

Optimal transport with 3D shapes

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6th of December, 2023
SMAI-SIGMA day
Laboratoire Jacques-Louis Lions, Jussieu

Who am I?

Background in **mathematics** and **data sciences**:

2012–2016 ENS Paris, mathematics.

2014–2015 M2 mathematics, vision, learning at ENS Cachan.

2016–2019 PhD thesis in **medical imaging** with Alain Trouve at ENS Cachan.

2019–2021 **Geometric deep learning** with Michael Bronstein at Imperial College.

2021+ **Medical data analysis** in the HeKA INRIA team (Paris).

Hôpitaux
Inria Inserm
Universités



My main motivation

Develop **robust and efficient** software that **stimulates other researchers**:

1. Speed up **geometric machine learning** on GPUs:
⇒ **pyKeOps** library for distance and kernel matrices, 500k+ downloads.
2. Scale up **pharmacovigilance** to the full French population:
⇒ **survivalGPU**, a fast re-implementation of the R survival package.
3. Ease access to modern statistical **shape analysis**:
⇒ **GeomLoss**, truly scalable optimal transport in Python.
⇒ **scikit-shapes**, to be released soon.

Today's talk – assuming that you would enjoy some applied maths

1. The **optimal transport** problem.
2. Efficient discrete **solvers**.
3. **Applications** and **open** problems.

Optimal transport?

Optimal transport (OT) generalizes sorting to spaces of dimension D > 1

If $A = (x_1, \dots, x_N)$ and $B = (y_1, \dots, y_N)$
are two clouds of N points in \mathbb{R}^D , we define:

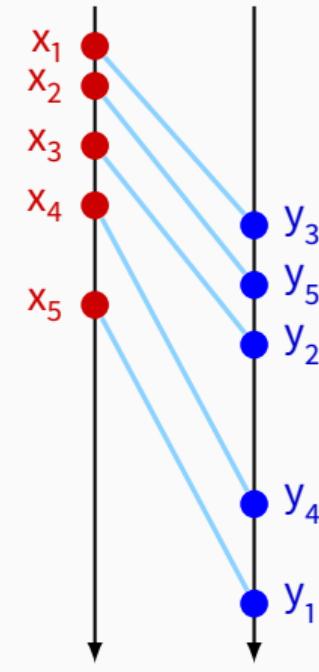
$$\text{OT}(A, B) = \min_{\sigma \in \mathcal{S}_N} \frac{1}{2N} \sum_{i=1}^N \|x_i - y_{\sigma(i)}\|^2$$

Generalizes **sorting** to metric spaces.

Linear problem on the permutation matrix P:

$$\text{OT}(A, B) = \min_{P \in \mathbb{R}^{N \times N}} \frac{1}{2N} \sum_{i,j=1}^N P_{i,j} \cdot \|x_i - y_j\|^2,$$

s.t. $P_{i,j} \geq 0$ $\underbrace{\sum_j P_{i,j} = 1}_{\text{Each source point...}}$ $\underbrace{\sum_i P_{i,j} = 1}_{\text{is transported onto the target.}}$



assignment
 $\sigma : [1, 5] \rightarrow [1, 5]$

Practical use

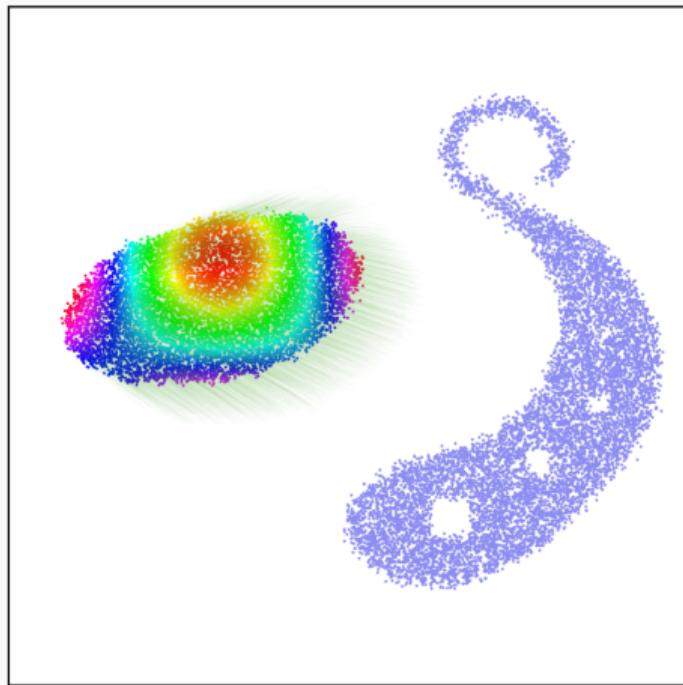
Alternatively, we understand OT as:

- Nearest neighbor **projection + incompressibility** constraint.
- Fundamental example of **linear optimization** over the transport plan $P_{i,j}$.

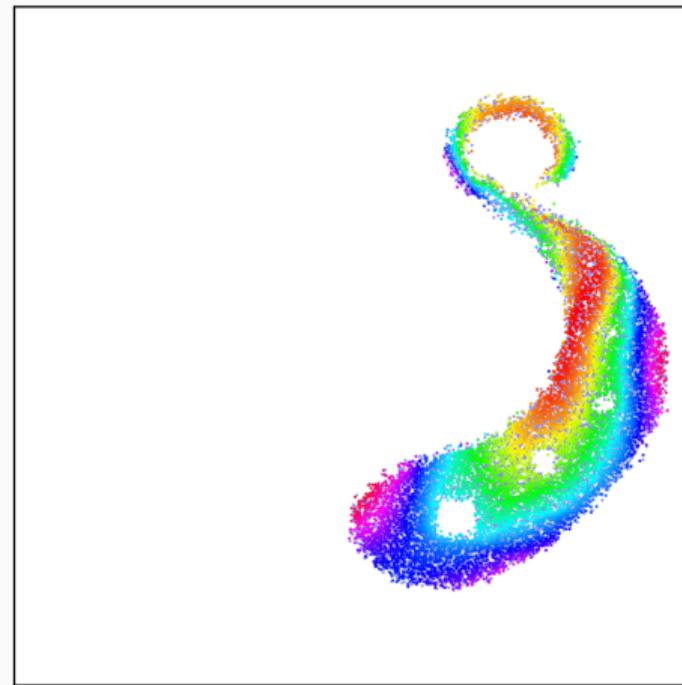
This theory induces two main quantities:

- The transport plan $P_{i,j} \simeq$ the optimal mapping $x_i \mapsto y_{\sigma(i)}$.
- The “Wasserstein” distance $\sqrt{OT(A, B)}$.

The optimal transport plan

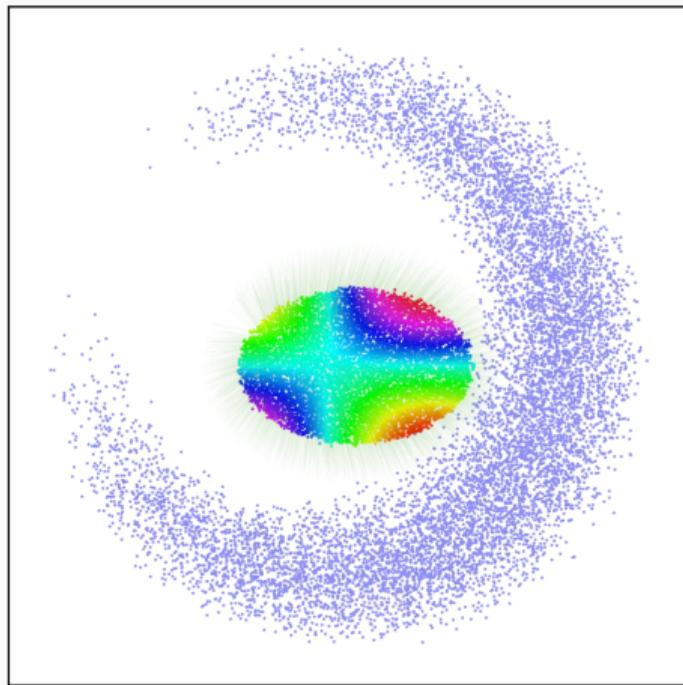


Before

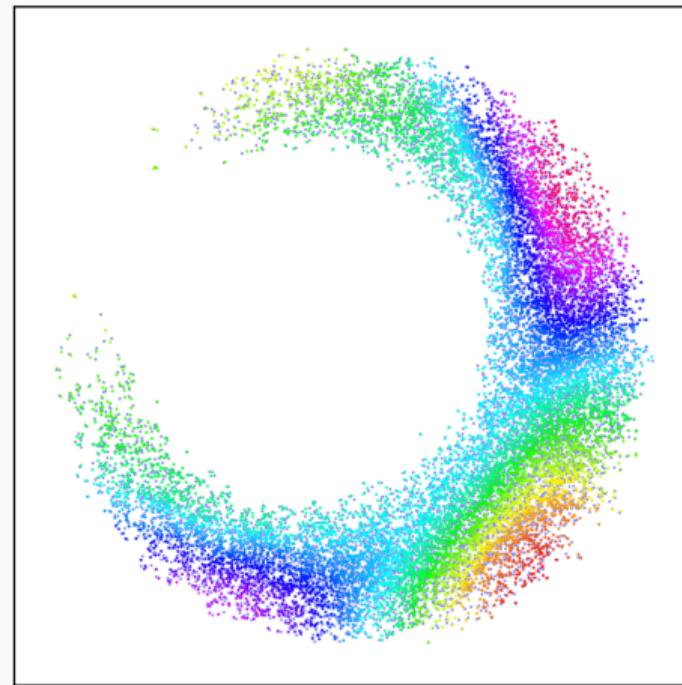


After

The optimal transport plan

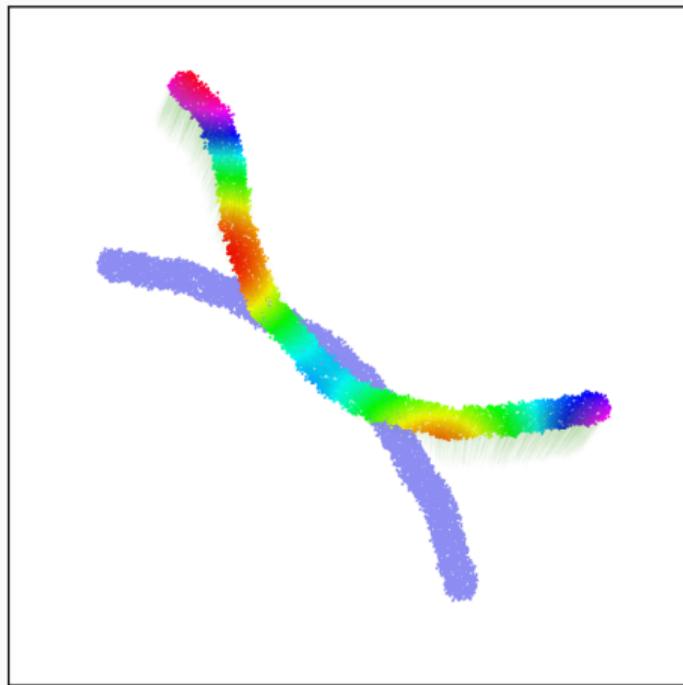


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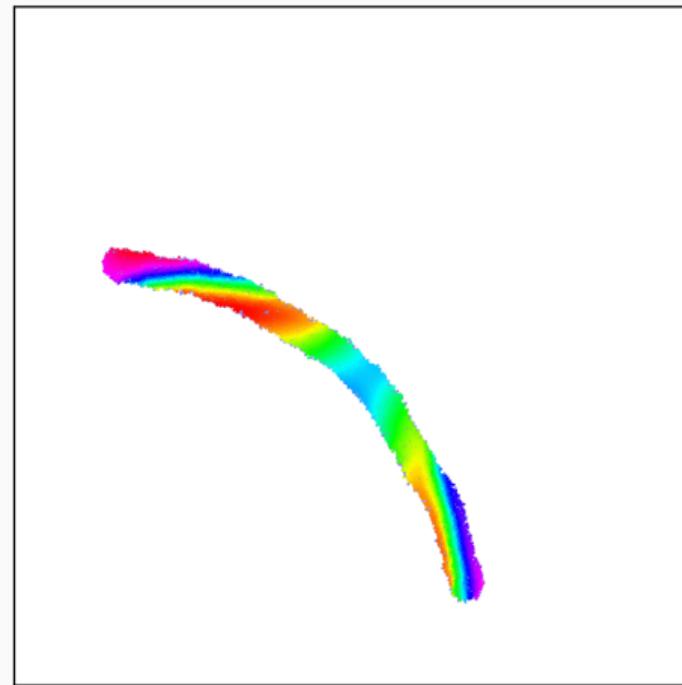


After

The optimal transport plan

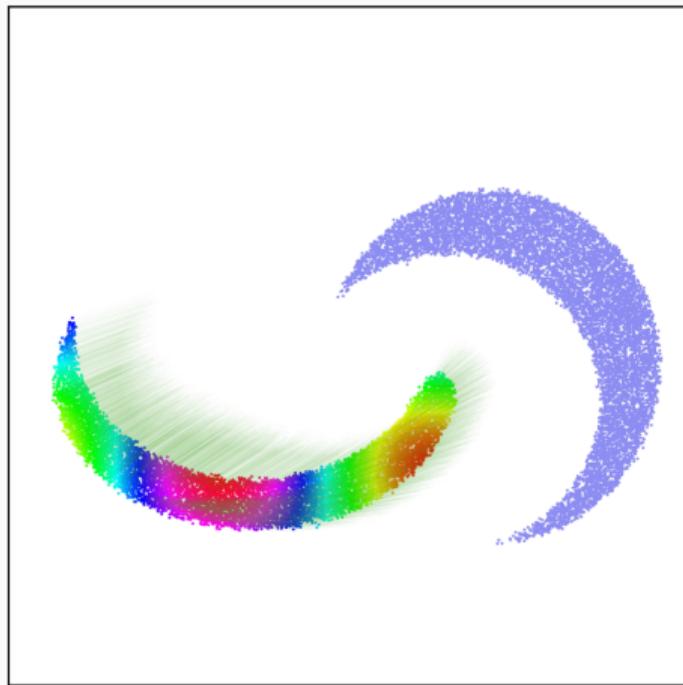


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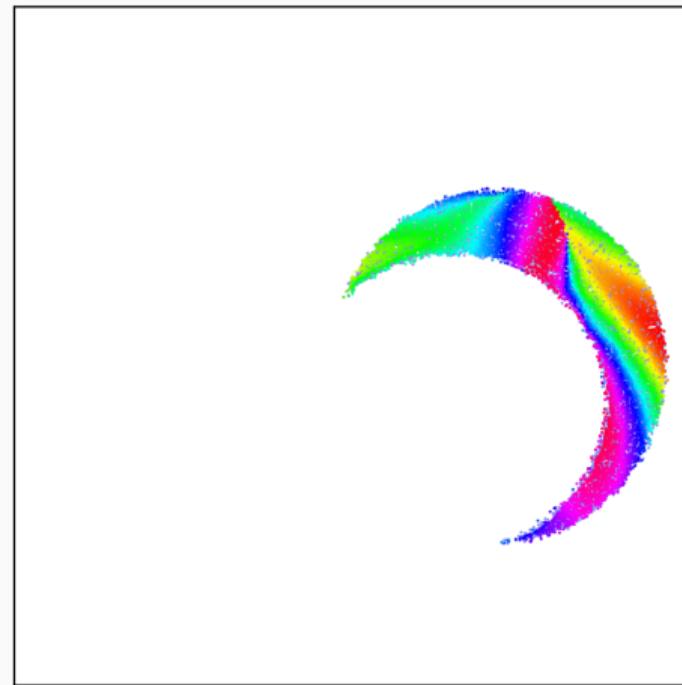


After

The optimal transport plan



Before

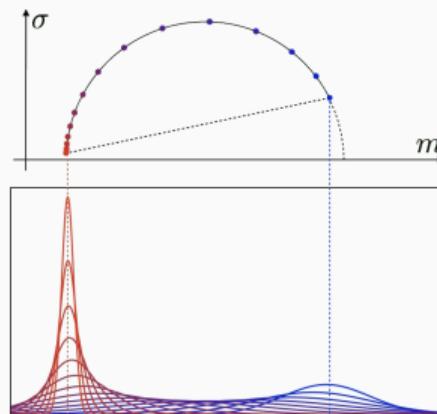


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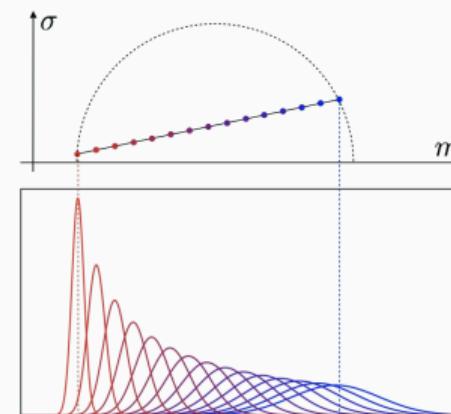
OT induces a geometry-aware distance between probability distributions [PC18]

Gauss map $\mathcal{N} : (m, \sigma) \in \mathbb{R} \times \mathbb{R}_{\geq 0} \mapsto \mathcal{N}(m, \sigma) \in \mathbb{P}(\mathbb{R})$.

If the space of **probability distributions** $\mathbb{P}(\mathbb{R})$ is endowed with a given metric,
what is the “pull-back” geometry on the space of **parameters** (m, σ) ?



Fisher-Rao (\simeq relative entropy) on $\mathcal{N}(m, \sigma)$
 \rightarrow Hyperbolic **Poincaré** metric on (m, σ) .



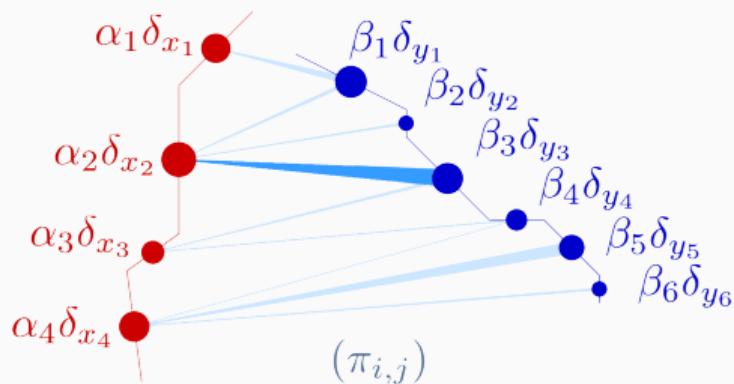
OT on $\mathcal{N}(m, \sigma)$
 \rightarrow Flat **Euclidean** metric on (m, σ) .

How should we solve the OT problem?

Duality: central planning with NM variables \simeq outsourcing with $N + M$ variables

$$\text{OT}(\mathbf{A}, \mathbf{B}) = \min_{\pi} \langle \pi, \mathbf{C} \rangle, \text{ with } \mathbf{C}(\mathbf{x}_i, \mathbf{y}_j) = \frac{1}{p} \|\mathbf{x}_i - \mathbf{y}_j\|^p \quad \rightarrow \text{ Assignment}$$

s.t. $\pi \geq 0, \quad \pi \mathbf{1} = \mathbf{A}, \quad \pi^\top \mathbf{1} = \mathbf{B}$

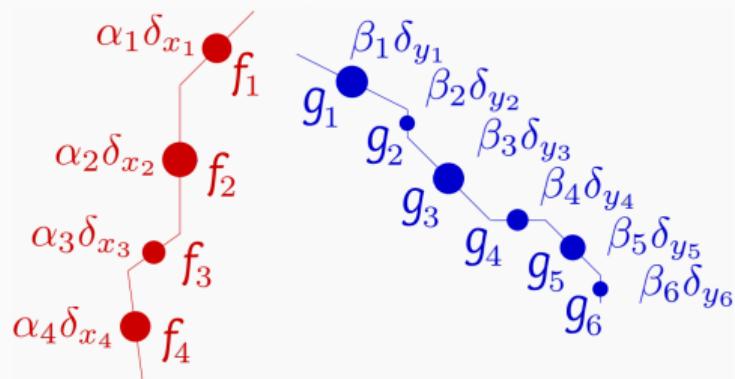


$$\sum_{i,j} \pi_{i,j} \mathbf{C}(\mathbf{x}_i, \mathbf{y}_j)$$

Duality: central planning with NM variables \simeq outsourcing with $N + M$ variables

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$$\sum_{i,j} \pi_{i,j} \mathbf{C}(\mathbf{x}_i, \mathbf{y}_j)$$

$$\max_{\mathbf{f}, \mathbf{g}} \quad \langle \mathbf{A}, \mathbf{f} \rangle + \langle \mathbf{B}, \mathbf{g} \rangle$$

s.t. $f(x_i) + g(y_j) \leq \mathbf{C}(\mathbf{x}_i, \mathbf{y}_j),$



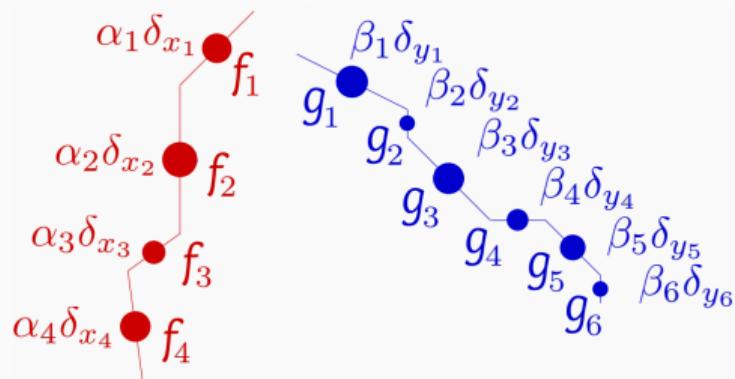
$$\sum_i \mathbf{A}_i f_i + \sum_j \mathbf{B}_j g_j$$

\rightarrow FedEx

Duality: central planning with NM variables \simeq outsourcing with $N + M$ variables

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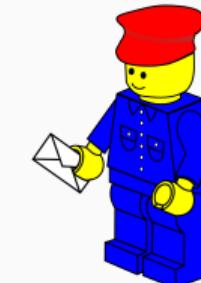
s.t. $\pi \geq 0, \quad \pi \mathbf{1} = \mathbf{A}, \quad \pi^\top \mathbf{1} = \mathbf{B}$



$$\sum_{i,j} \pi_{i,j} \mathbf{C}(\mathbf{x}_i, \mathbf{y}_j)$$

$$= \max_{\mathbf{f}, \mathbf{g}} \quad \langle \mathbf{A}, \mathbf{f} \rangle + \langle \mathbf{B}, \mathbf{g} \rangle$$

s.t. $f(x_i) + g(y_j) \leq \mathbf{C}(\mathbf{x}_i, \mathbf{y}_j),$



$$\sum_i \mathbf{A}_i f_i + \sum_j \mathbf{B}_j g_j$$

\rightarrow FedEx

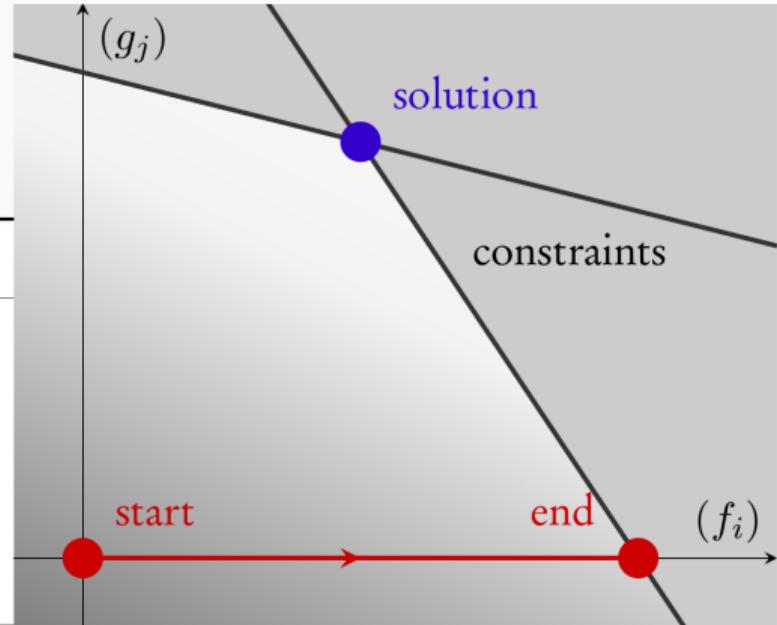
Being too greedy... doesn't work!

$$\text{OT}(\alpha, \beta) = \max_{\substack{(f_i) \in \mathbb{R}^N \\ (g_j) \in \mathbb{R}^M}} \sum_{i=1}^N \alpha_i f_i + \sum_{j=1}^M \beta_j g_j$$

s.t. $\forall i, j, f_i + g_j \leq \mathbf{C}(x_i, y_j)$

Algorithm 3.1: Naive greedy algorithm

- 1: $f_i, g_j \leftarrow \mathbf{0}_{\mathbb{R}^N}, \mathbf{0}_{\mathbb{R}^M}$
 - 2: **repeat**
 - 3: $f_i \leftarrow \min_{j=1}^M [\mathbf{C}(x_i, y_j) - g_j]$
 - 4: $g_j \leftarrow \min_{i=1}^N [\mathbf{C}(x_i, y_j) - f_i]$
 - 5: **until** convergence.
 - 6: **return** f_i, g_j
-



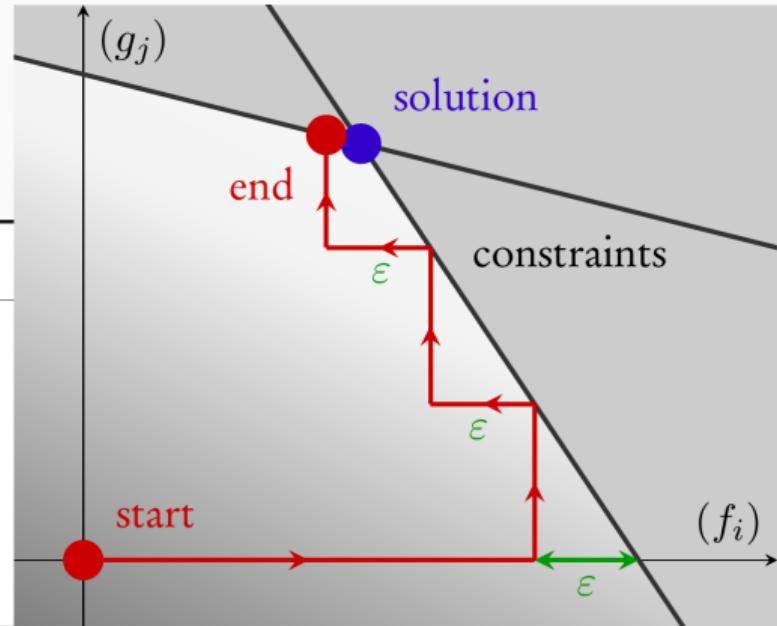
The auction algorithm: take it easy with a slackness $\varepsilon > 0$

$$\text{OT}(\alpha, \beta) = \max_{\substack{(f_i) \in \mathbb{R}^N \\ (g_j) \in \mathbb{R}^M}} \sum_{i=1}^N \alpha_i f_i + \sum_{j=1}^M \beta_j g_j$$

s.t. $\forall i, j, f_i + g_j \leq \mathbf{C}(x_i, y_j)$

Algorithm 3.2: Pseudo-auction algorithm

```
1:  $f_i, g_j \leftarrow \mathbf{0}_{\mathbb{R}^N}, \mathbf{0}_{\mathbb{R}^M}$ 
2: repeat
3:    $f_i \leftarrow \min_{j=1}^M [\mathbf{C}(x_i, y_j) - g_j] - \varepsilon$ 
4:    $g_j \leftarrow \min_{i=1}^N [\mathbf{C}(x_i, y_j) - f_i]$ 
5: until  $\forall i, \exists j, f_i + g_j \geq \mathbf{C}(x_i, y_j) - \varepsilon$ .
6: return  $f_i, g_j$ 
```



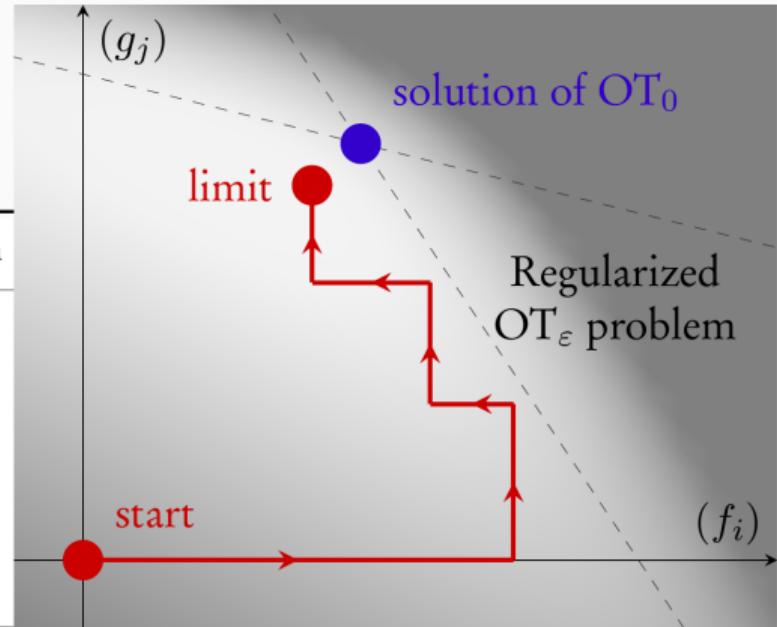
The Sinkhorn algorithm: use a softmin, get a well-defined optimum

$$\text{OT}(\alpha, \beta) = \max_{\substack{(f_i) \in \mathbb{R}^N \\ (g_j) \in \mathbb{R}^M}} \sum_{i=1}^N \alpha_i f_i + \sum_{j=1}^M \beta_j g_j$$

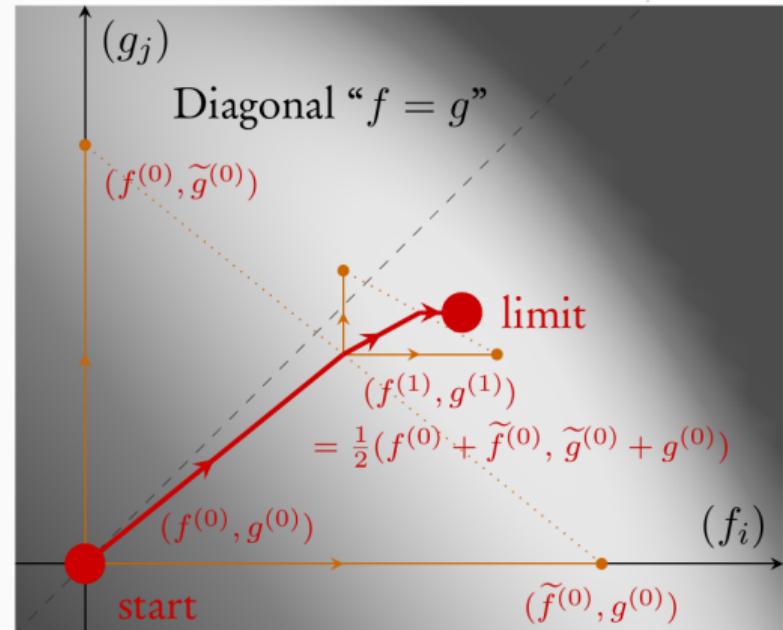
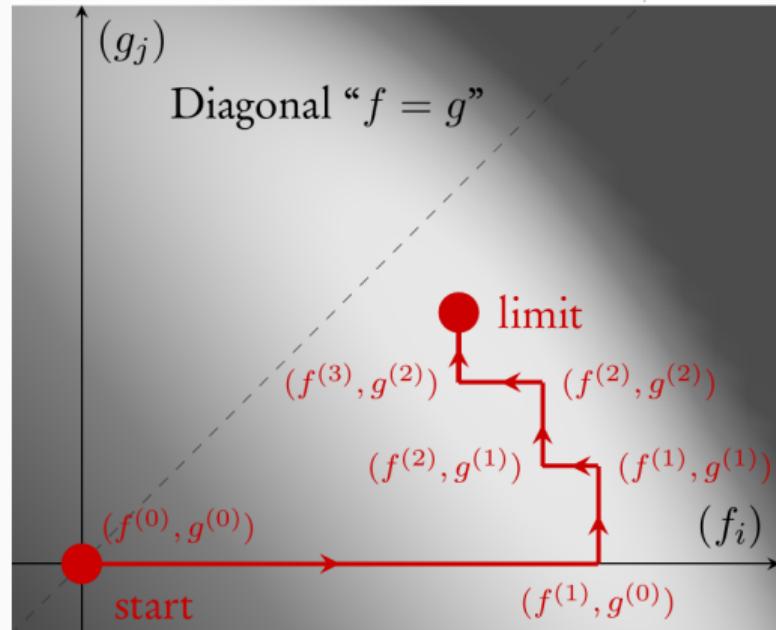
s.t. $\forall i, j, f_i + g_j \leq \mathbf{C}(x_i, y_j)$

Algorithm 3.3: Sinkhorn or “soft-auction” algorithm

- 1: $f_i, g_j \leftarrow \mathbf{0}_{\mathbb{R}^N}, \mathbf{0}_{\mathbb{R}^M}$
- 2: **repeat**
- 3: $f_i \leftarrow -\varepsilon \log \sum_{j=1}^M \beta_j \exp \frac{1}{\varepsilon} [g_j - \mathbf{C}(x_i, y_j)]$
- 4: $g_j \leftarrow -\varepsilon \log \sum_{i=1}^N \alpha_i \exp \frac{1}{\varepsilon} [f_i - \mathbf{C}(x_i, y_j)]$
- 5: **until** convergence up to a set tolerance.
- 6: **return** f_i, g_j



The symmetric Sinkhorn algorithm: stay close to the diagonal if $A \simeq B$



Remark 1: a streamlined algorithm

One key operation – the soft, **weighted distance transform**:

$$\forall i \in [1, N], \quad f(x_i) \leftarrow \min_{y \sim \beta} [\mathbf{C}(x_i, y) - g(y)] = -\varepsilon \log \sum_{j=1}^M \beta_j \exp \frac{1}{\varepsilon} [g_j - \mathbf{C}(x_i, y_j)].$$

Similar to the chamfer distance transform, convolution with a Gaussian kernel...

Fast implementations with **pyKeOps**:

- If $\mathbf{C}(x_i, y_j)$ is a closed formula: **bruteforce** scales to $N, M \simeq 100k$ in 10ms on a GPU.
- If **A** and **B** have a low-dimensional support:
use a clustering and **truncation** strategy to get a x10 speed-up.
- If **A** and **B** are supported on a 2D or 3D grid and $\mathbf{C}(x_i, y_j) = \frac{1}{2} \|x_i - y_j\|^2$:
use a **separable** distance transform to get a second x10 speed-up.
(N.B.: FFTs run into numerical accuracy issues.)

Remark 2: annealing works!

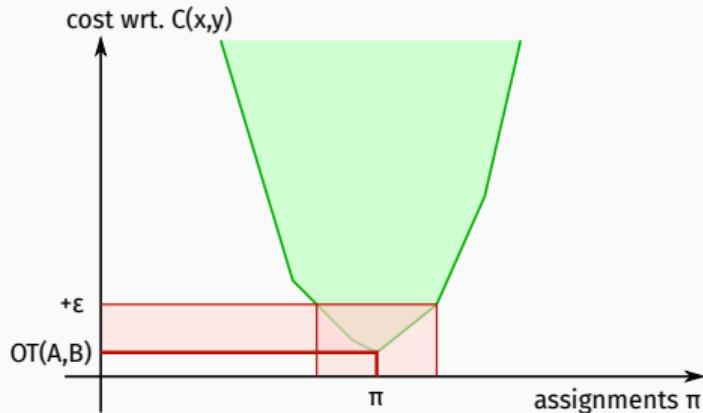
The **Auction/Sinkhorn** algorithms:

- Improve the dual cost by at least ε at each (early) step.
- Reach an ε -optimal solution with $(\max C) / \varepsilon$ steps.

Simple heuristic: run the optimization with **decreasing values** of ε .

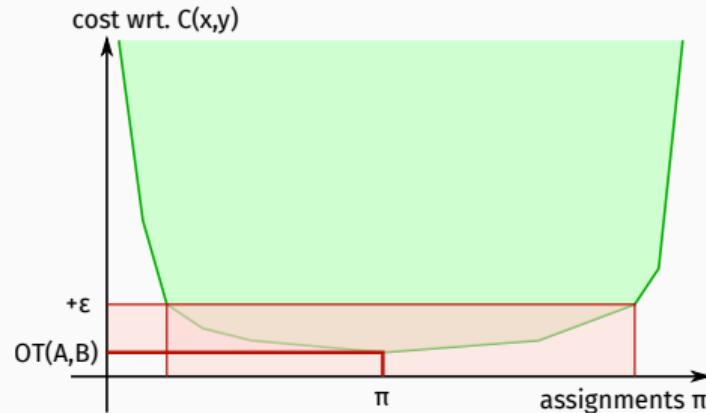
ε -scaling
= **simulated annealing**
= **multiscale** strategy
= **divide and conquer**

Remark 3: the curse of dimensionality



In **low dimension**:

- $\|x - y\|$ takes large and small values.
- The OT objective is **peaky** wrt. π .
- ε -optimal solutions are **useful**.
- $OT(\text{discrete samples}) \simeq OT(\text{underlying distributions})$



In **high dimension**:

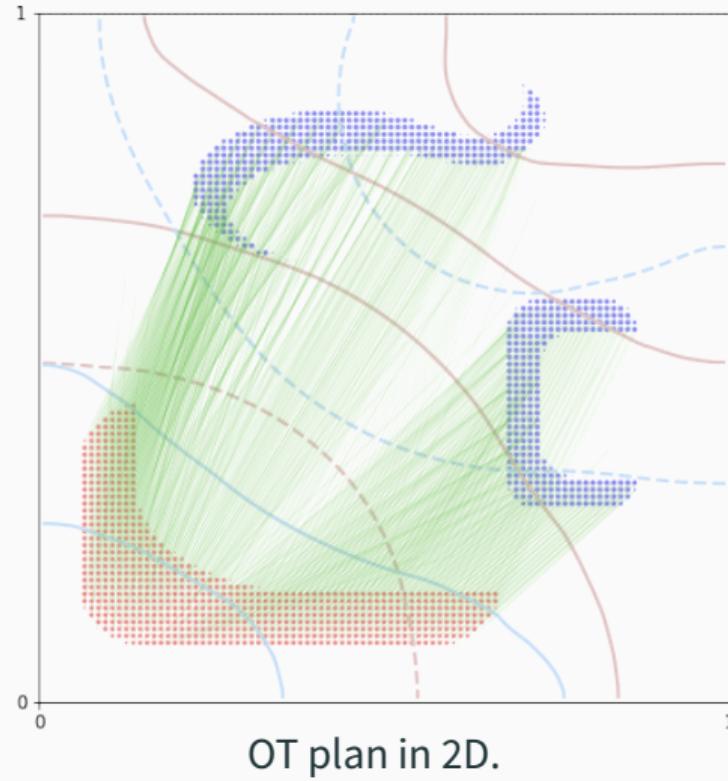
- $\|x - y\|$ gets closer to a constant.
- The OT objective is **flat** wrt. π .
- ε -optimal solutions are **random**.
- $OT(\text{discrete samples}) \neq OT(\text{underlying distributions})$

To recap 80+ years of work...

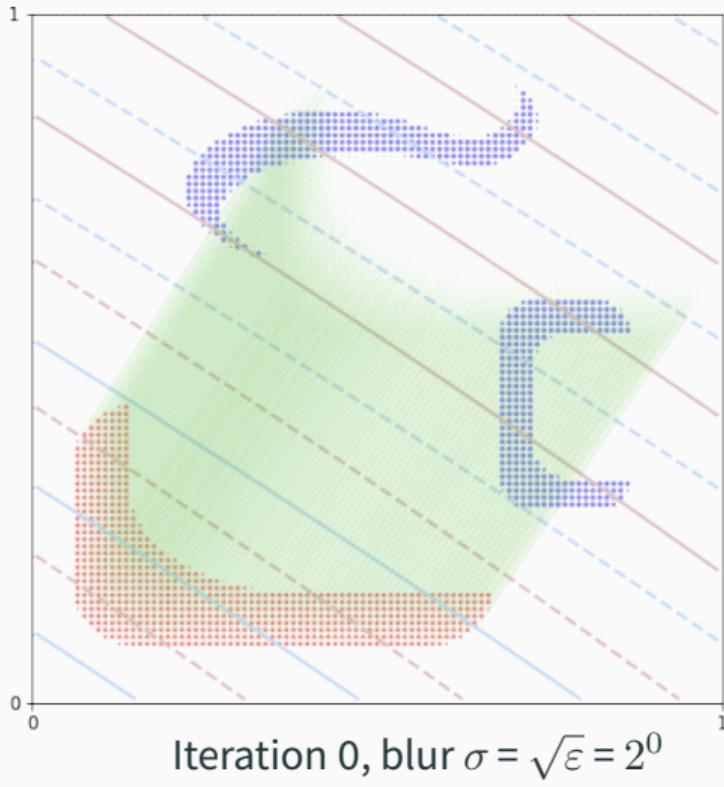
Key dates for discrete optimal transport with N points:

- [Kan42]: **Dual** problem of Kantorovitch.
- [Kuh55]: **Hungarian** methods in $O(N^3)$.
- [Ber79]: **Auction** algorithm in $O(N^2)$.
- [KY94]: **SoftAssign** = Sinkhorn + simulated annealing, in $O(N^2)$.
- [GRL⁺98, CR00]: **Robust Point Matching** = Sinkhorn as a loss.
- [Cut13]: Start of the **GPU era**.
- [Mér11, Lév15, Sch19]: **multi-scale** solvers in $O(N \log N)$.
- **Solution**, today: **Multiscale Sinkhorn algorithm, on the GPU**.
 ⇒ Generalized **QuickSort** algorithm.

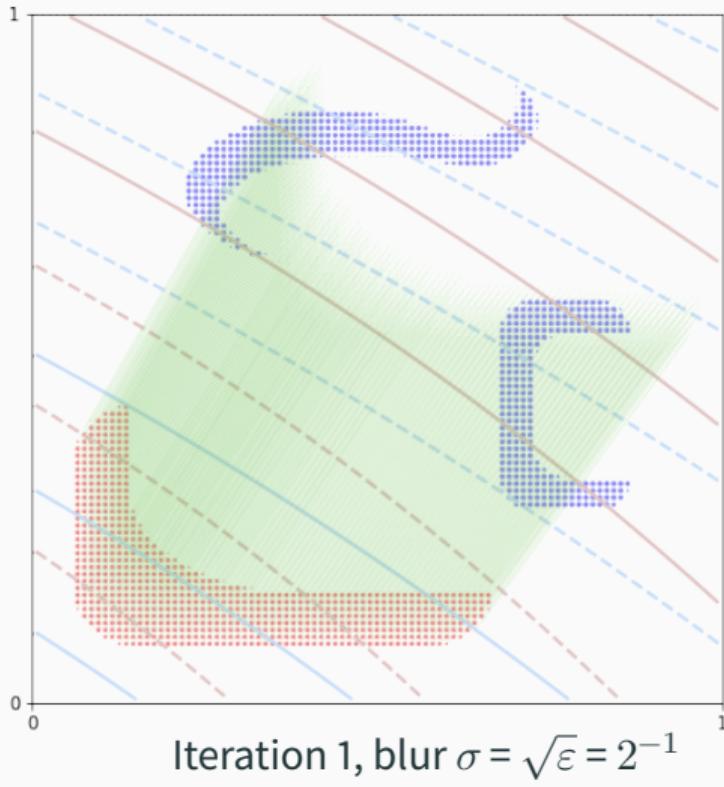
Visualizing F , G and the Brenier map $\nabla F(x_i) = -\frac{1}{\alpha_i} \partial_{x_i} \mathbf{OT}(\alpha, \beta)$



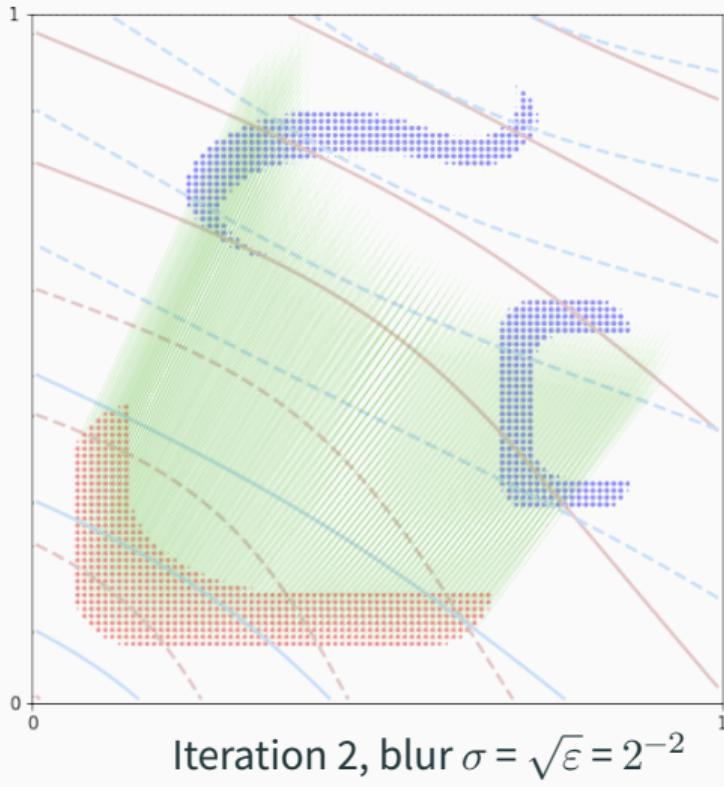
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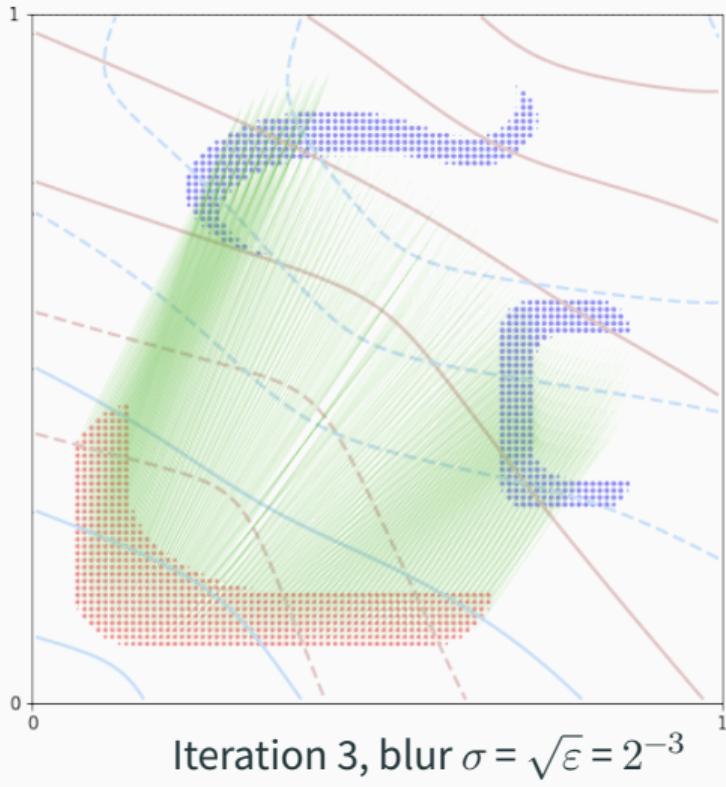
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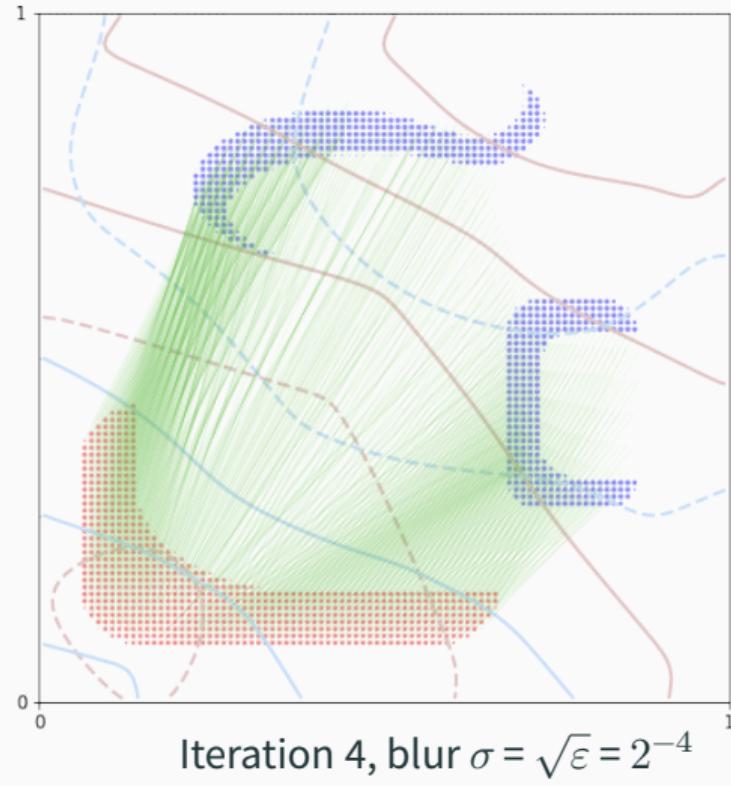
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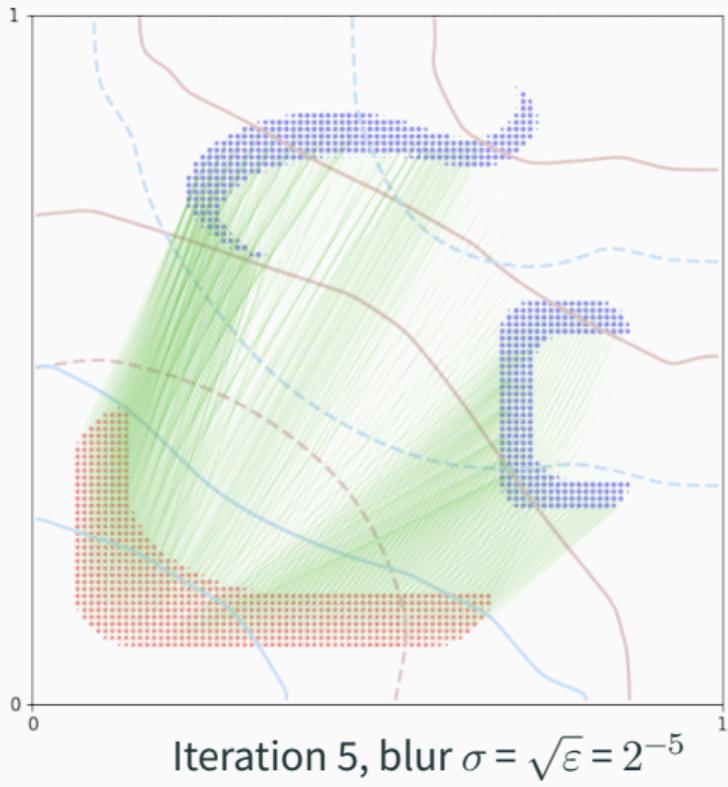
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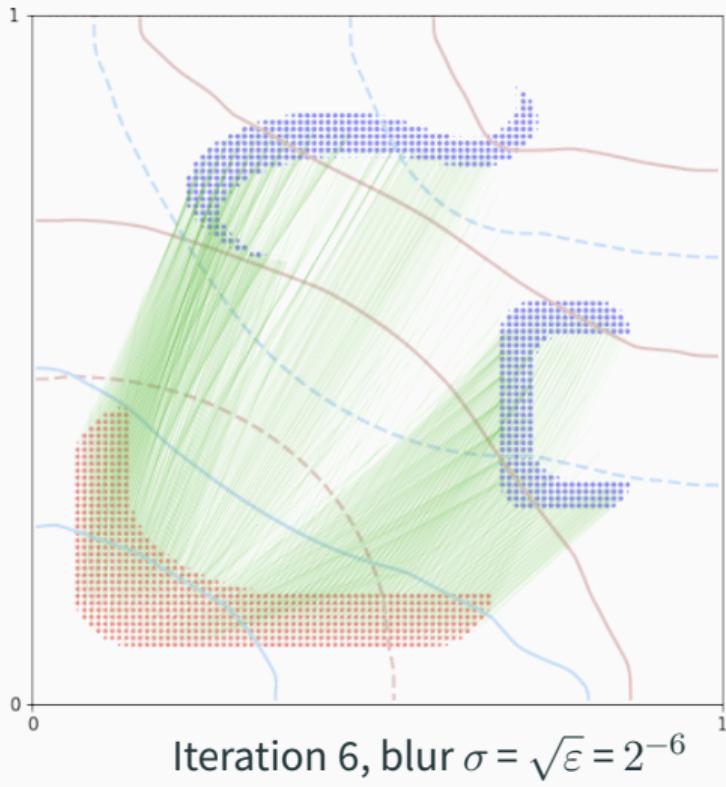
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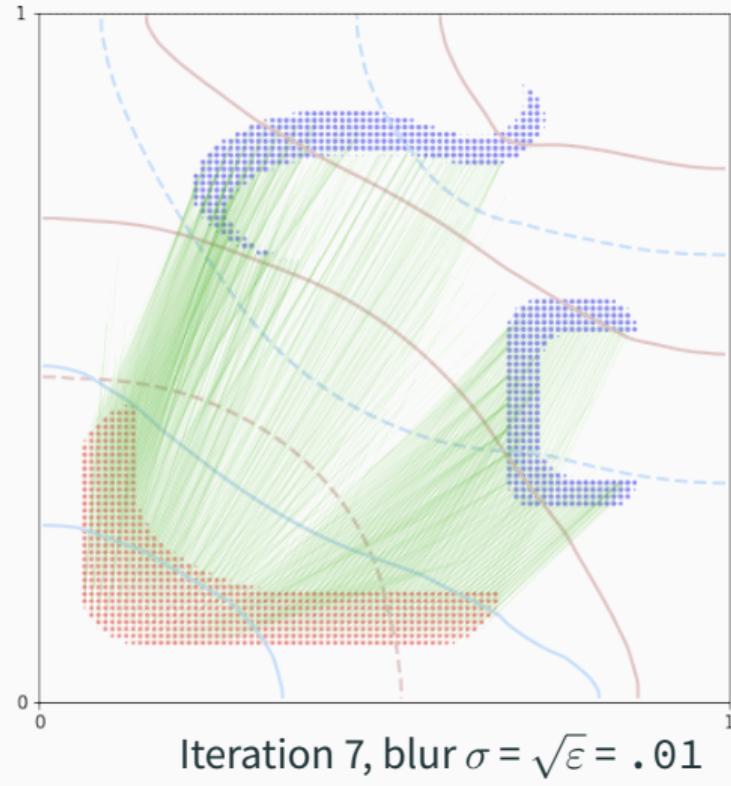
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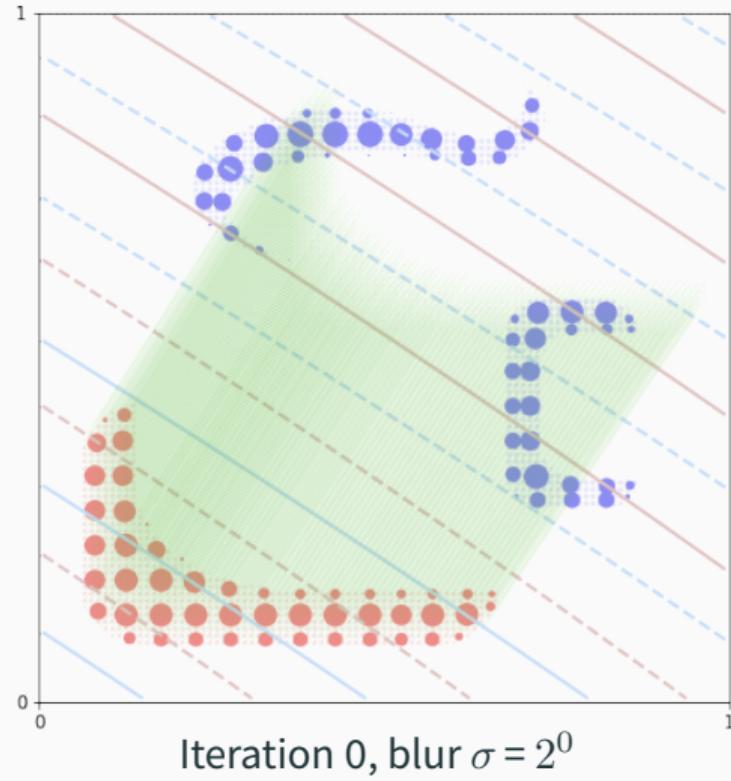
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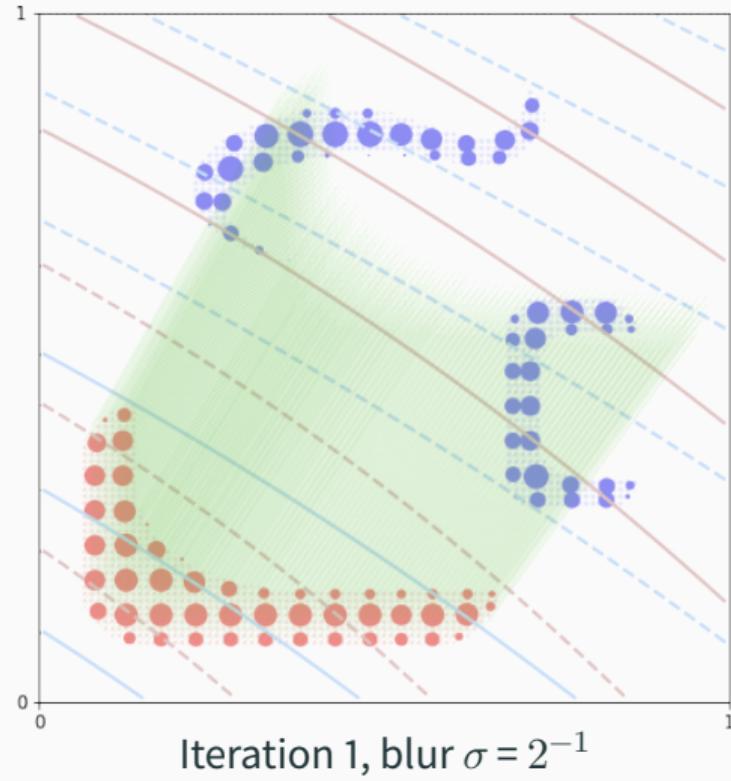
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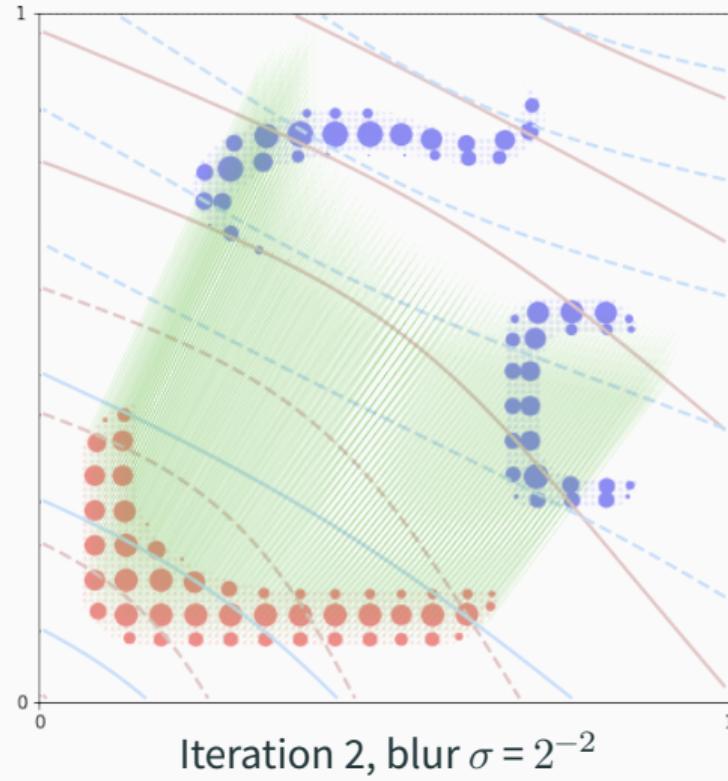
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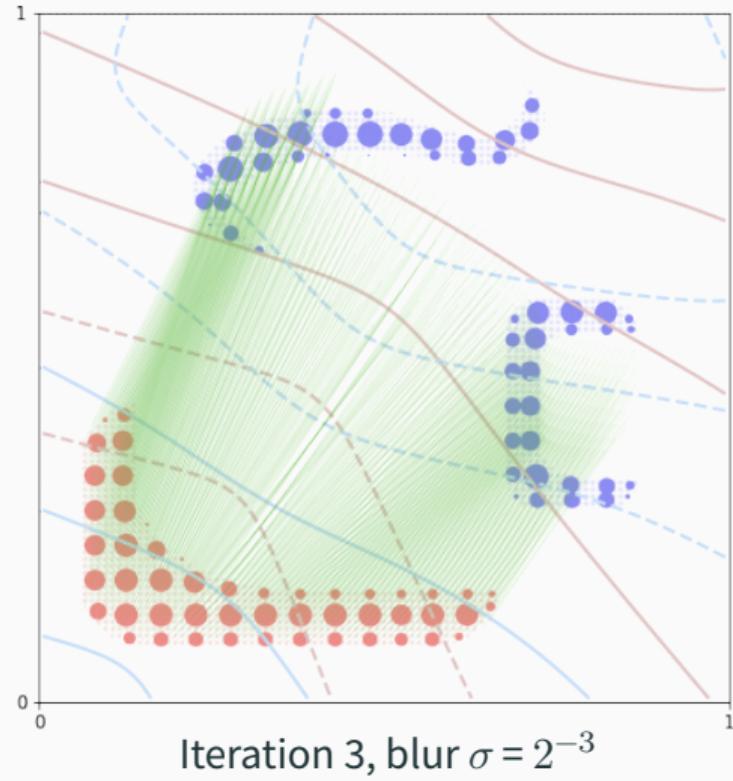
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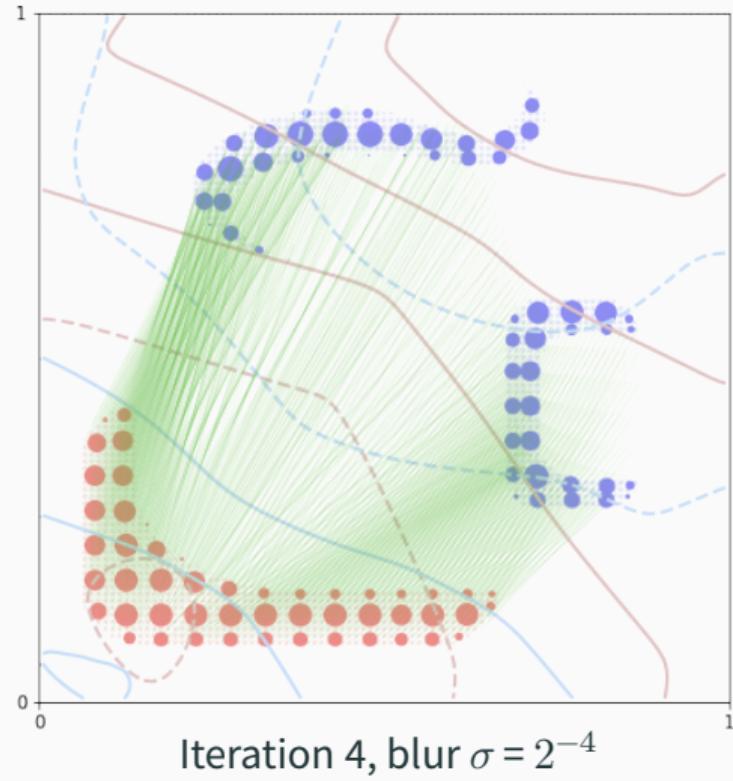
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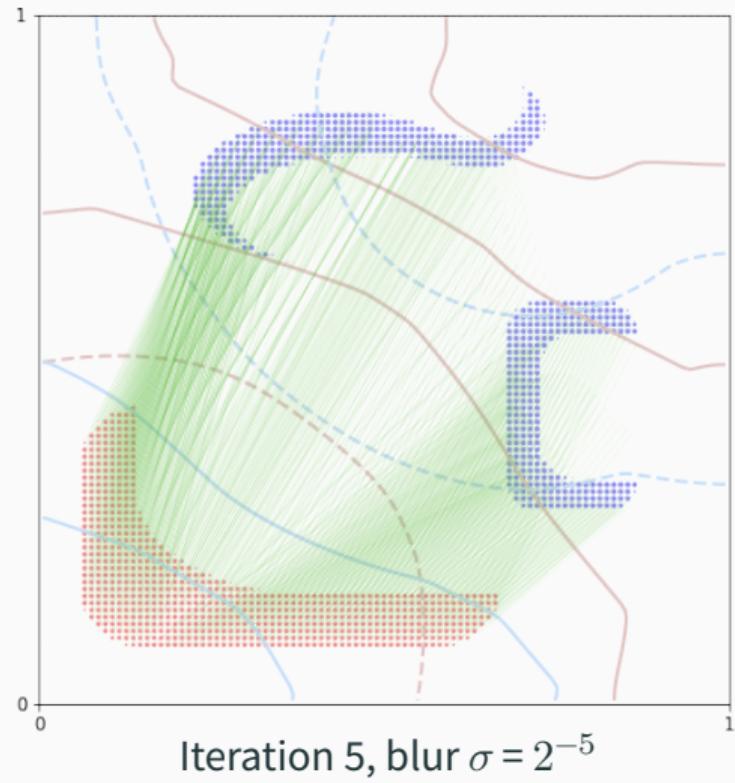
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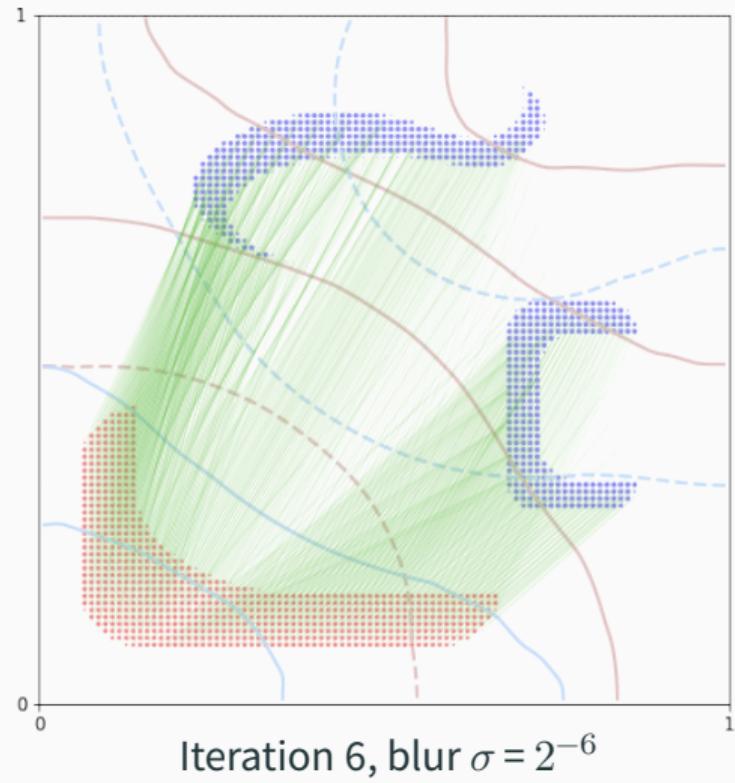
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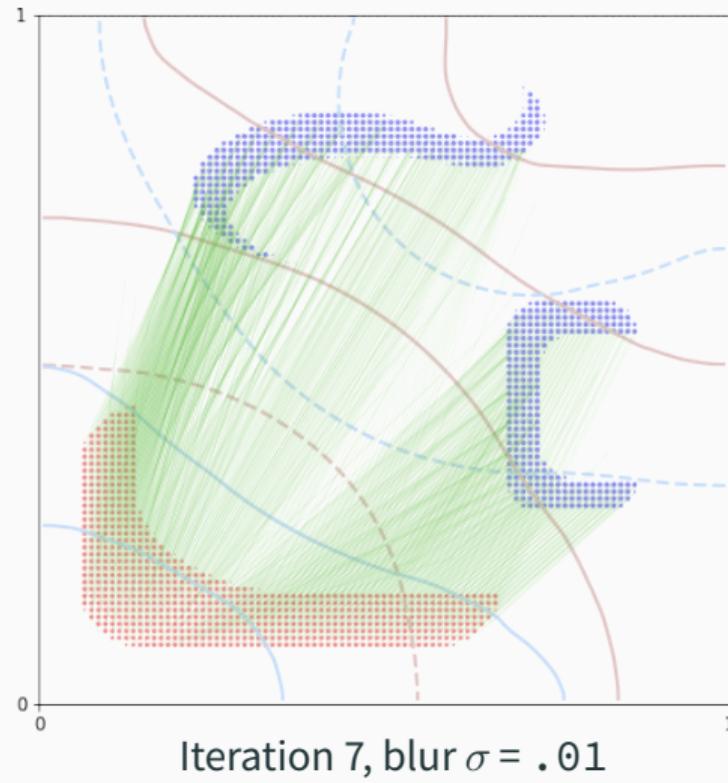
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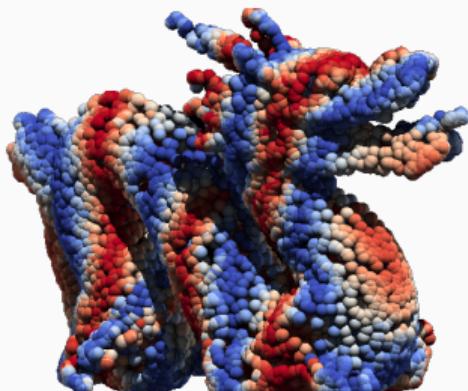
Scaling up optimal transport to anatomical data

Progresses of the last decade add up to a $\times 100$ - $\times 1000$ acceleration:

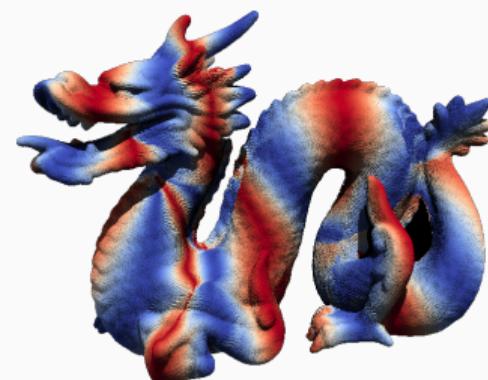
Sinkhorn GPU $\xrightarrow{\times 10}$ + KeOps $\xrightarrow{\times 10}$ + Annealing $\xrightarrow{\times 10}$ + Multi-scale

With a precision of 1%, on a modern gaming GPU:

pip install
geomloss
+
modern GPU
(1 000 €)



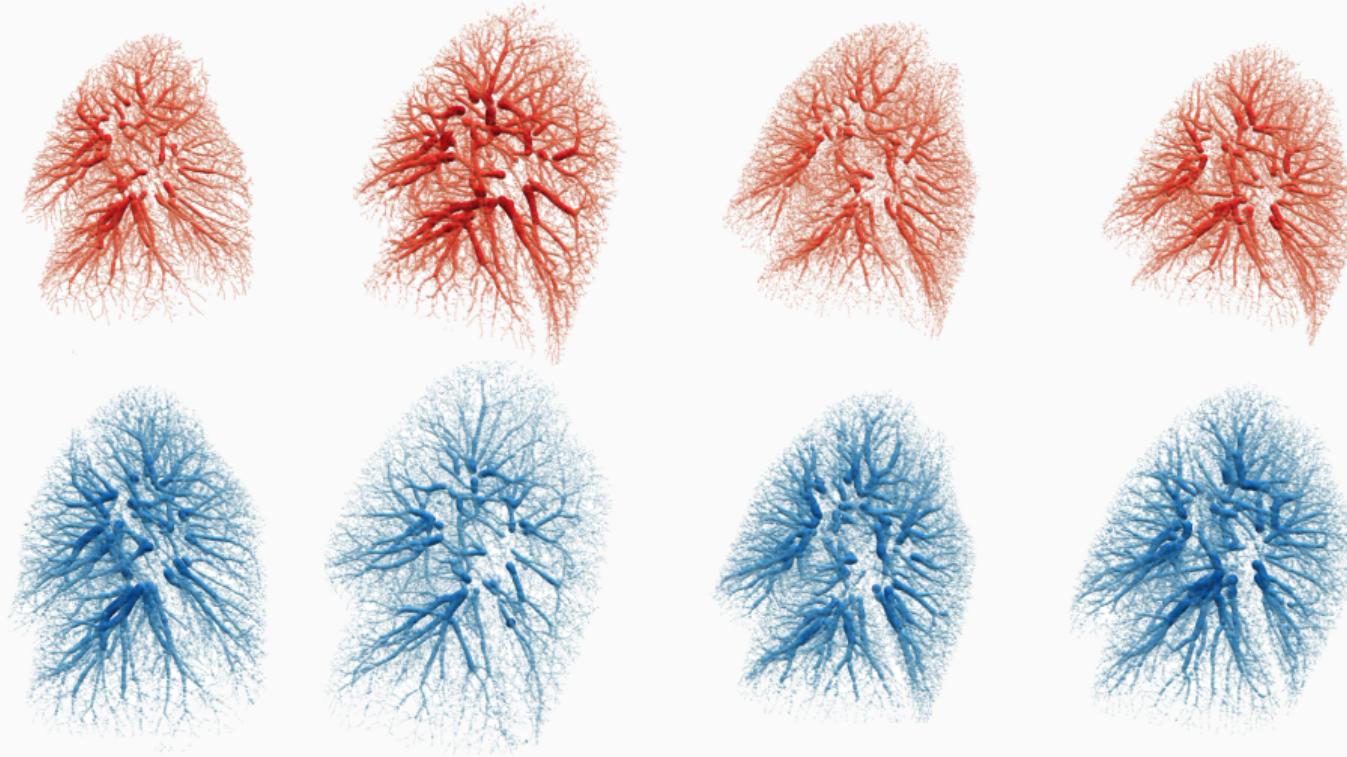
10k points in 30-50ms



100k points in 100-200ms

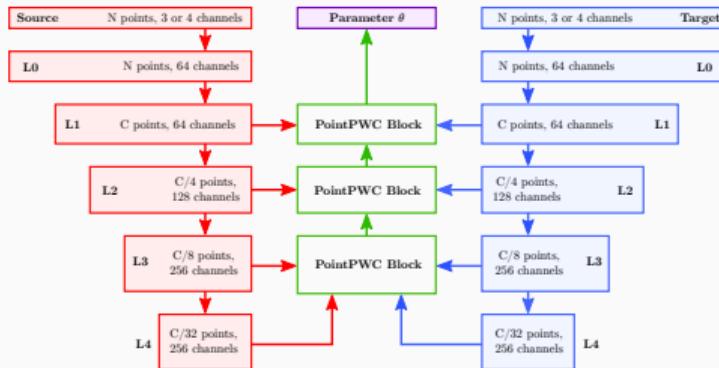
Applications

A typical example in anatomy: lung registration “Exhale – Inhale”



Complex deformations, high **resolution** (50k–300k points), high **accuracy** (<1mm).

State-of-the-art networks – and their limitations



Multi-scale convolutional
point neural network.

Point neural nets, **in practice**:

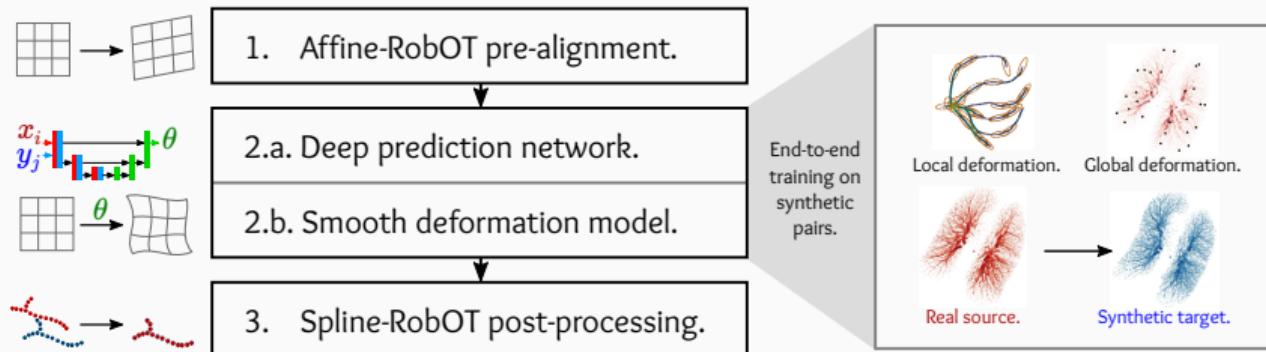
- Compute **descriptors** at all scales.
- **Match** them using geometric layers.
- Train on **synthetic** deformations.

Strengths and weaknesses:

- Good at **pairing** branches.
- Hard to train to high **accuracy**.

⇒ **Complementary** to OT.

Three-steps registration

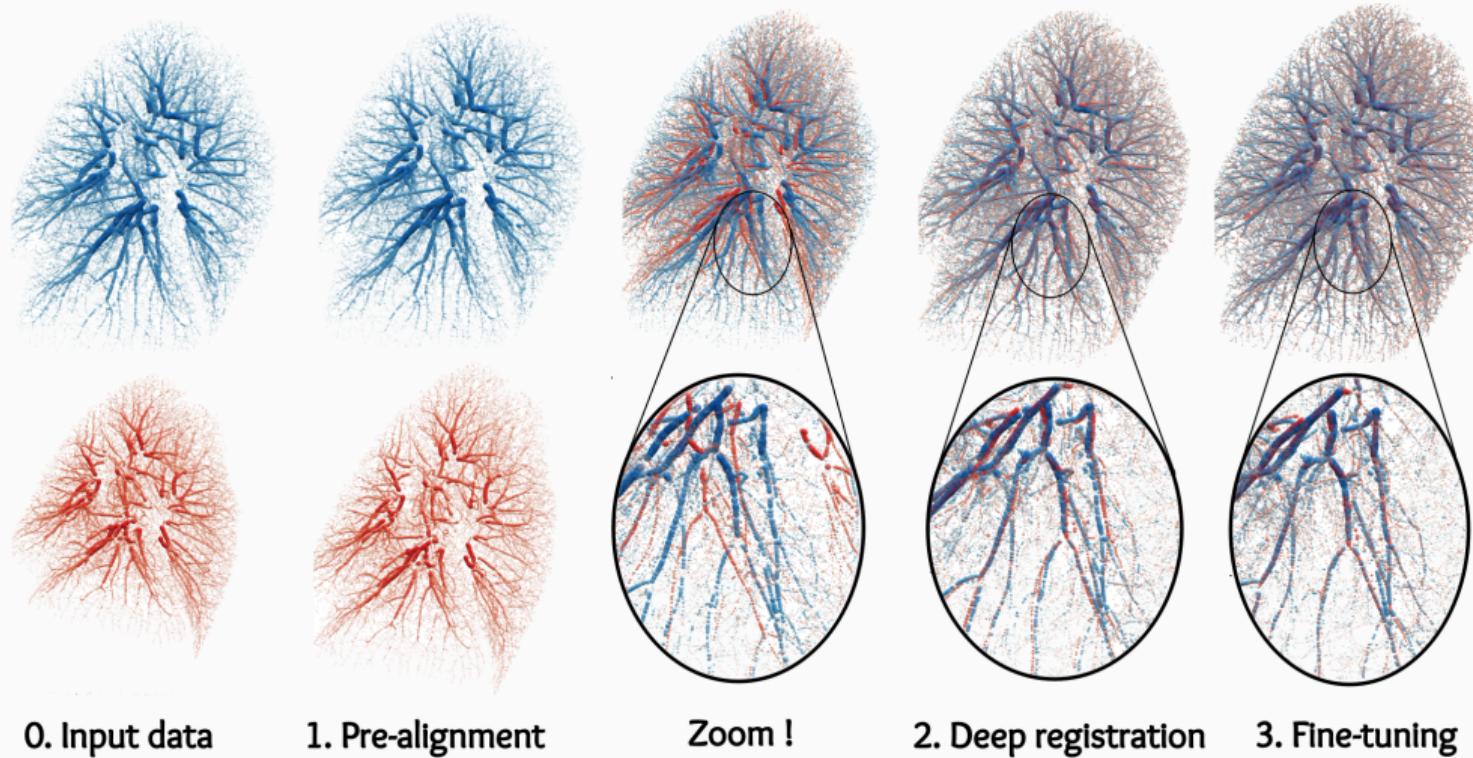


This **pragmatic** method:

- Is **easy to train** on synthetic data.
- Scales up to high-resolution: 100k points in 1s.
- Excellent results: **KITTI** (outdoors scans) and **DirLab** (lungs).

*Accurate point cloud registration with **robust** optimal transport,*
Shen, Feydy et al., NeurIPS 2021.

Three-steps registration



0. Input data

1. Pre-alignment

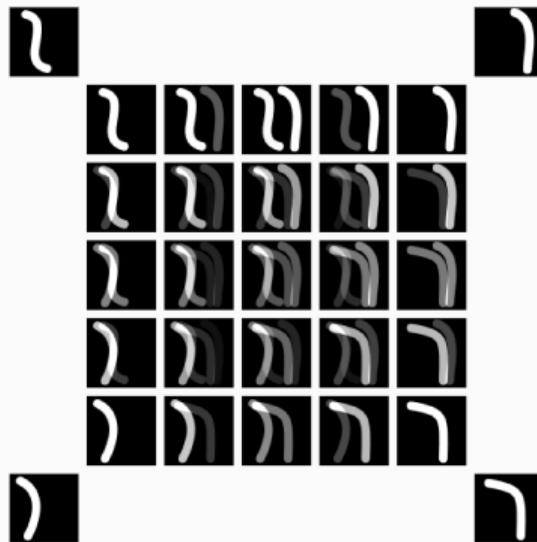
Zoom !

2. Deep registration

3. Fine-tuning

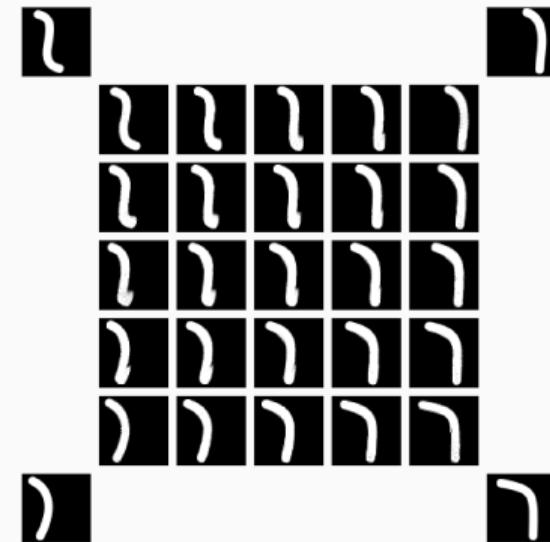
Wasserstein barycenters [AC11]

$$\text{Barycenter } \mathbf{A}^* = \arg \min_{\mathbf{A}} \sum_{i=1}^4 \lambda_i \text{Loss}(\mathbf{A}, \mathbf{B}_i).$$



Euclidean barycenters.

$$\text{Loss}(\mathbf{A}, \mathbf{B}) = \|\mathbf{A} - \mathbf{B}\|_{L^2}^2$$



Wasserstein barycenters.

$$\text{Loss}(\mathbf{A}, \mathbf{B}) = \text{OT}(\mathbf{A}, \mathbf{B})$$

Wasserstein barycenters

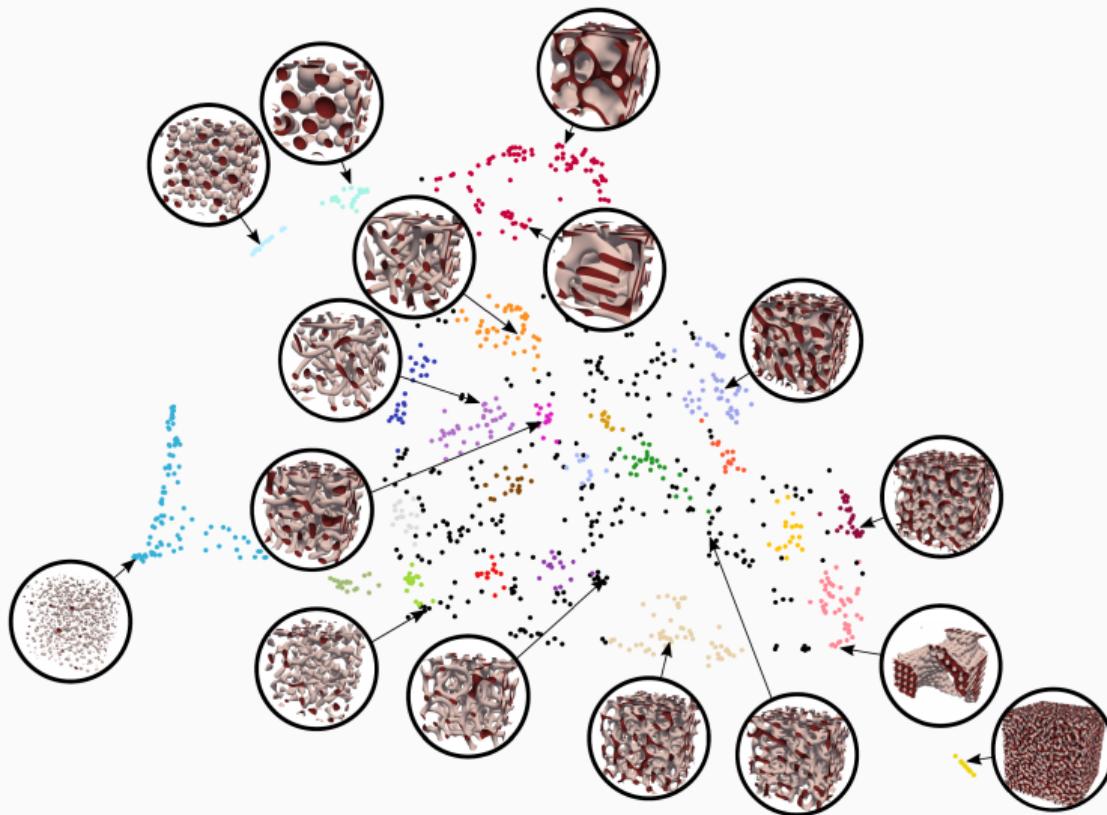
From a computational perspective:

- The problem is **convex** (easy) wrt. the weights.
- The support of the barycenter lies in the **convex hull** of the input distributions.

The **curse of dimensionality** hits hard:

- In high dimension, identifying the support can become **NP-hard**.
- In dimensions 2 and 3, we can just use a grid and recover **super fast** algorithms.
Computing OT distances and barycenters between **density maps** is a solved problem.
 \implies We can now **easily** do manifold learning with e.g. UMAP in Wasserstein spaces of **2D and 3D** distributions.

An example this afternoon: Anna Song's presentation on 3D shape textures



Conclusion

Genuine team work



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Thibault Séjourné



F.-X. Vialard



Gabriel Peyré



Alain Trouvé



Marc Niethammer



Shen Zhengyang



Olga Mula



Hieu Do

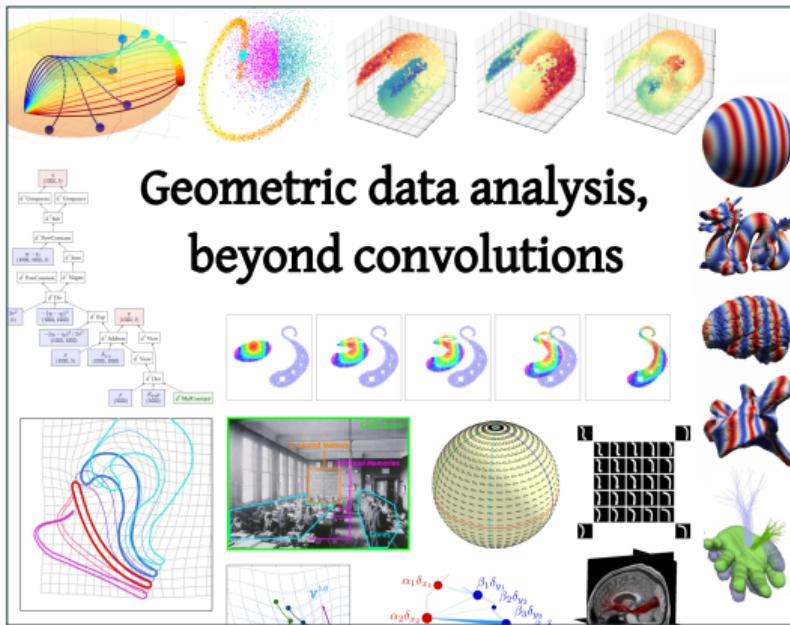
Key points

- Optimal Transport = **generalized sorting** :
 - Super-fast solvers on **simple domains** (esp. 2D/3D spaces).
 - Simple registration for shapes that are close to each other.
 - **Fundamental tool** at the intersection of geometry and statistics.
 - Can we extend recent computational advances to **topology-aware** metrics?
- GPUs are more **versatile** than you think.
 - Ongoing work to provide **fast GPU backends** to researchers, going beyond what Google and Facebook are ready to pay for.

Documentation and tutorials are available online



www.kernel-operations.io



www.jeanfeydy.com/geometric_data_analysis.pdf

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