Global divergences between measures: from Hausdorff distance to Optimal Transport

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Curves and Surfaces, Arcachon – 2 juillet 2018

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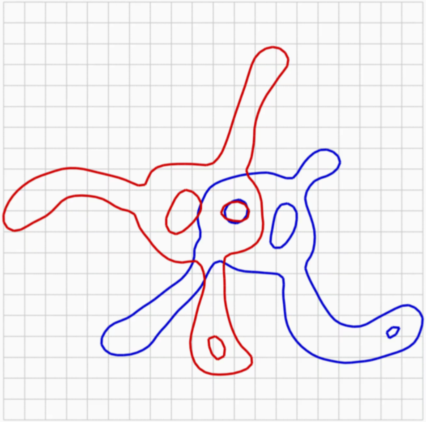
Collaboration with B. Charlier, J. Glaunès, F.-X. Vialard, G. Peyré

Today: focus on shape registration

Source A, target B,



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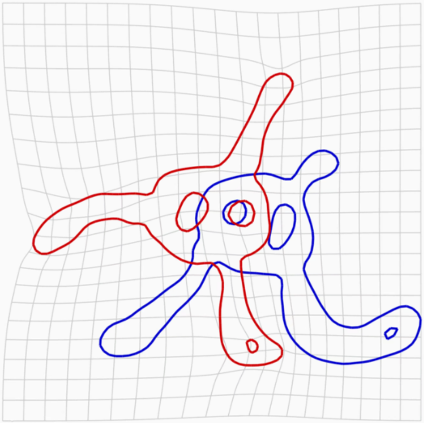
Source A, target B, mapping φ



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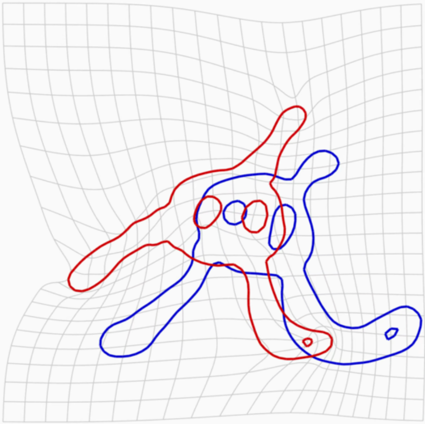

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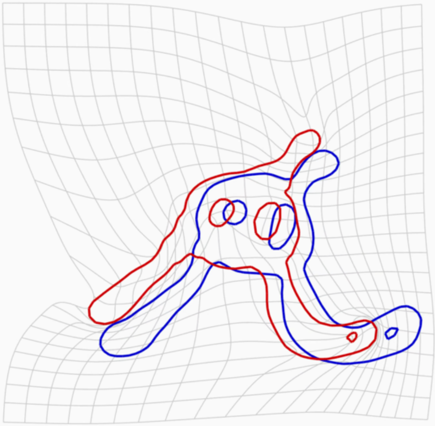

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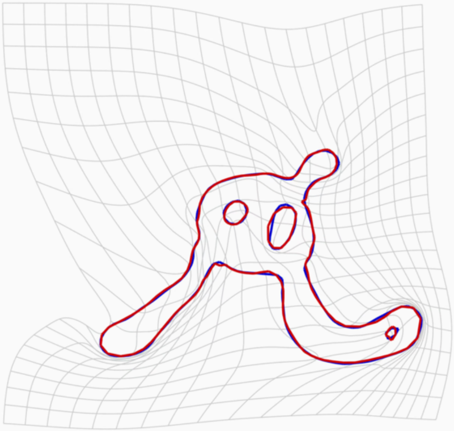

In practice: gradient descent on the deformation

$$\text{Cost}(\varphi) = \underbrace{\text{Reg}(\varphi)}_{\text{regularization}} + \underbrace{\text{d}(\varphi(A), B)}_{\text{fidelity}}$$

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If A and B are labeled vectors of $\mathbb{R}^{N\times D}$, you can use

$$\text{Affine registration:} \qquad \text{Cost}(\varphi) = 1_{\text{affine}}(\varphi) + \|\varphi(A) - B\|_2^2$$

$$\text{Thin Plate Splines:} \qquad \text{Cost}(\varphi) = \lambda \, \|\Delta\varphi\|_2^2 + \|\varphi(A) - B\|_2^2$$

In practice: gradient descent on the deformation

$$\text{Cost}(\varphi) \;=\; \underbrace{\text{Reg}(\varphi)}_{\text{regularization}} \;+\; \underbrace{\text{d}(\varphi(A)\,,B)}_{\text{fidelity}}$$

Iterative Matching Algorithm

$\varphi \leftarrow \text{Id}$
while updates $>$ tol **do**
 “$\varphi \leftarrow \varphi \;-\; \alpha \cdot \big(\nabla_\varphi \text{Reg}(\varphi) + \nabla_\varphi\, [\text{d}(\varphi(A), B)]\,\big)$”
return φ

Output : matching transformation φ.

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Output : matching transformation φ.

$\Rightarrow$ The fidelity's gradient **drives** the registration

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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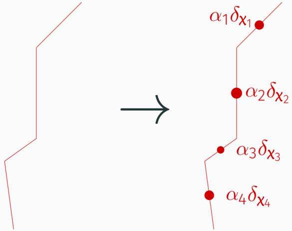

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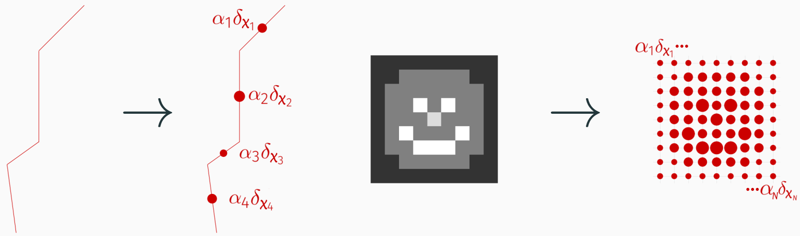
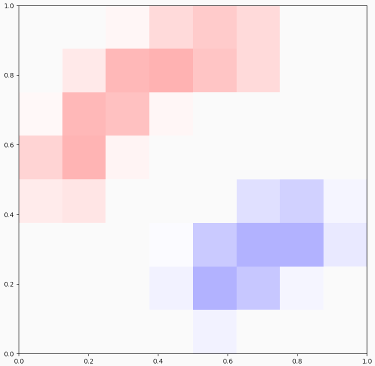


A baseline setting: density registration



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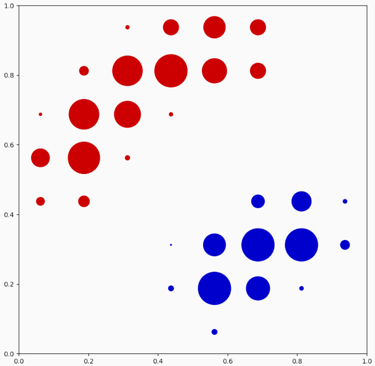

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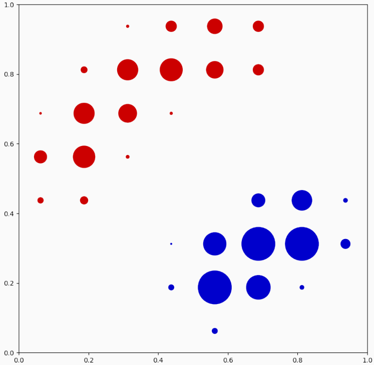

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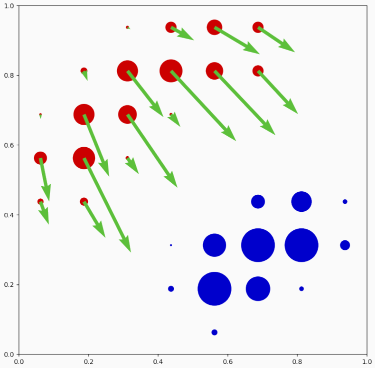

$$\alpha = \sum_{i=1}^{N} \alpha_i \delta_{x_i} , \quad \beta = \sum_{j=1}^{M} \beta_j \delta_{y_j} .$$

$$\sum_{i=1}^{N} \alpha_i = 1 = \sum_{j=1}^{M} \beta_j$$

Display $v = -\nabla_{x_i} \mathrm{d}(\alpha, \beta)$.

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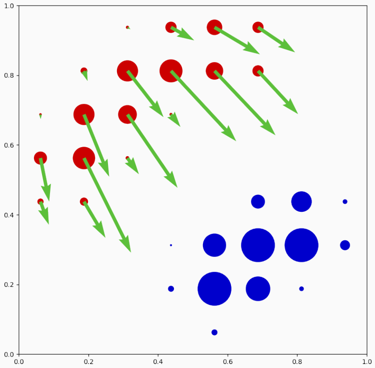

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Display $v \;=\; -\nabla_{x_i} \mathrm{d}(\alpha, \beta)$.

$\rightarrow$ seamless extensions to $\sum_i \alpha_i \neq \sum_j \beta_j$ [Chizat et al., 2018], curves and surfaces [Kaltenmark et al., 2017].

Overview

Computing fidelities between **measures**:

1. **Statistics:** kernel distances
2. **Computer graphics:** Hausdorff distances
3. **Optimal Transport:** Sinkhorn divergences

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1. **Statistics:** kernel distances
2. **Computer graphics:** Hausdorff distances
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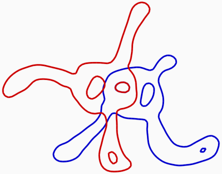
4. Efficient GPU routines: **KeOps**

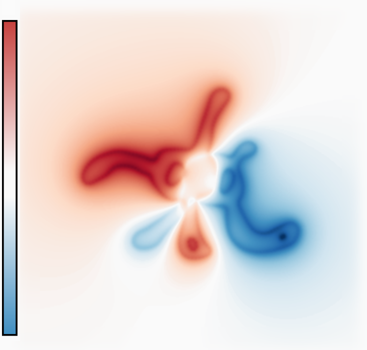
An idea from statistics:
Kernel distances

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



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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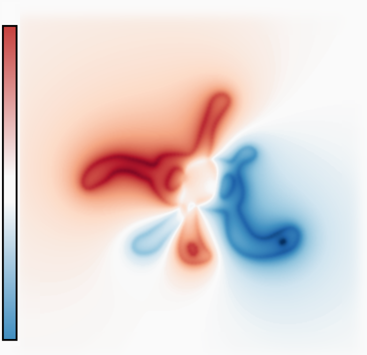

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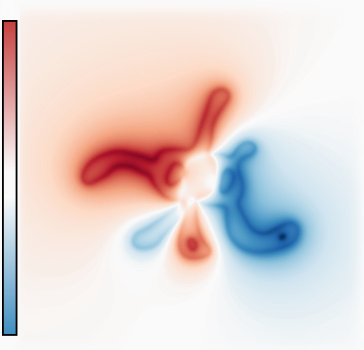

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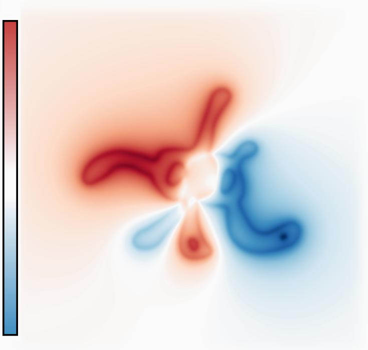

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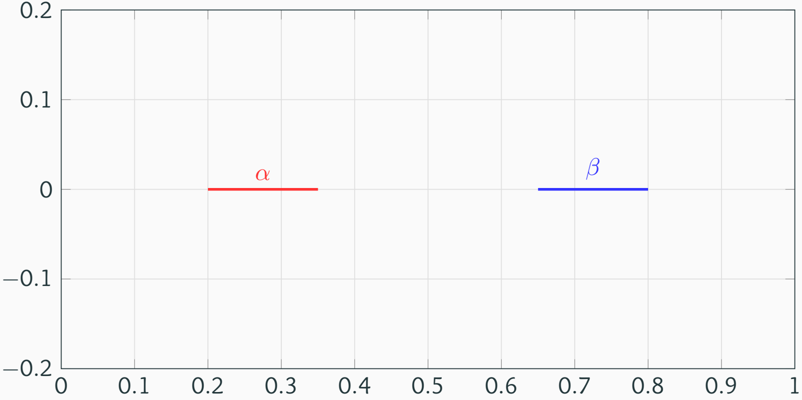
$$\begin{aligned} \mathrm{d}_k(\alpha, \beta) &= \| g \star \alpha - g \star \beta \|^2_{L^2} \\ &= \langle \alpha - \beta \mid k \star (\alpha - \beta) \rangle \\ &= -2 \sum_{i,j} k(x_i, y_j)\, \alpha_i \beta_j + \cdots \\ &= \langle \alpha - \beta \mid b^k - a^k \rangle \end{aligned}$$

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

The registration flows along the gradient of $b^k - a^k$

$$k(x-y) = \exp(-\|x-y\|^2/.2^2)$$



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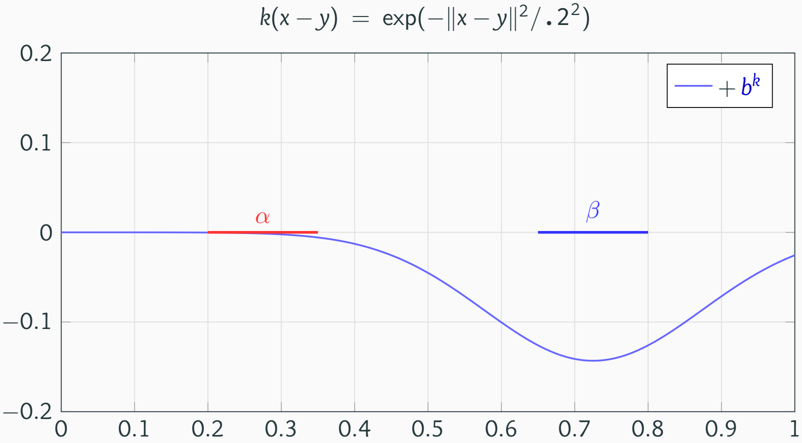

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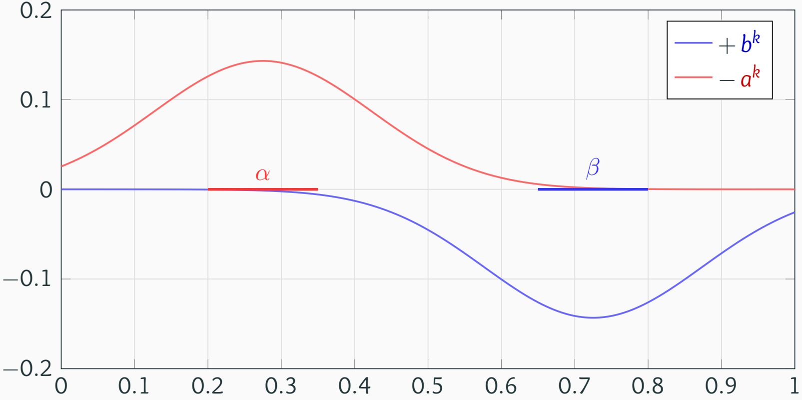

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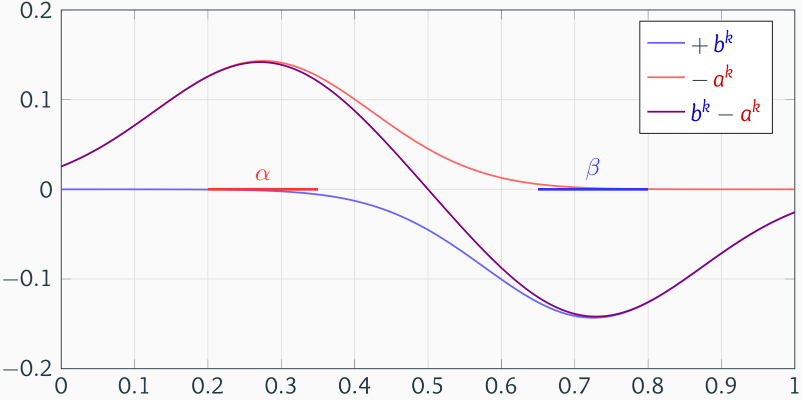

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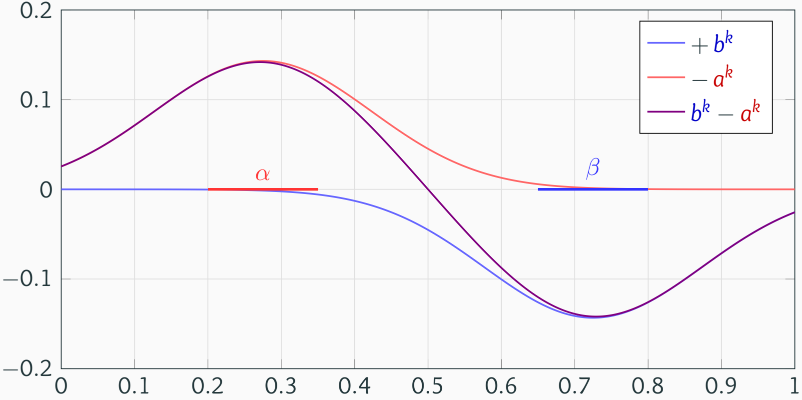

$$\mathrm{d}_k(\alpha,\beta) \;=\; \big\langle\, \alpha-\beta \,|\, k\star(\alpha-\beta)\,\big\rangle$$

$$\tfrac{1}{2}\nabla_{x_i}\mathrm{d}_k(\alpha,\beta) \;=\; \nabla\big[k\star(\alpha-\beta)\big](x_i) \;=\; \nabla b^k(x_i) - \nabla a^k(x_i)$$

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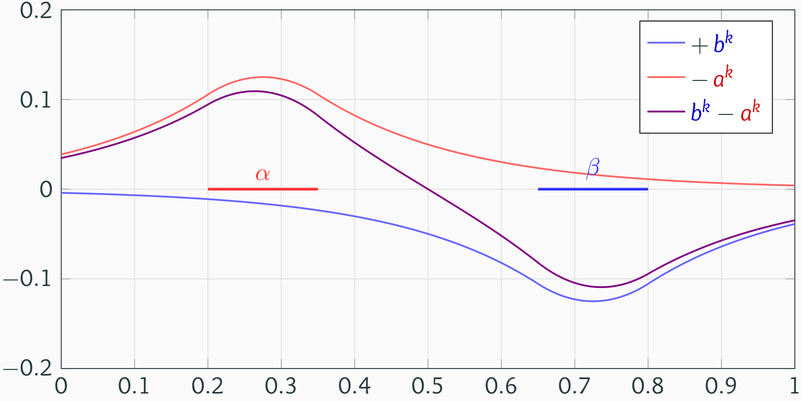

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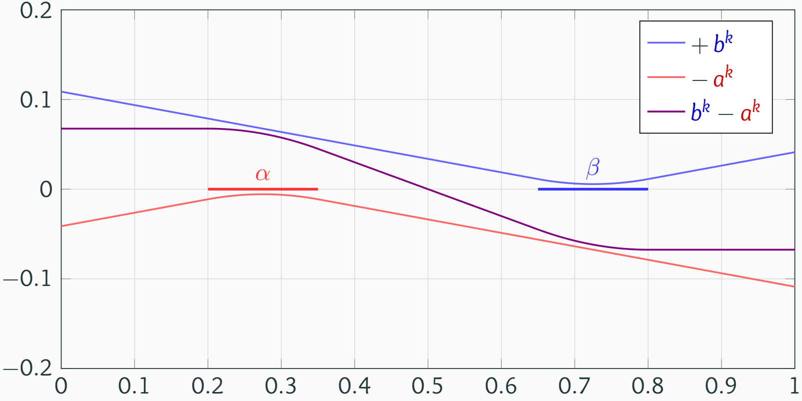

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The Energy Distance is scale-invariant, robust

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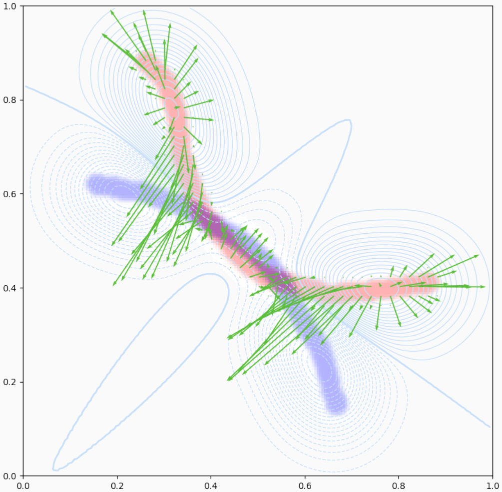

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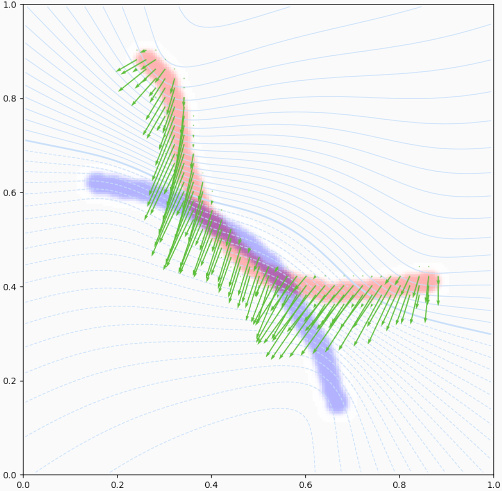

An idea from computer graphics: Hausdorff distances

Can we go further?

$$\begin{array}{c} \\ \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_N \end{array} \begin{array}{c} \begin{array}{cccc} \beta_1 & \beta_2 & \cdots & \beta_M \end{array} \\ \begin{pmatrix} \|x_1 - y_1\| & \|x_1 - y_2\| & \cdots & \|x_1 - y_M\| \\ \|x_2 - y_1\| & \|x_2 - y_2\| & \cdots & \|x_2 - y_M\| \\ \vdots & \vdots & \ddots & \vdots \\ \|x_N - y_1\| & \|x_N - y_2\| & \cdots & \|x_N - y_M\| \end{pmatrix} \end{array}$$

Can we go further?

$$
\begin{array}{cc}
 & \begin{array}{cccc} \beta_1 & \beta_2 & \cdots & \beta_M \end{array} \\
\begin{array}{c} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_N \end{array} &
\begin{pmatrix}
\|x_1 - y_1\| & \|x_1 - y_2\| & \cdots & \|x_1 - y_M\| \\
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\end{array}
$$

Can we go further?

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\begin{array}{c}
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\end{array}
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\begin{pmatrix}
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\vdots & \vdots & \ddots & \vdots \\
\|x_N - y_1\| & \|x_N - y_2\| & \cdots & \|x_N - y_M\|
\end{pmatrix}
\end{array}
\begin{array}{l}
 \\ \to \quad \sum_j \beta_j \|x_1 - y_j\| \\
\to \quad \sum_j \beta_j \|x_2 - y_j\| \\
\vdots \\
\to \quad \sum_j \beta_j \|x_N - y_j\|
\end{array}
$$

Energy Distance : $\sum_j \beta_j \|x_i - y_j\| = b^k(x_i)$

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\end{pmatrix}
\begin{array}{l}
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\end{array}
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Energy Distance : $\sum_j \beta_j \|x_i - y_j\| \quad = \quad b^k(x_i)$

Hausdorff Distance : $\min_j \|x_i - y_j\| \quad = \quad d(x_i, \mathrm{supp}(\beta))$

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$$
\begin{array}{cc}
 & \begin{array}{cccc} \beta_1 & \beta_2 & \cdots & \beta_M \end{array} \\
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\begin{pmatrix}
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\end{pmatrix}
\begin{array}{cl}
\rightarrow & \mathrm{Smin}_{\varepsilon, y\sim\beta} \|x_1 - y\| \\
\rightarrow & \mathrm{Smin}_{\varepsilon, y\sim\beta} \|x_2 - y\| \\
\vdots & \\
\rightarrow & \mathrm{Smin}_{\varepsilon, y\sim\beta} \|x_N - y\|
\end{array}
\end{array}
$$

Energy Distance	:	$\sum_j \beta_j \, \|x_i - y_j\|$	$=$	$b^k(x_i)$
ε-SoftMin	:	$\mathrm{Smin}_{\varepsilon, y\sim\beta} \, \|x_i - y\,\|$	$=$	$b^\varepsilon(x_i)$
Hausdorff Distance	:	$\min_j \, \|x_i - y_j\|$	$=$	$\mathrm{d}(x_i, \mathrm{supp}(\beta))$

The log-sum-exp trick

$$\log(e^{c_1} + e^{c_2}) = c_{\max} + \log\big(\underbrace{e^{c_1 - c_{\max}} + e^{c_2 - c_{\max}}}_{\in [1,2]}\big)$$

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Building on this, we define

$$b^{\varepsilon}(x) = \text{Smin}_{\varepsilon, y \sim \beta} \, \| x - y \|$$

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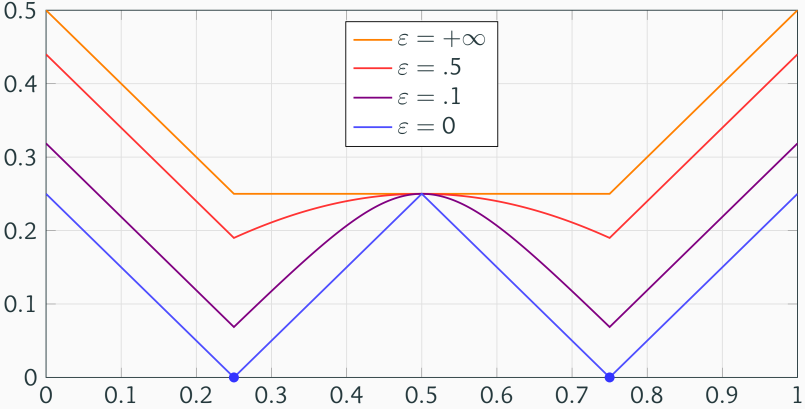
&\xrightarrow{\varepsilon \to +\infty} \sum_{j=1}^{M} \beta_j \, \|x - y_j\| \\
&\xrightarrow{\varepsilon \to 0} \min_j \|x - y_j\|
\end{aligned}$$

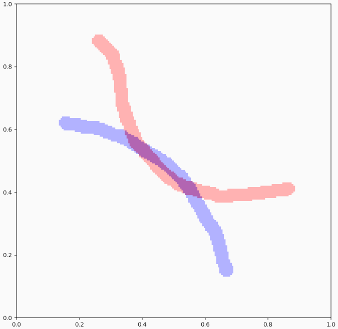
Smin_ε interpolates between a sum and a minimum

$x \mapsto \text{Smin}_{\varepsilon, y\sim\beta} |x - y|$, with $\beta = \frac{1}{2}\delta_{.25} + \frac{1}{2}\delta_{.75}$



The ε-SoftMin fidelity interpolates between ED and Hausdorff

$$\mathrm{d}_{\varepsilon\text{-SoftMin}}(\alpha, \beta) \quad = \quad \langle \alpha - \beta,\ b^{\varepsilon} - a^{\varepsilon} \rangle$$



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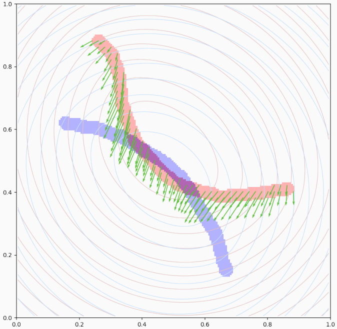

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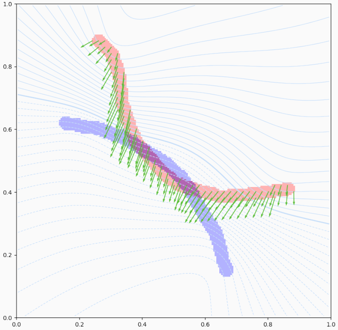

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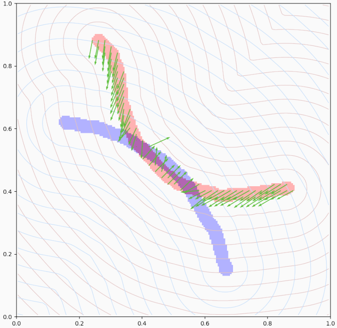
$$\xrightarrow{\varepsilon \to 0} \sum_i \alpha_i \min_{y \sim \beta} \|x_i - y\| \ + \ \sum_j \beta_j \min_{x \sim \alpha} \|x - y_j\|$$



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$$
\begin{aligned}
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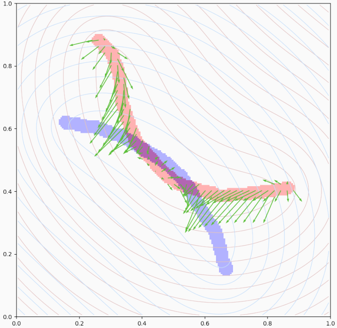

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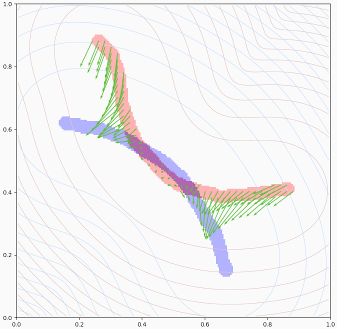
You can also use it with $C(x, y) = \|x - y\|^2$, etc.



Shape registration isn't *always* about naive projections...

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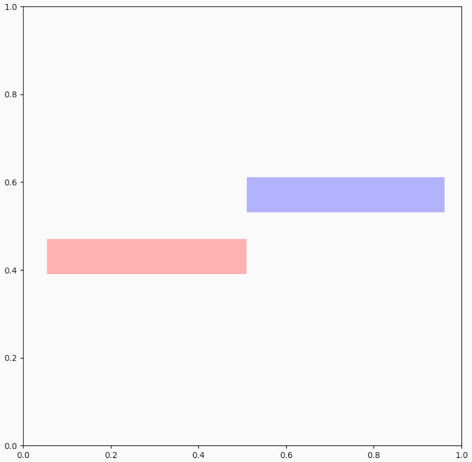

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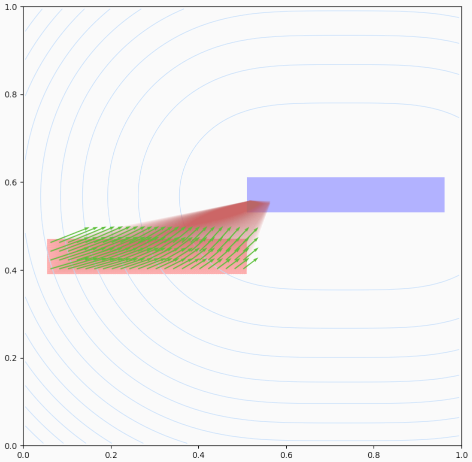

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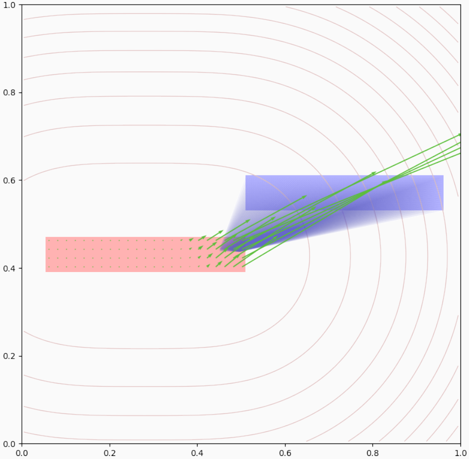

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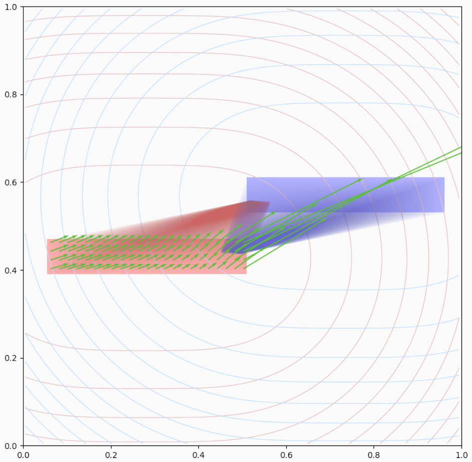

An idea from optimal transport theory: Sinkhorn and Wasserstein divergences

Optimal Transport = Hausdorff + mass repartition constraint

Computational Optimal Transport
[Cuturi, 2013, Peyré and Cuturi, 2018]:

Enforce a **mass repartition** constraint through alternating projections onto α and β.

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Baseline algorithm:

Use this **Sinkhorn** loop to compute $a^{\alpha\to\beta}$ and $b^{\beta\to\alpha}$.

Define $\mathcal{W}_\varepsilon(\alpha,\beta) = \langle\, \alpha\, ,\, b^{\beta\to\alpha}\, \rangle + \langle\, \beta\, ,\, a^{\alpha\to\beta}\, \rangle$

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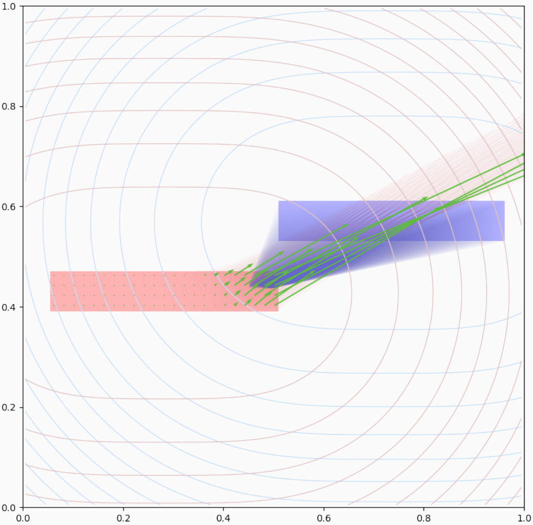
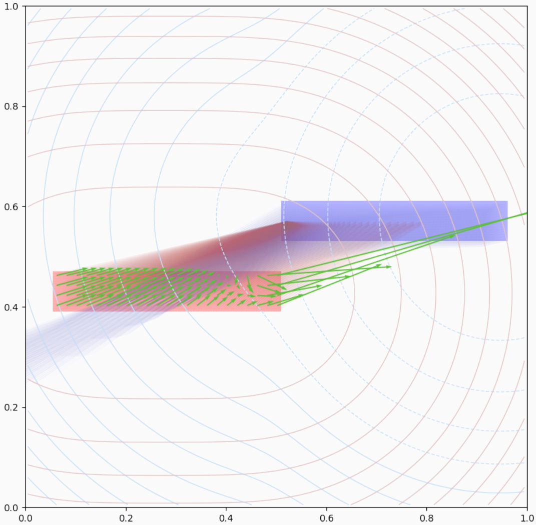
The core operation is still $\textbf{Smin}_\varepsilon$, for some $\varepsilon > 0$.

The Sinkhorn algorithm, in practice; $C(x, y) = \|x - y\|^2$, $\sqrt{\varepsilon} = .1$



Iteration 1/2

The Sinkhorn algorithm, in practice; $C(x,y) = \|x-y\|^2$, $\sqrt{\varepsilon} = .1$



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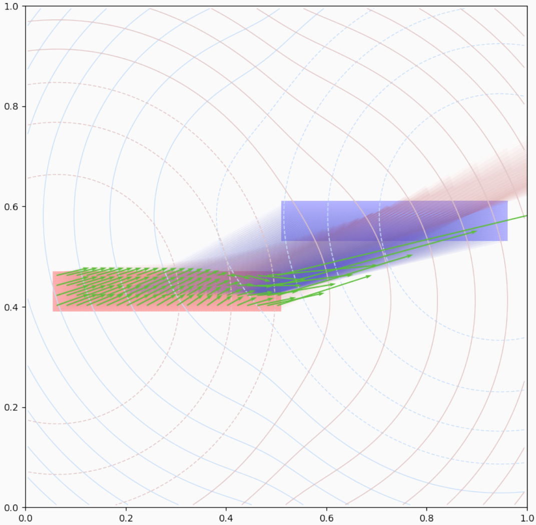
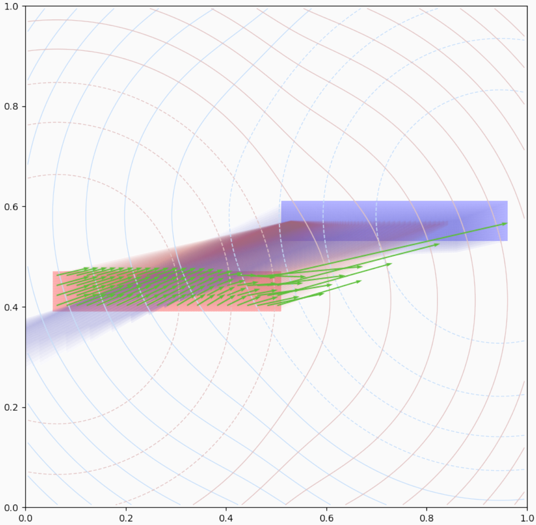


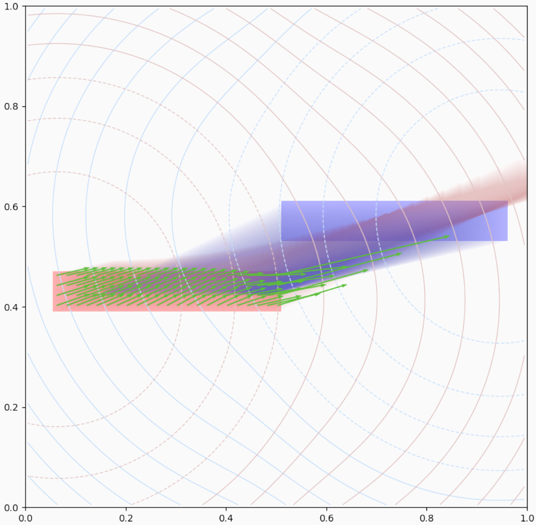
Iteration 1 ½

The Sinkhorn algorithm, in practice; $C(x, y) = \|x - y\|^2$, $\sqrt{\varepsilon} = .1$



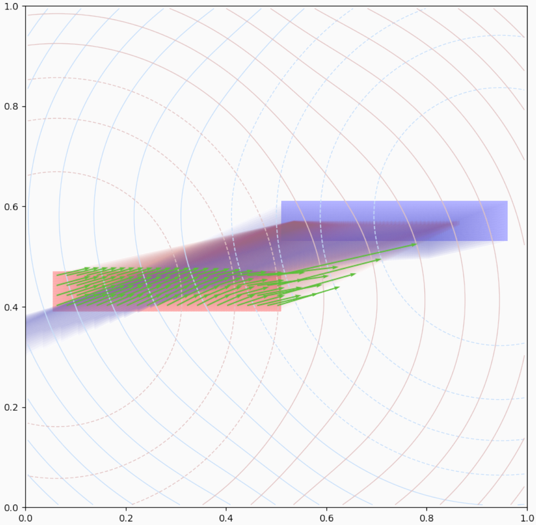
Iteration 2

The Sinkhorn algorithm, in practice; $C(x, y) = \|x - y\|^2$, $\sqrt{\varepsilon} = .1$



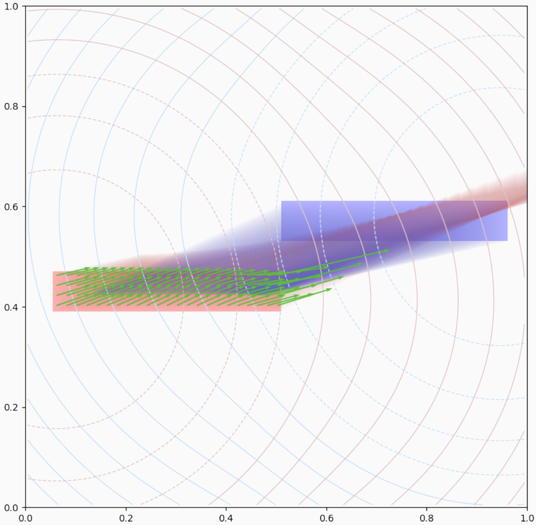
Iteration 2 ½

The Sinkhorn algorithm, in practice; $C(x,y) = \|x-y\|^2$, $\sqrt{\varepsilon} = .1$



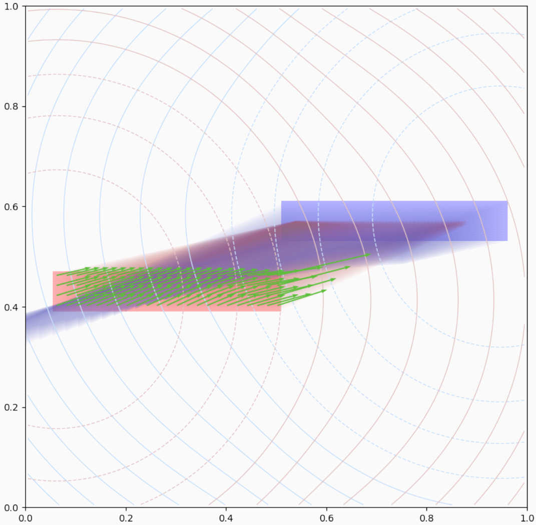
Iteration 3

The Sinkhorn algorithm, in practice; $C(x,y) = \|x-y\|^2$, $\sqrt{\varepsilon} = .1$



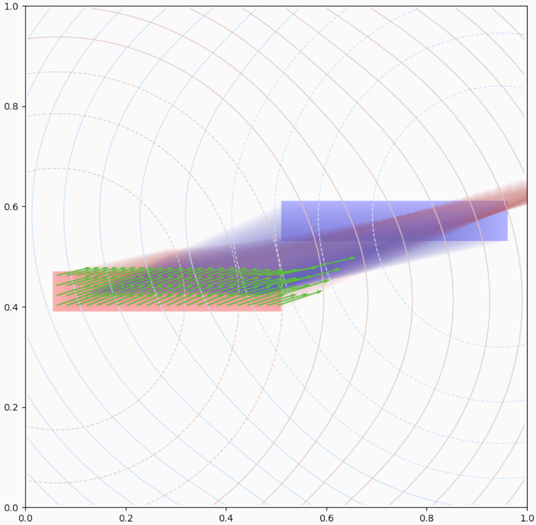
Iteration 3 ½

The Sinkhorn algorithm, in practice; $C(x,y) = \|x-y\|^2$, $\sqrt{\varepsilon} = .1$



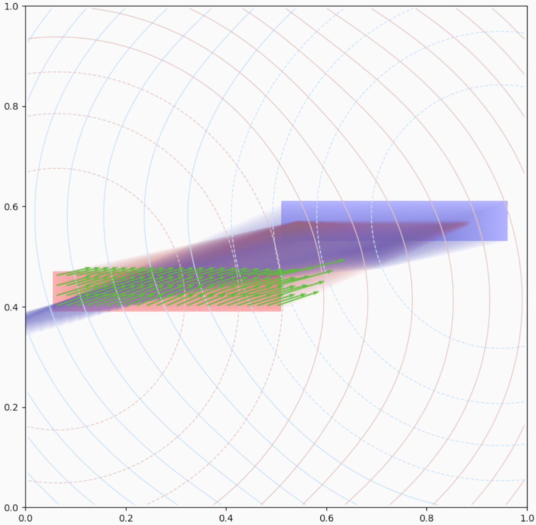
Iteration 4

The Sinkhorn algorithm, in practice; $C(x, y) = \|x - y\|^2$, $\sqrt{\varepsilon} = .1$

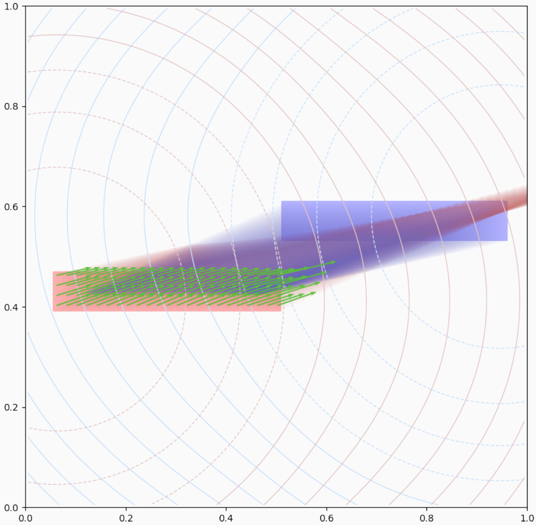


Iteration 4 ½

The Sinkhorn algorithm, in practice; $C(x,y) = \|x-y\|^2$, $\sqrt{\varepsilon} = .1$

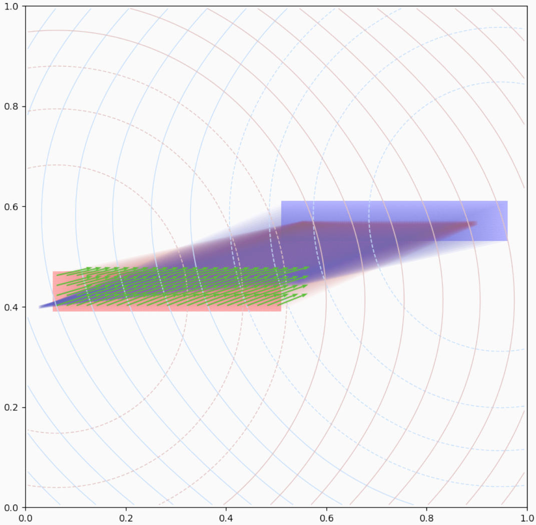


Iteration 5



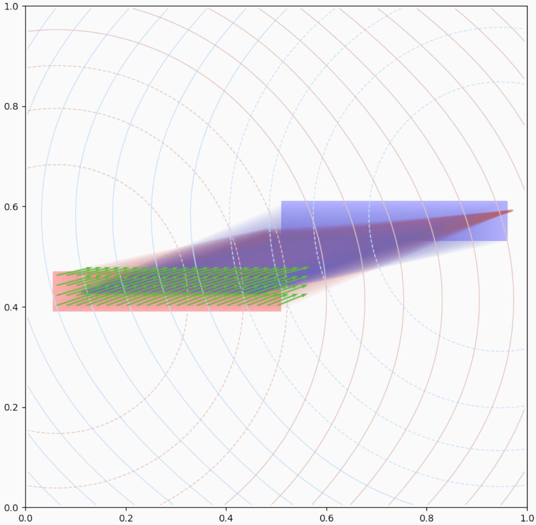
Iteration 5 ½

The Sinkhorn algorithm, in practice; $C(x,y) = \|x-y\|^2$, $\sqrt{\varepsilon} = .1$



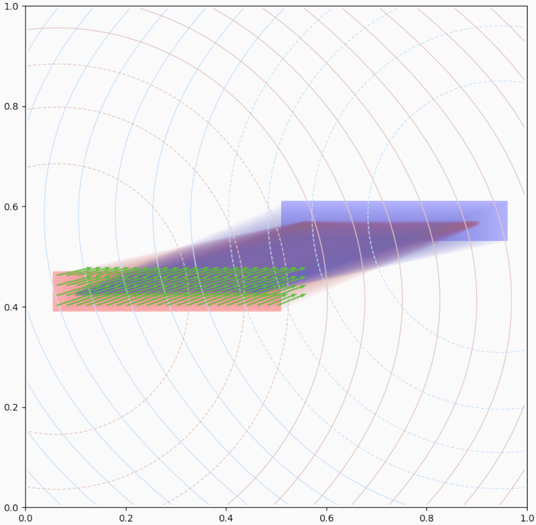
Iteration 10

The Sinkhorn algorithm, in practice; $C(x,y) = \|x-y\|^2$, $\sqrt{\varepsilon} = .1$



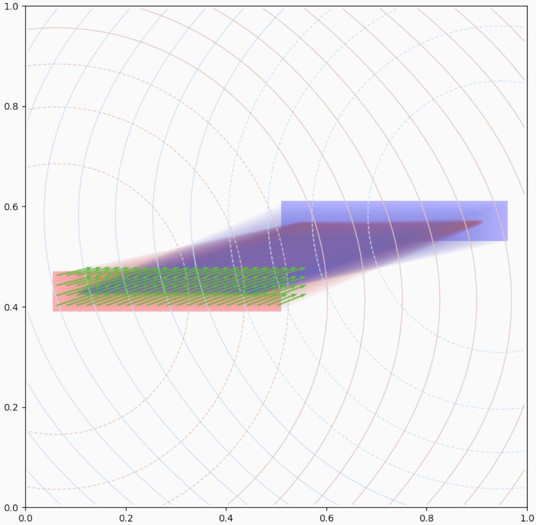
Iteration 10 ½

The Sinkhorn algorithm, in practice; $C(x,y) = \|x-y\|^2$, $\sqrt{\varepsilon} = .1$



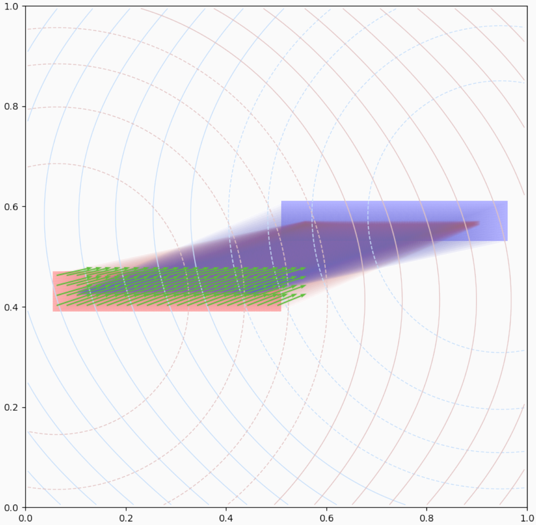
Iteration 20

The Sinkhorn algorithm, in practice; $C(x,y) = \|x-y\|^2$, $\sqrt{\varepsilon} = .1$



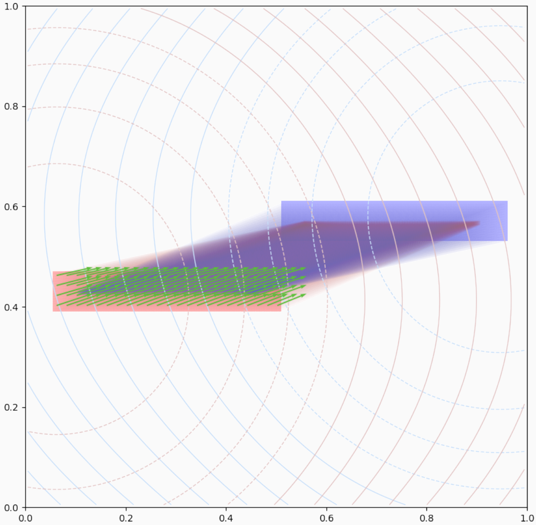
Iteration 20 ½

The Sinkhorn algorithm, in practice; $C(x,y) = \|x-y\|^2$, $\sqrt{\varepsilon} = .1$



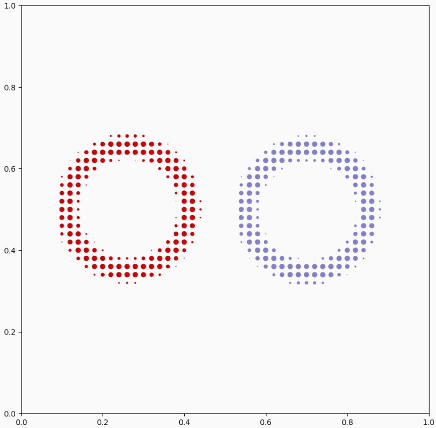
Iteration 30

The Sinkhorn algorithm, in practice; $C(x,y) = \|x-y\|^2$, $\sqrt{\varepsilon} = .1$

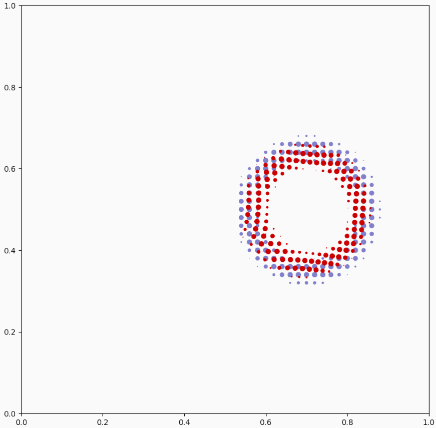


Iteration 30 ½

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



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



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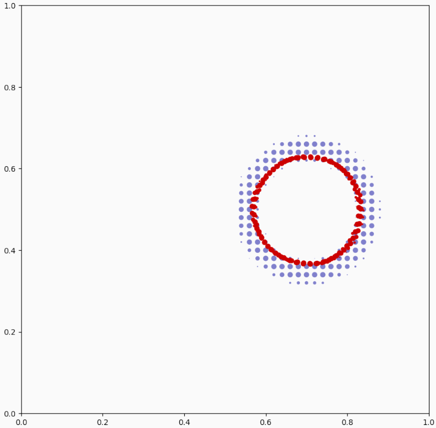
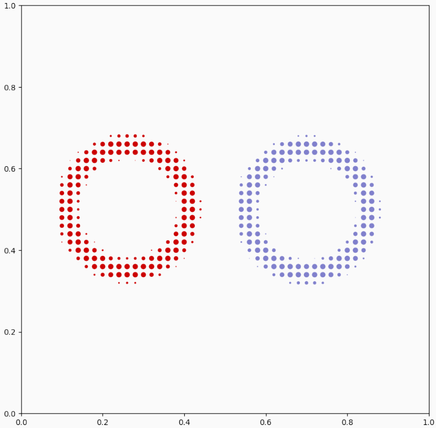
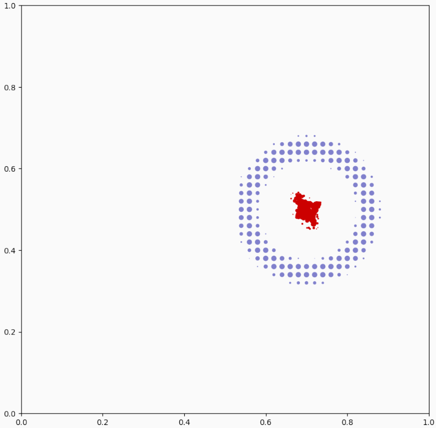


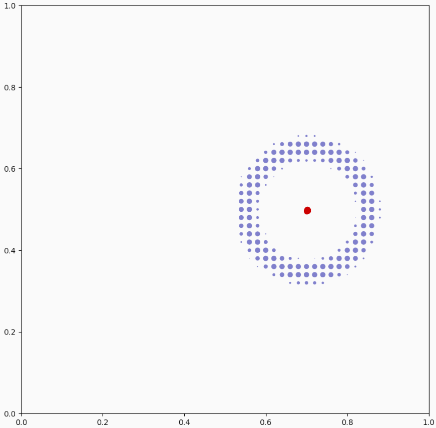
Registrating circles; $C(x, y) = \|x - y\|^2$, $\sqrt{\varepsilon} = 0.2$



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



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



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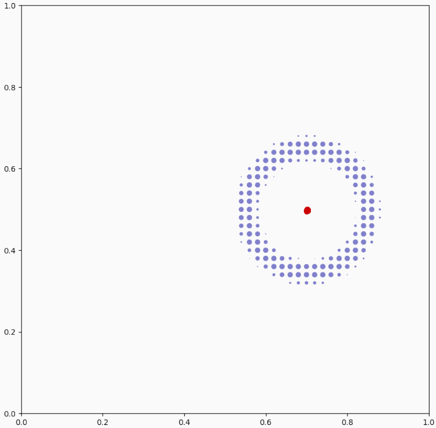

Bad news: for $0 < \varepsilon < +\infty$, we converge towards α such that

$$\mathcal{W}_\varepsilon(\alpha, \beta) \;<\; \mathcal{W}_\varepsilon(\beta, \beta).$$

In our paper: theoretical guarantees

Solution: Use an unbiased divergence [Genevay et al., 2018]

$$\mathrm{d}_{\varepsilon\text{-Sinkhorn}}(\alpha, \beta) \;=\; \mathcal{W}_\varepsilon(\alpha, \beta) - \tfrac{1}{2}\mathcal{W}_\varepsilon(\alpha, \alpha) - \tfrac{1}{2}\mathcal{W}_\varepsilon(\beta, \beta).$$

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Theorem (Positivity ; F., Vialard)

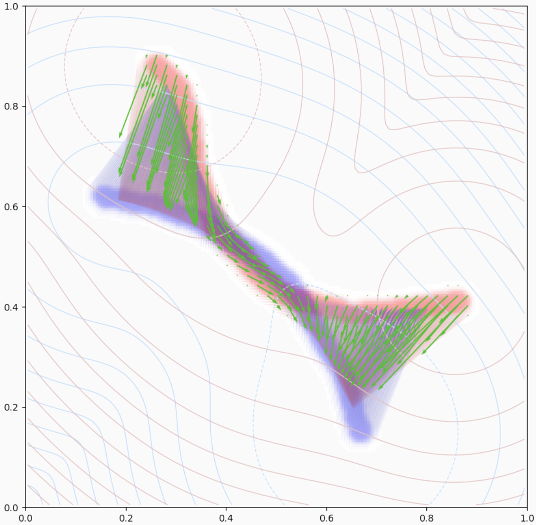
We define $\mathrm{d}_{\varepsilon\text{-Hausdorff}}(\alpha, \beta) \simeq \mathrm{d}_{\varepsilon\text{-SoftMin}}(\alpha, \beta)$. *Then, if*

$$k_\varepsilon(x, y) \;=\; \exp\big(-\tfrac{1}{\varepsilon}\mathrm{C}(x, y)\big)$$

defines a positive kernel, we have

$$0 \;\leqslant\; \mathrm{d}_{\varepsilon\text{-Hausdorff}}(\alpha, \beta) \;\leqslant\; \mathrm{d}_{\varepsilon\text{-Sinkhorn}}(\alpha, \beta).$$

The ε-Sinkhorn divergence; $C(x, y) = \|x - y\|^2$, $\sqrt{\varepsilon} = .1$



A high-quality gradient.

Conclusion

How do I implement this on real shapes?

$$
\begin{array}{c} \\ \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_N \end{array}
\begin{array}{c}
\begin{array}{cccc} \beta_1 & \beta_2 & \cdots & \beta_M \end{array} \\
\begin{pmatrix}
\|x_1 - y_1\| & \|x_1 - y_2\| & \cdots & \|x_1 - y_M\| \\
\|x_2 - y_1\| & \|x_2 - y_2\| & \cdots & \|x_2 - y_M\| \\
\vdots & \vdots & \ddots & \vdots \\
\|x_N - y_1\| & \|x_N - y_2\| & \cdots & \|x_N - y_M\|
\end{pmatrix}
\end{array}
\begin{array}{ll}
\\
\rightarrow & \text{Smin}_{\varepsilon, y\sim\beta} \|x_1 - y\| \\
\rightarrow & \text{Smin}_{\varepsilon, y\sim\beta} \|x_2 - y\| \\
\vdots & \\
\rightarrow & \text{Smin}_{\varepsilon, y\sim\beta} \|x_N - y\|
\end{array}
$$

How do I implement this on real shapes?

$$\begin{array}{c} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_N \end{array}
\overset{\begin{array}{cccc} \beta_1 & \beta_2 & \cdots & \beta_M \end{array}}{\begin{pmatrix}
\|x_1 - y_1\| & \|x_1 - y_2\| & \cdots & \|x_1 - y_M\| \\
\|x_2 - y_1\| & \|x_2 - y_2\| & \cdots & \|x_2 - y_M\| \\
\vdots & \vdots & \ddots & \vdots \\
\|x_N - y_1\| & \|x_N - y_2\| & \cdots & \|x_N - y_M\|
\end{pmatrix}}
\begin{array}{l} \rightarrow \quad \text{Smin}_{\varepsilon, y \sim \beta} \|x_1 - y\| \\ \rightarrow \quad \text{Smin}_{\varepsilon, y \sim \beta} \|x_2 - y\| \\ \vdots \\ \rightarrow \quad \text{Smin}_{\varepsilon, y \sim \beta} \|x_N - y\| \end{array}$$

Huge 100,000-by-100,000 matrices just don't fit into GPU memories.

How do I implement this on real shapes?

$$
\begin{array}{c}
 \\ \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_N
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\begin{pmatrix}
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\|x_2 - y_1\| & \|x_2 - y_2\| & \cdots & \|x_2 - y_M\| \\
\vdots & \vdots & \ddots & \vdots \\
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\begin{array}{l}
 \\ \to \quad \mathrm{Smin}_{\varepsilon, y\sim\beta} \|x_1 - y\| \\
\to \quad \mathrm{Smin}_{\varepsilon, y\sim\beta} \|x_2 - y\| \\
\vdots \\
\to \quad \mathrm{Smin}_{\varepsilon, y\sim\beta} \|x_N - y\|
\end{array}
$$

Huge 100,000-by-100,000 matrices just don’t fit into GPU memories.

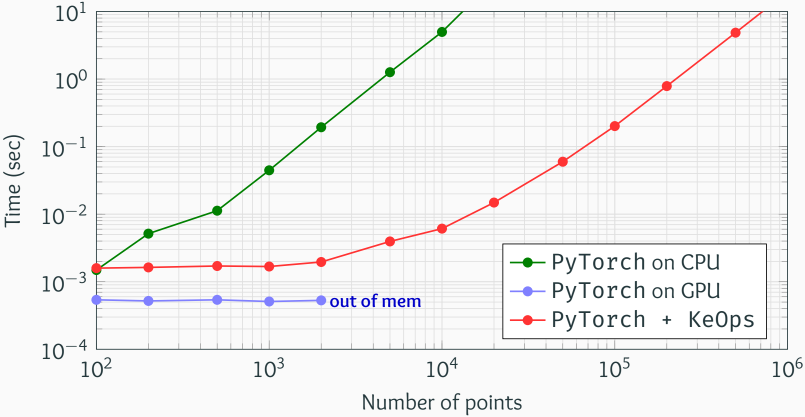
We need online map-reduce routines.

KErnel OPerationS, with autodiff, without memory overflows

$\Longrightarrow$ `pip install pykeops` $\Longleftarrow$

(Thanks Benjamin and Joan!)

Time needed to compute an N-by-N Gaussian convolution in $\mathbb{R}^3$



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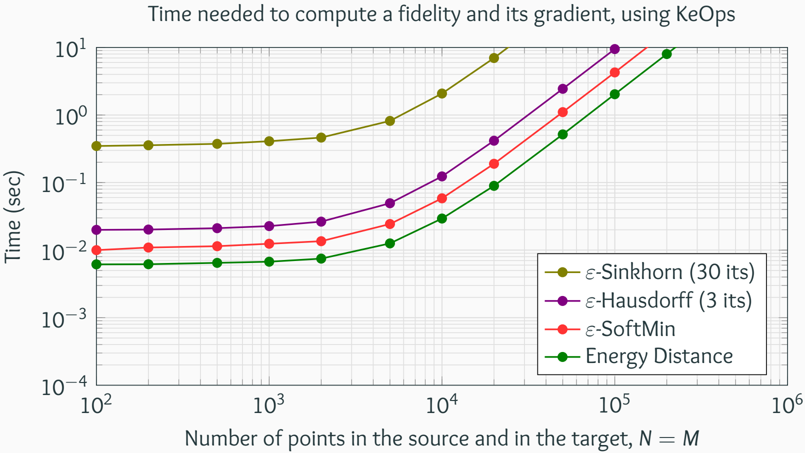
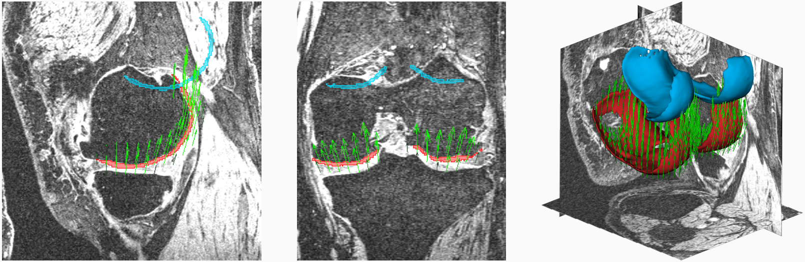


On real data, from the OsteoArthritris Initiative



Gradient of the Energy Distance, computed in 0.5s on my laptop.
(52,319 and 34,966 voxels – out of a 192-192-160 volume)

Conclusion

- Try using $k(x, y) = -\|x - y\|$!

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Our contributions:

- Statistics $\longleftrightarrow$ Computer Graphics $\longleftrightarrow$ Optimal Transport

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- New ε-**Hausdorff** fidelity, metric entropy.

Conclusion

- Try using $k(x, y) = -\|x - y\|$!

Our contributions:

- Statistics $\longleftrightarrow$ Computer Graphics $\longleftrightarrow$ Optimal Transport
- New ε-**Hausdorff** fidelity, metric entropy.
- First proof that the ε-Sinkhorn divergence (from ML) is **positive**.

Conclusion

- Try using $k(x,y) \;=\; -\|x-y\|$!

Our contributions:

- Statistics $\longleftrightarrow$ Computer Graphics $\longleftrightarrow$ Optimal Transport
- New ε-**Hausdorff** fidelity, metric entropy.
- First proof that the ε-Sinkhorn divergence (from ML) is **positive**.
- **KeOps**: efficient online map-reduce routines

CUDA + Matlab, numpy, PyTorch

References

Our code is available:

`plmlab.math.cnrs.fr/jeanfeydy/shapes_toolbox`

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Our papers:

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- *Optimal Transport for diffeomorphic registration*, F., Charlier, Vialard, Peyré, 2017

Thank you for your attention.

Any questions ?

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