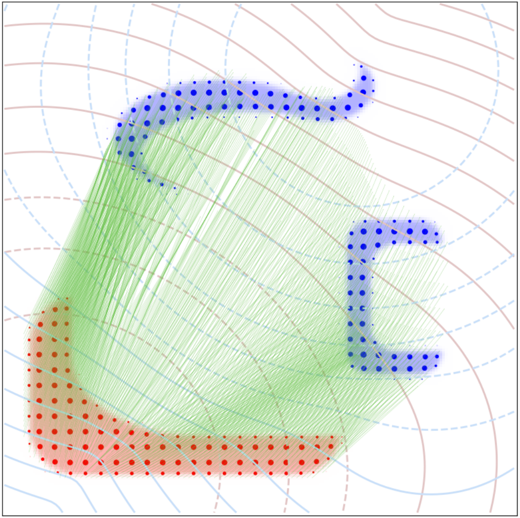

Iteration 5

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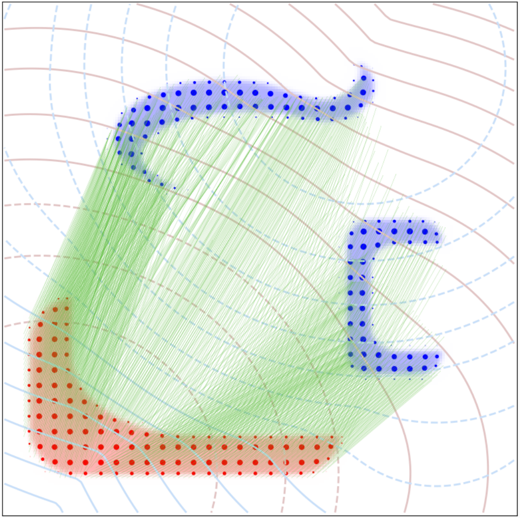

Iteration 6

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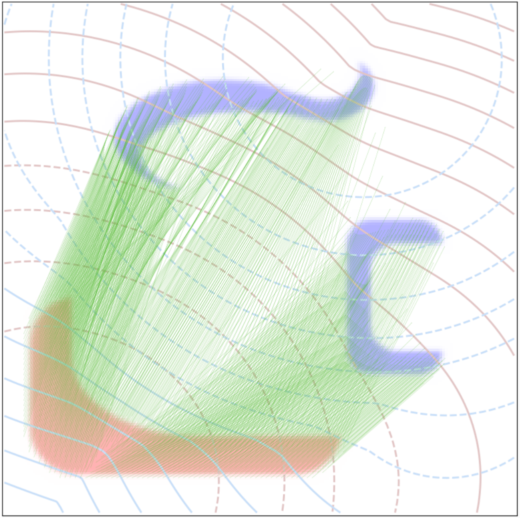

Iteration 7

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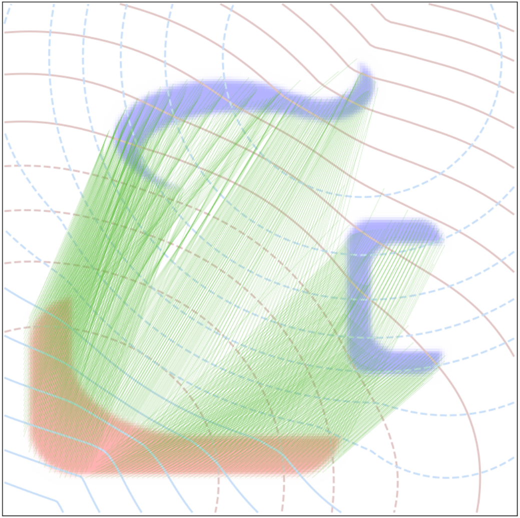


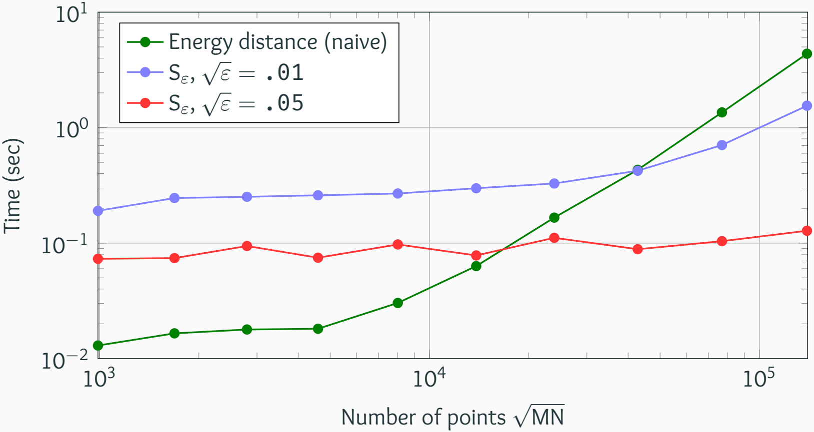
Iteration 8

A new, super-fast GPU implementation (not public just yet)

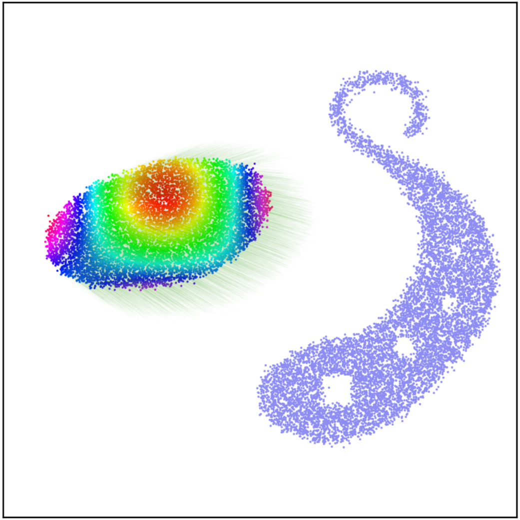
Leverages the KeOps library [Charlier et al., 2018]:

$$\Longrightarrow \texttt{pip install pykeops} \Longleftarrow$$

Loss + gradient in 3D, on a cheap laptop's GPU (GTX960M)



Gradient flow as a toy registration problem



$t = .00$

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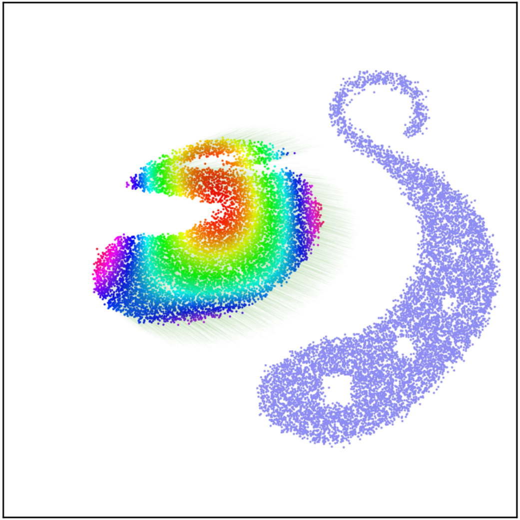
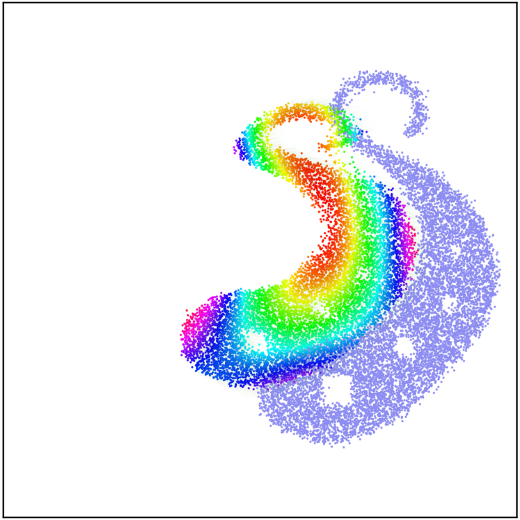


$t = .25$

Gradient flow as a toy registration problem

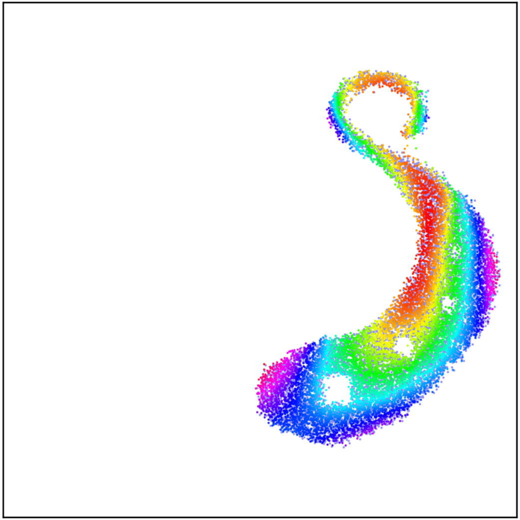
$t = .50$

Gradient flow as a toy registration problem



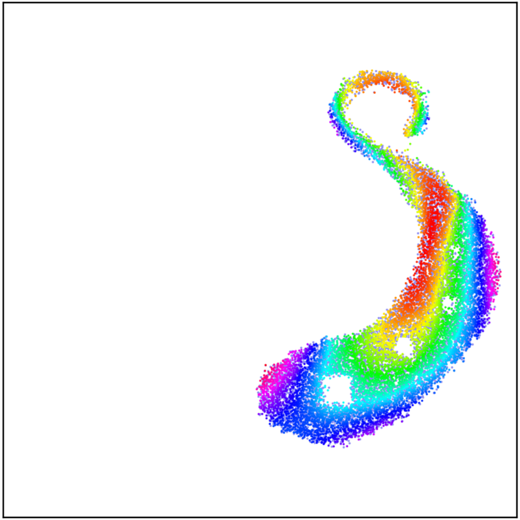
$t = 1.00$

Gradient flow as a toy registration problem



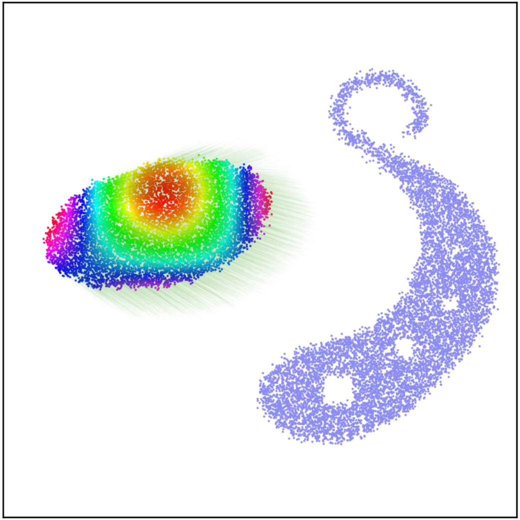
$t = 5.00$

Gradient flow as a toy registration problem



$t = 10.00$

Gradient descent on S_ε: cheap'n easy registration?



Iteration 0

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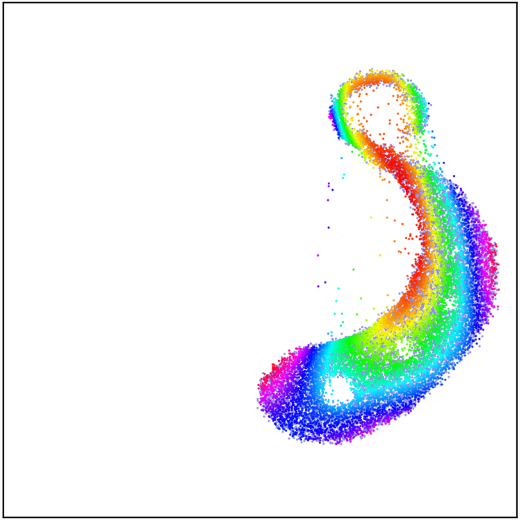

Iteration 1

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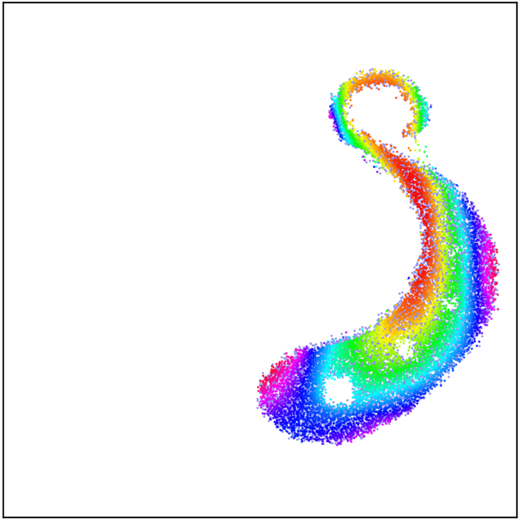
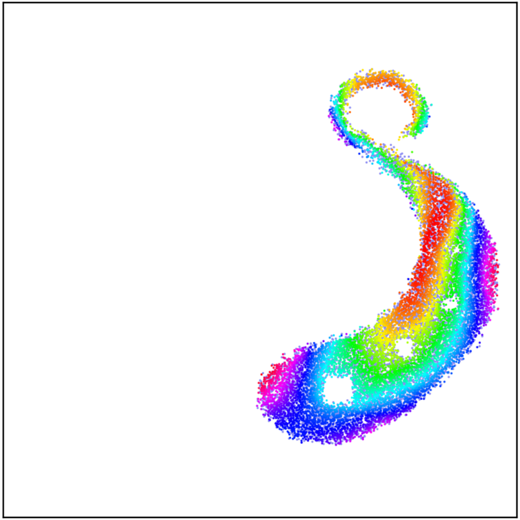


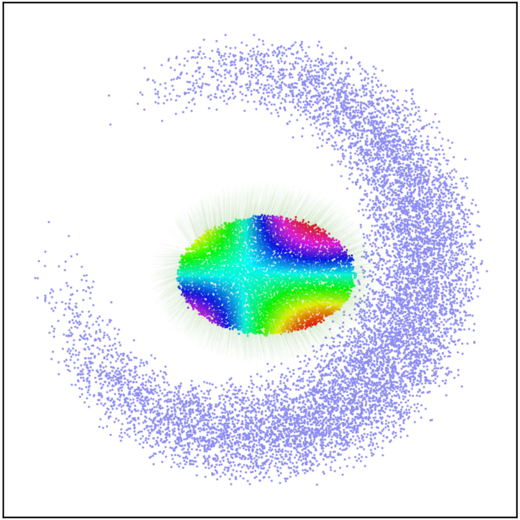
Iteration 2

Gradient descent on S_ε: cheap'n easy registration?



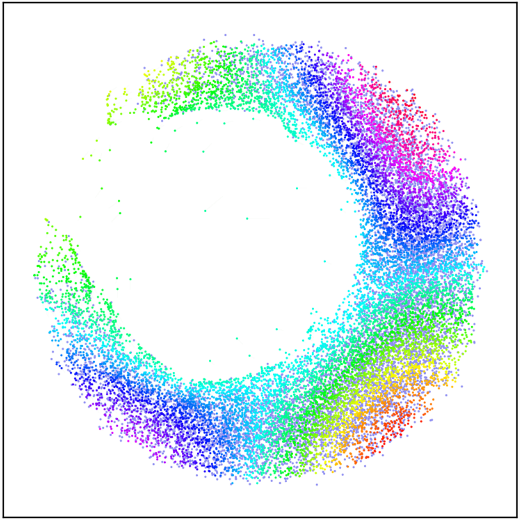
Iteration 10

Gradient descent on S_ε: cheap'n easy registration?



Iteration 0

Gradient descent on S_ε: cheap'n easy registration?



Iteration 1

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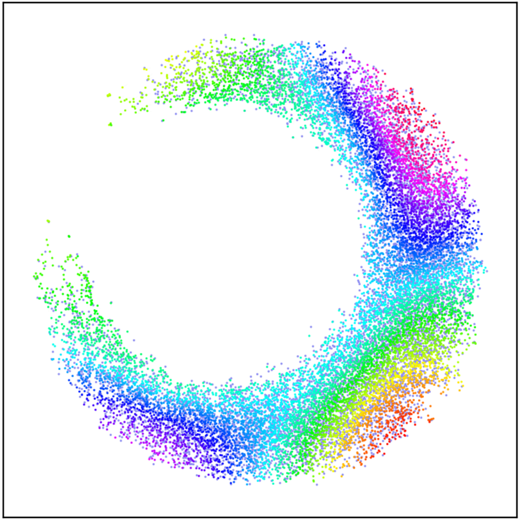
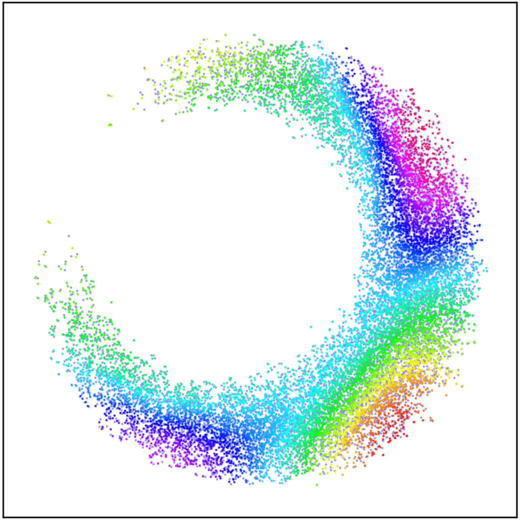


Iteration 2

Gradient descent on S_ε: cheap'n easy registration?



Iteration 10

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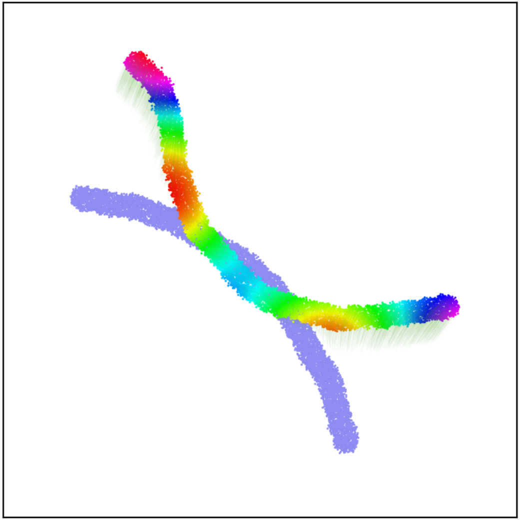


Iteration 0

Gradient descent on S_ε: cheap'n easy registration?

Iteration 1

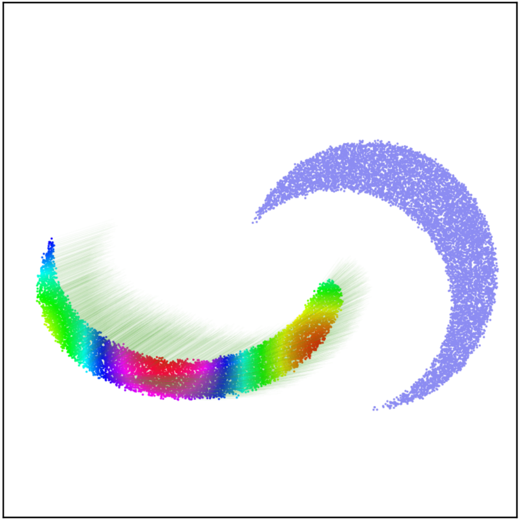
Gradient descent on S_ε: cheap'n easy registration?

Iteration 2

Gradient descent on S_ε: cheap'n easy registration?

Iteration 10

Gradient descent on S_ε: cheap'n easy registration? Beware!



Iteration 0

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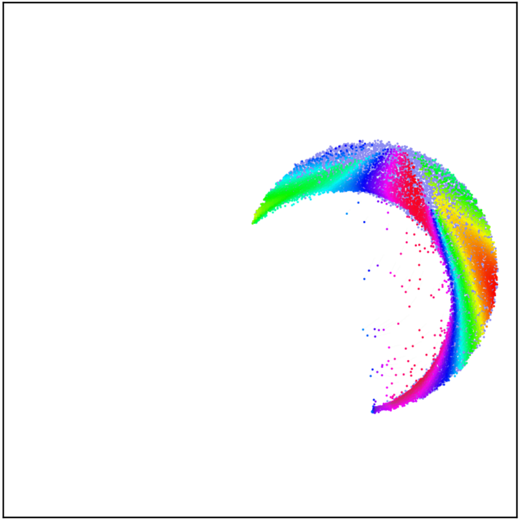

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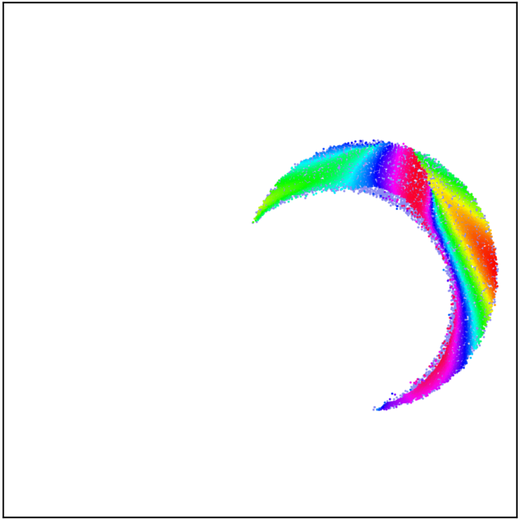

Iteration 2

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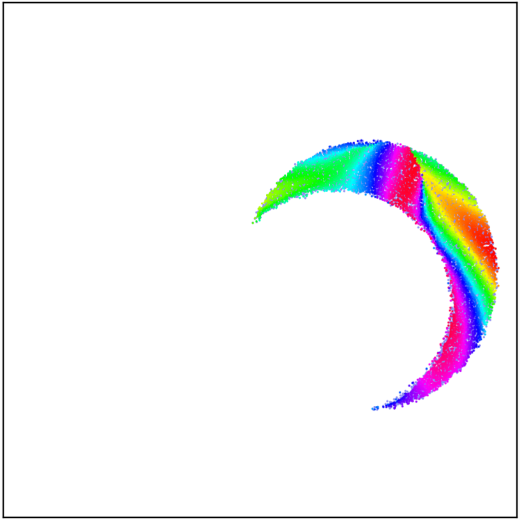

Iteration 10

Conclusion

A significant result

The **true** OT_0 problem is **hard**.

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The **true** OT_0 problem is **hard**.
Approximating it with **subsampling** or **smoothing** is easy:
this is what **SoftAssign** is all about.

A significant result

The **true** OT_0 problem is **hard**.
Approximating it with **subsampling** or **smoothing** is easy:
this is what **SoftAssign** is all about.

Remarkably, $\mathrm{S}_\varepsilon(\alpha, \beta)$ is a cheap approximation of $\mathrm{OT}_0(\alpha, \beta)$
that defines a **positive definite** cost between the **discrete samples**.
It is the first known way of doing so.

Dual norms - link with the GANs literature

$$\text{Loss}(\alpha, \beta) = \max_{f \in B} \langle \alpha - \beta , f \rangle,$$

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- $B = \{ \| f \|_2^2 + \| \nabla f \|_2^2 + \cdots \leqslant 1 \} \implies$ Loss = kernel norm:
  - may saturate at infinity
  - **screening** artifacts

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  - can we provide relevant **insights** to the ML community?

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- Try using $k(x, y) \; = \; -\|x - y\|$!
- Remove the **entropic bias** from the SoftAssign algorithm!
- Sinkhorn $=$ Hausdorff + mass **spreading** constraint
  $\simeq$ best you can do without topology or landmarks
  $\simeq$ a handful of convolutions through the data
  $\rightarrow$ Is it worth it?

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- Miccai2017 : proof of concept

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  - link with statistics and **computer graphics**
  - reference **implementation** on sparse data
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- 2019 - available soon :
  - unbalanced formulation, to handle **outliers**
  - **evaluation** in varied settings
  - **octree**-like code on the GPU
  - separable **volumetric** implementation

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Open questions:

- Can we find a **Brenier-like** formulation for S_ε?

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- Interest in the **CVPR/SIGGRAPH** communities?

Thank you for your attention.

Any questions ?

References

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