Sorting points in dimension $D > 1$

Jean Feydy

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Imperial College London
Collaboration with B. Charlier, J. Glaunès (KeOps library);
F.-X. Vialard, G. Peyré, T. Séjourné, A. Trouvé (OT theory).

Who am I?

Quick CV:

- Typical French curriculum (ENS Maths + MVA + Siemens)

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$\Longrightarrow$ **Geometry**, mostly for medical imaging

The medical imaging pipeline [Ptr19, EPW+11]

Sensor data

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Raw image

Signal processing

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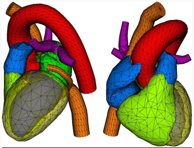

High-level description

Computational anatomy

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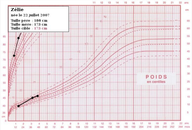
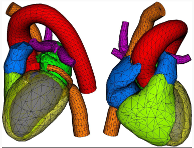


Valuable information

Statistics



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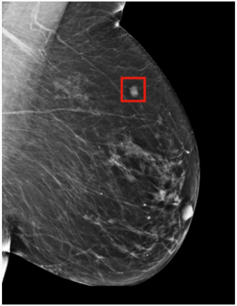
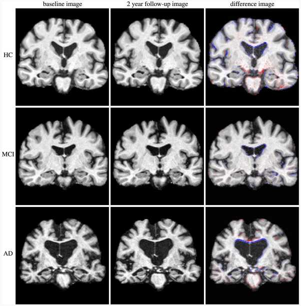
Computational anatomy [CSG19, LSG+18, CMN14]

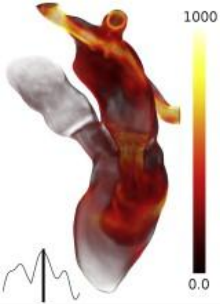
Three main problems:



Spot patterns

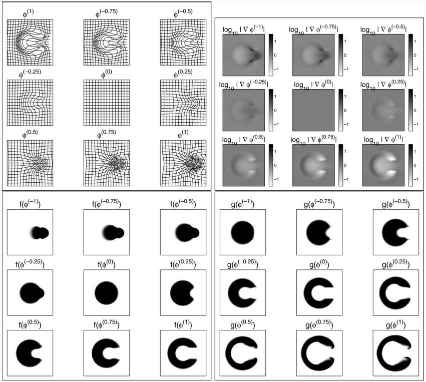


Analyze variations



Fit models

Shape analysis [Ash07, Gla05]



Advection $\neq$ Convolution

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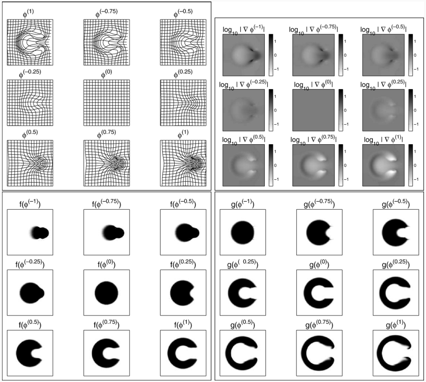

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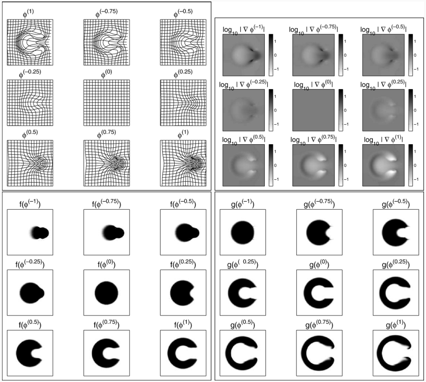

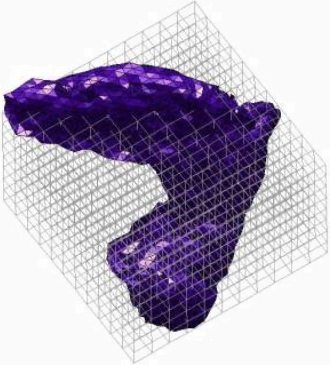

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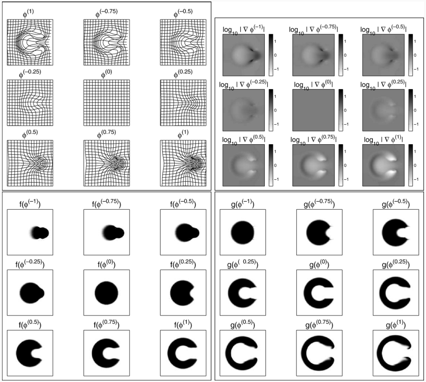

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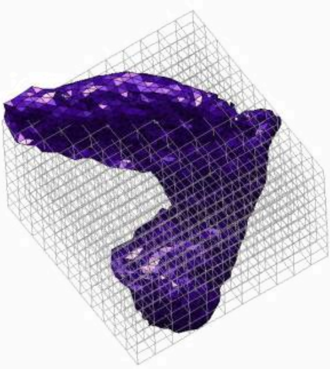

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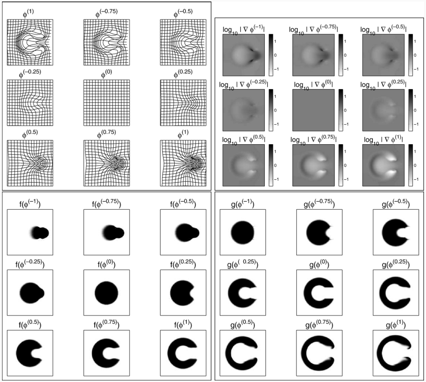

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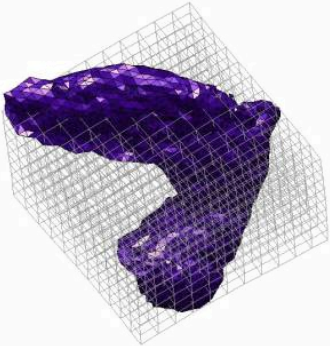

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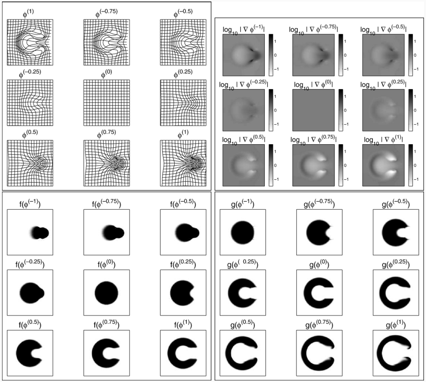

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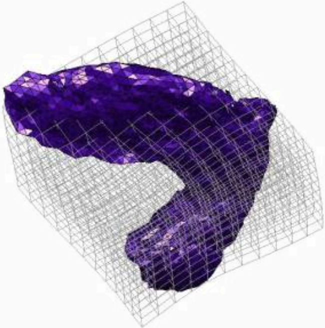

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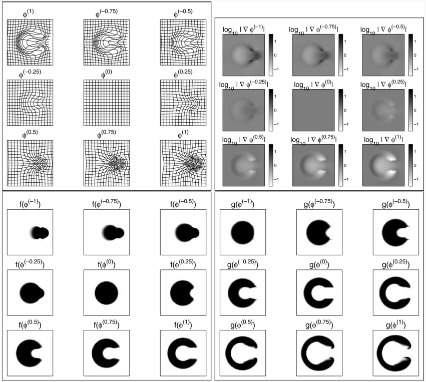

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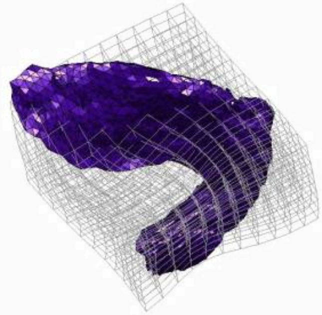

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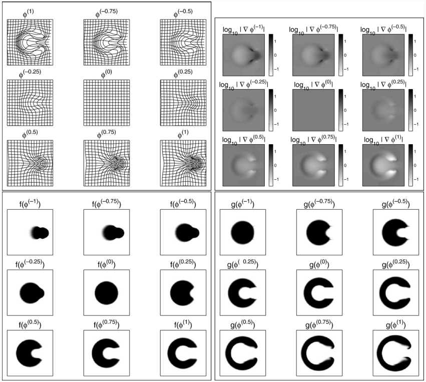
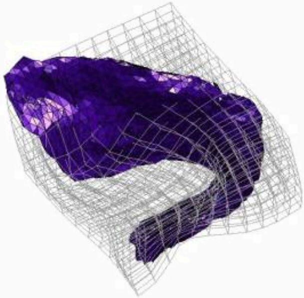


Advection ≠ Convolution



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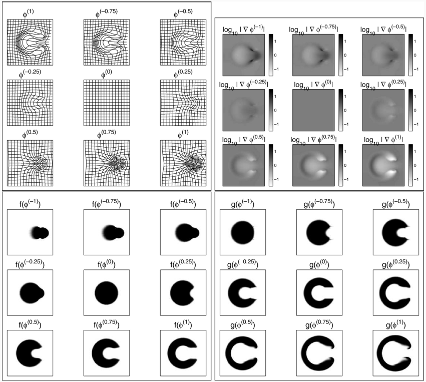

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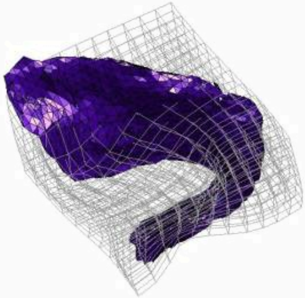
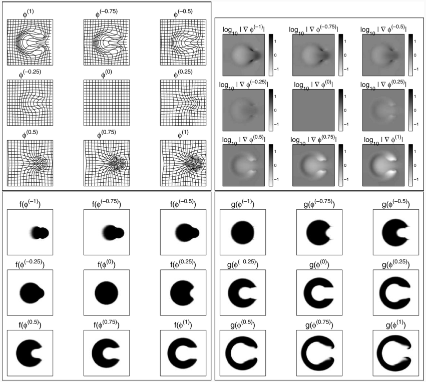


Mesh deformation

$\Longrightarrow$ We need **fast geometric primitives.**



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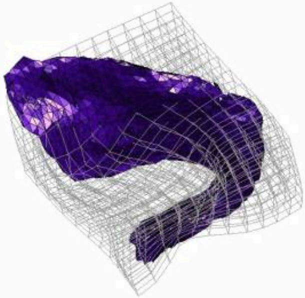

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Problem: not supported well by TensorFlow and PyTorch.

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Geometric data analysis, beyond convolutions

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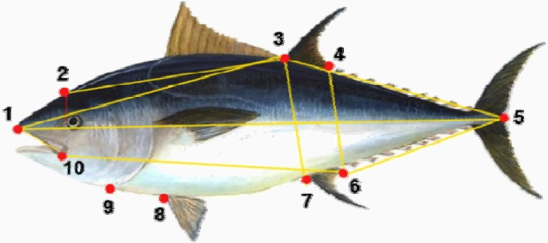
- **Geometric** loss functions
  $\longrightarrow$ Wasserstein distance = optimal transport = **sorting**.

Working with unlabeled point clouds

Life is easy when you have labels



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

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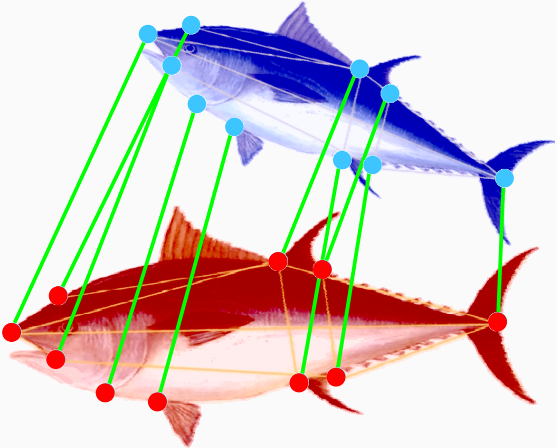

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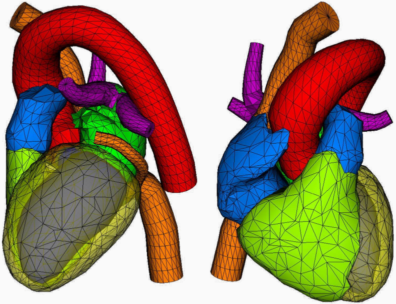
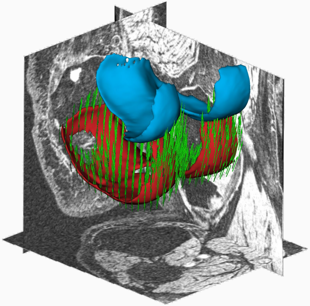
Unfortunately, medical data is often unlabeled [EPW+11]



Surface meshes



Segmentation masks

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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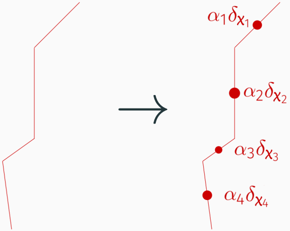

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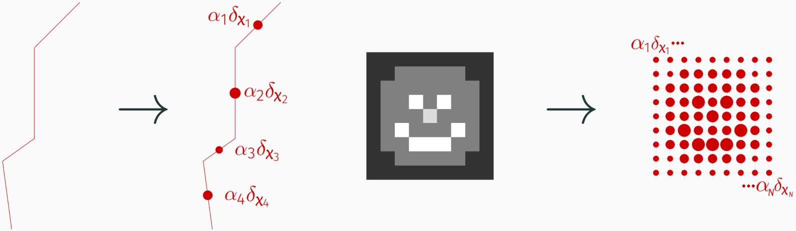
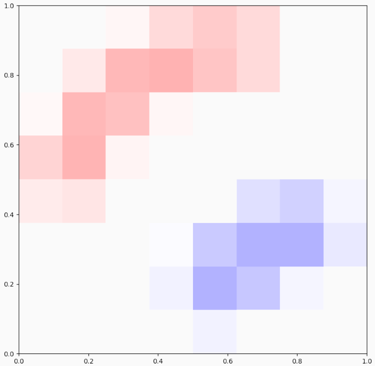


A baseline setting: density registration



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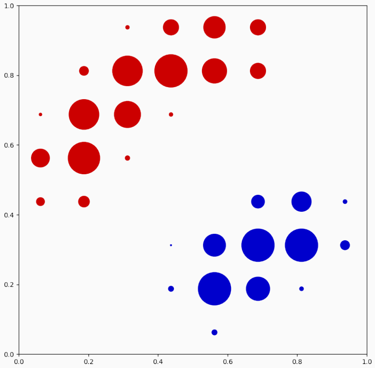

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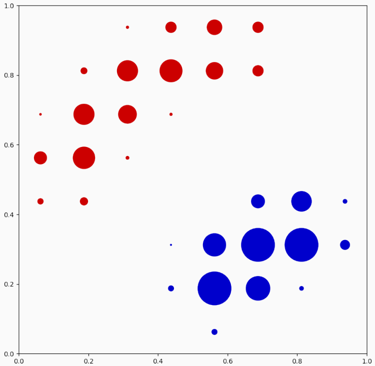

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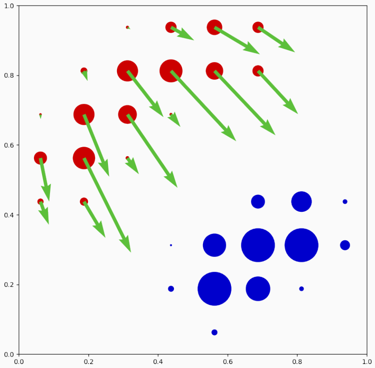

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Display $v_i \;=\; -\frac{1}{\alpha_i} \nabla_{x_i} \text{Loss}(\alpha, \beta)$.

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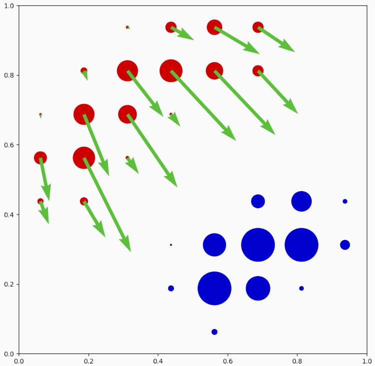

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Seamless extensions to:

- $\sum_i \alpha_i \neq \sum_j \beta_j$, outliers [CPSV18],
- curves and surfaces [KCC17],
- variable weights α_i.

Simple loss functions between measures

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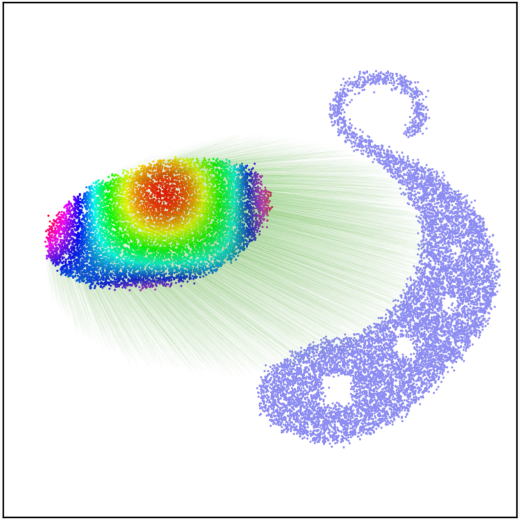
- Example: the Energy Distance, $k(x, y) = -\|x - y\|$:

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

Gradient flow as a toy registration problem



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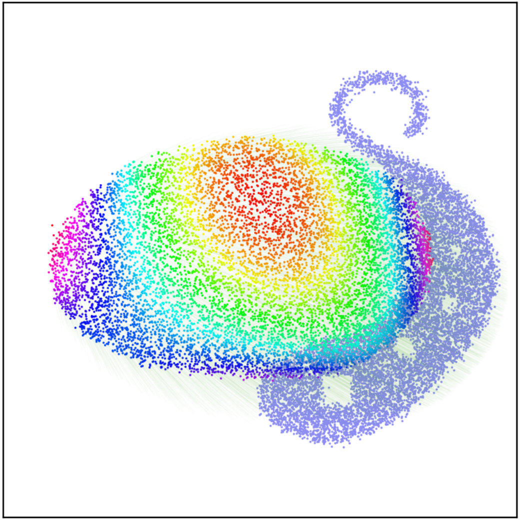
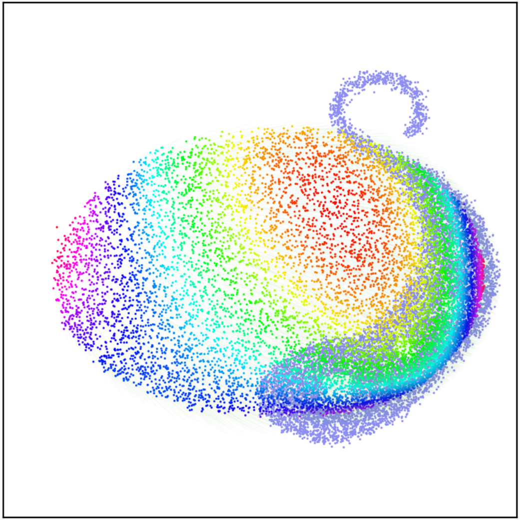


$t = .25$

Gradient flow as a toy registration problem



$t = .50$

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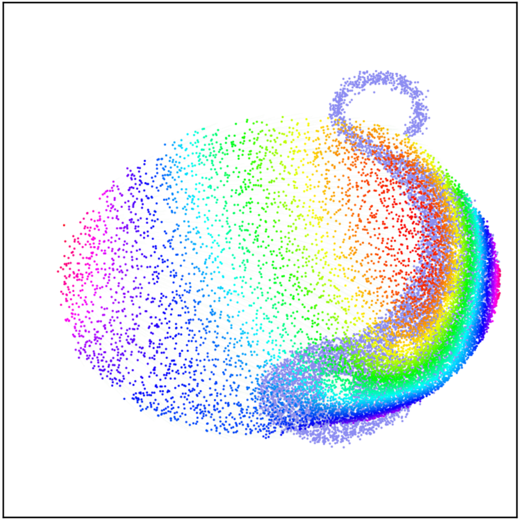

$t = 1.00$

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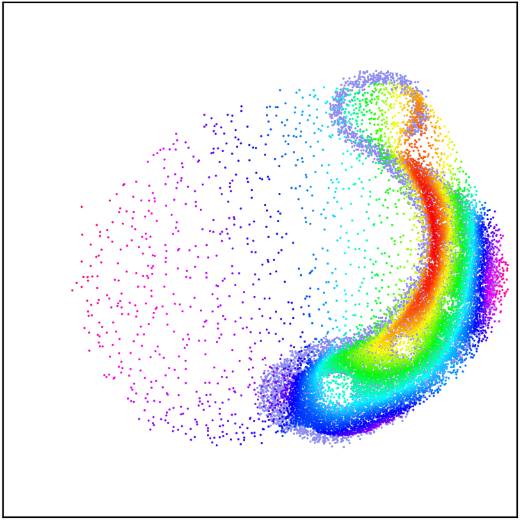

$t = 5.00$

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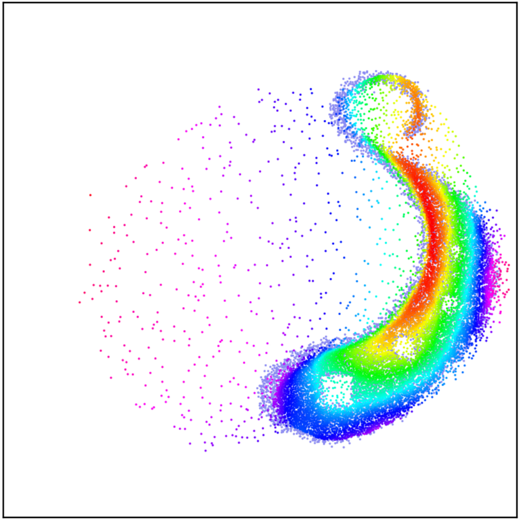

$t = 10.00$

The Wasserstein distance

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Simple toy example in 1D :

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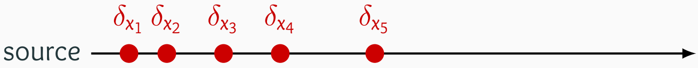

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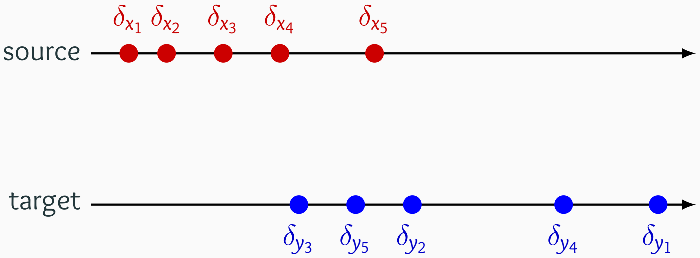

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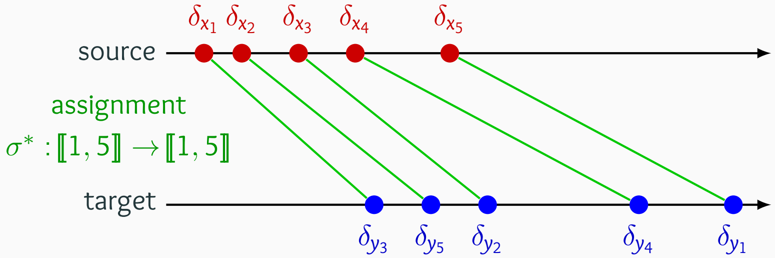

$$\text{OT}(\alpha, \beta) \;=\; \frac{1}{2N} \sum_{i=1}^{N} |x_i - y_{\sigma^*(i)}|^2$$

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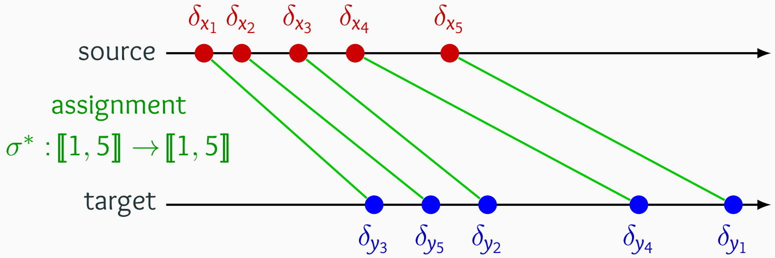

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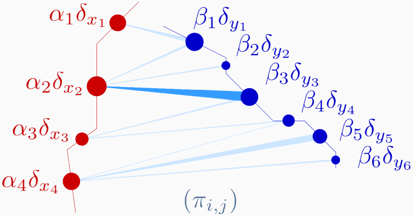
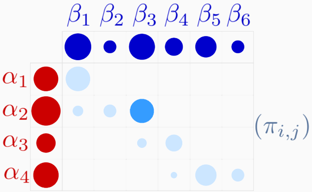
Optimal transport generalizes sorting to D > 1





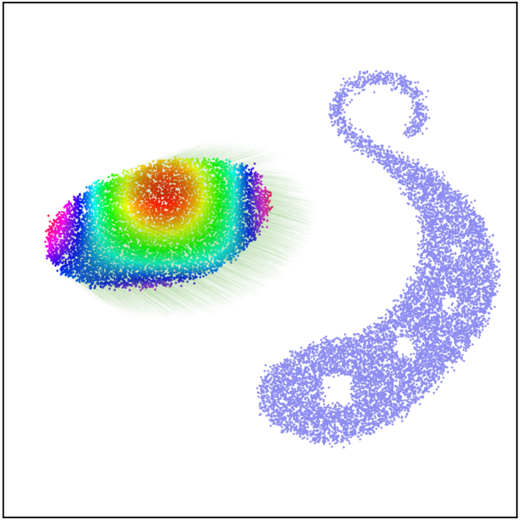
Minimize over *N*-by-*M* matrices (transport plans) π :

$$\text{OT}(\alpha, \beta) = \min_{\pi} \underbrace{\sum_{i,j} \pi_{i,j} \cdot \tfrac{1}{2}|x_i - y_j|^2}_{\text{transport cost}}$$

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

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

Wasserstein gradients are homogeneous



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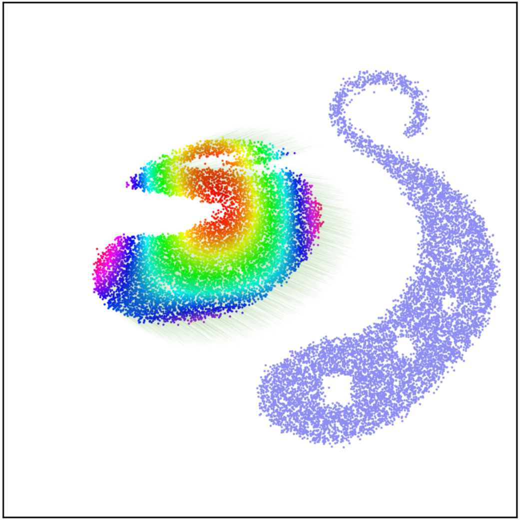

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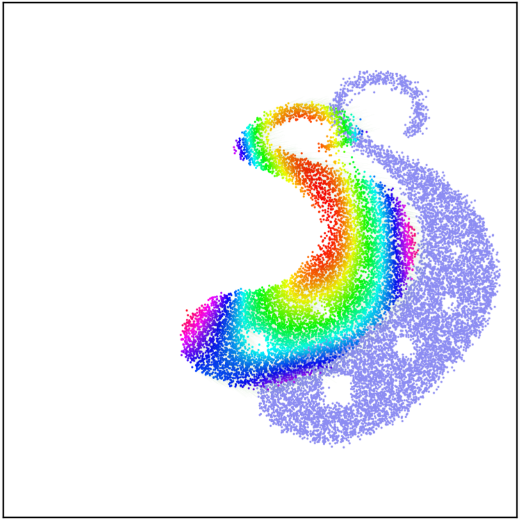
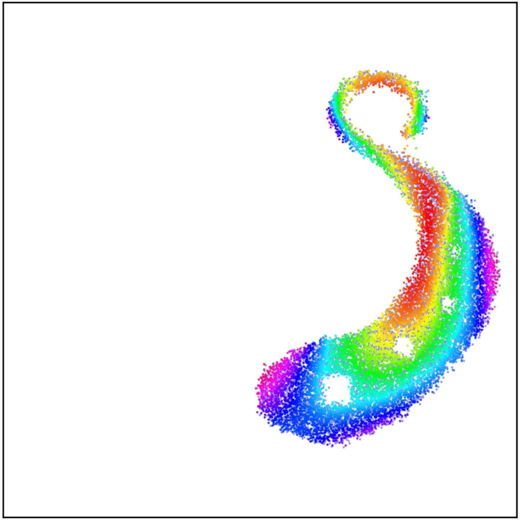
Wasserstein gradients are homogeneous



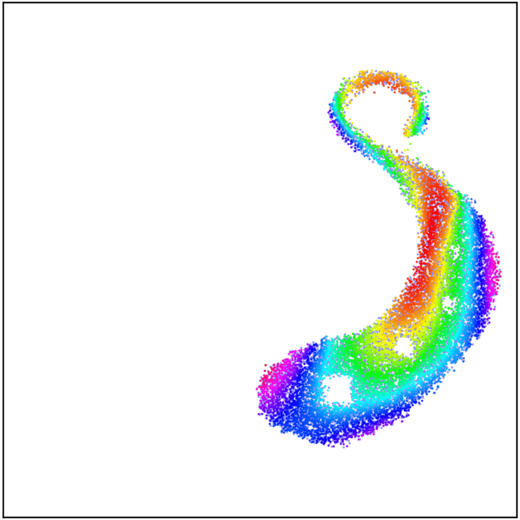
$t = 1.00$

Wasserstein gradients are homogeneous



$t = 5.00$

Wasserstein gradients are homogeneous



$t = \texttt{10.00}$

Key properties [Bre91]

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$\Longrightarrow$ Appealing generalization of an **increasing mapping.**

Can we scale all of this?

Kantorovitch's dual formulation

$$\mathrm{OT}(\alpha, \beta) = \min_{\pi} \langle \pi , \mathrm{C} \rangle, \text{ with } \mathrm{C}(x_i, y_j) = \frac{1}{p}\|x_i - y_j\|^p \quad \longrightarrow \text{Assignment}$$

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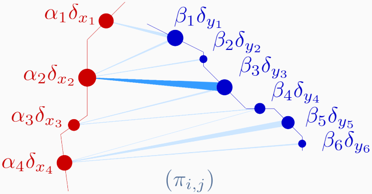
$\sum_{i,j} \pi_{i,j} C(x_i, y_j)$



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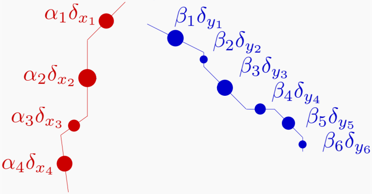

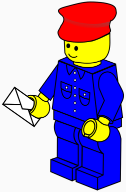

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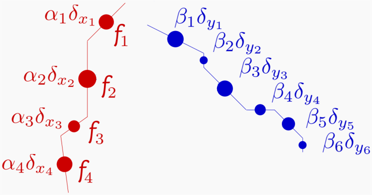

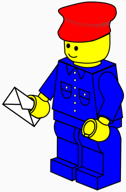

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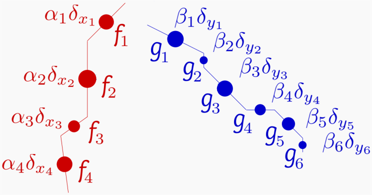

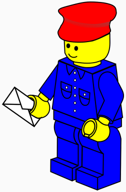

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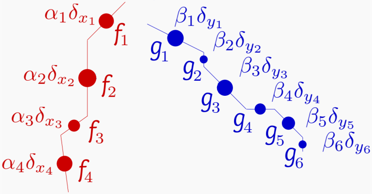

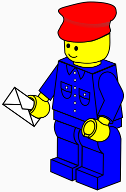

$\sum_{i,j} \pi_{i,j} \, \mathrm{C}(x_i,y_j)$

$\sum_i \alpha_i f_i + \sum_j \beta_j g_j$

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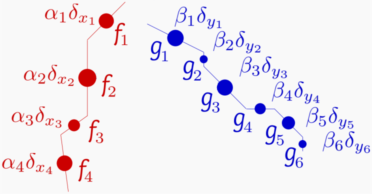

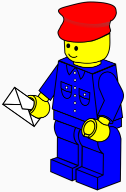

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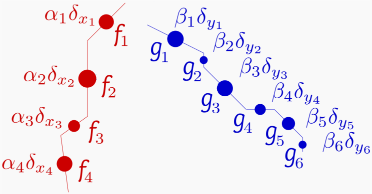

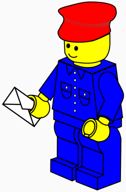

$\sum_{i,j} \pi_{i,j}\, \mathrm{C}(x_i,y_j)$ $\qquad$ $\sum_i \alpha_i f_i + \sum_j \beta_j g_j$

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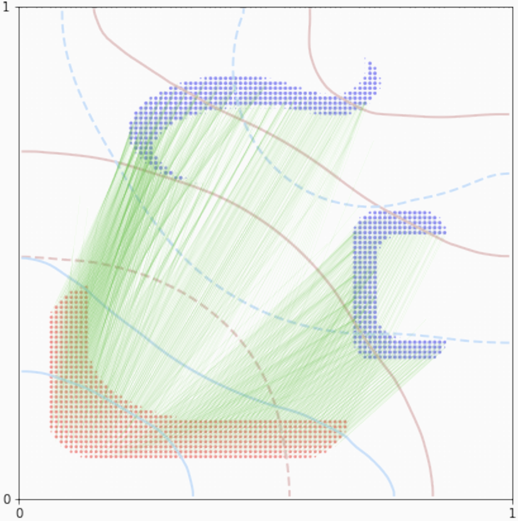
$\Longrightarrow$ Generalized **QuickSort** algorithm.

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



OT plan in 2D.

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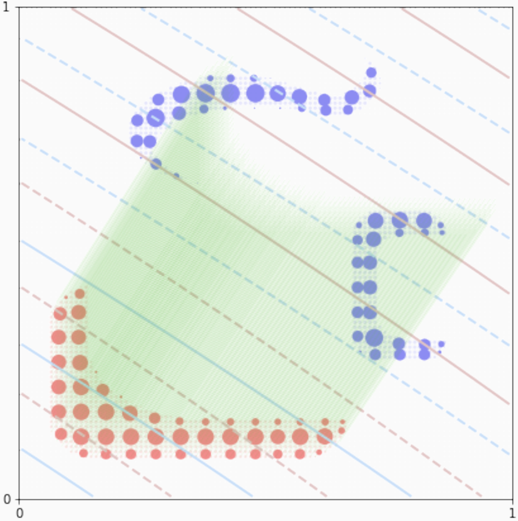

Iteration 0, blur = 2^0

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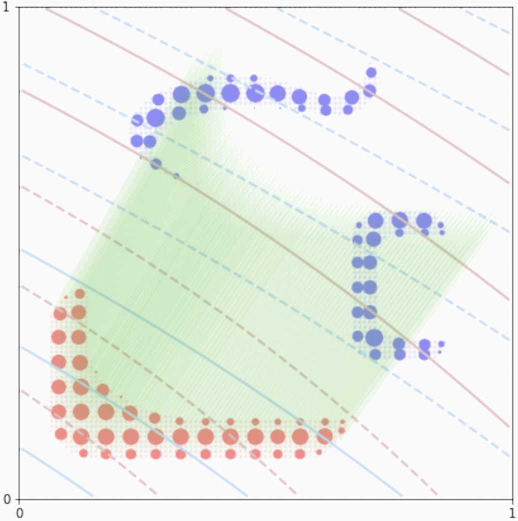

Iteration 1, blur = 2^{-1}

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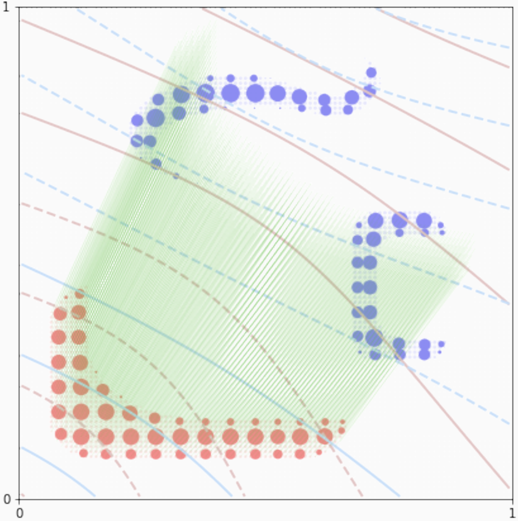

Iteration 2, blur = 2^{-2}

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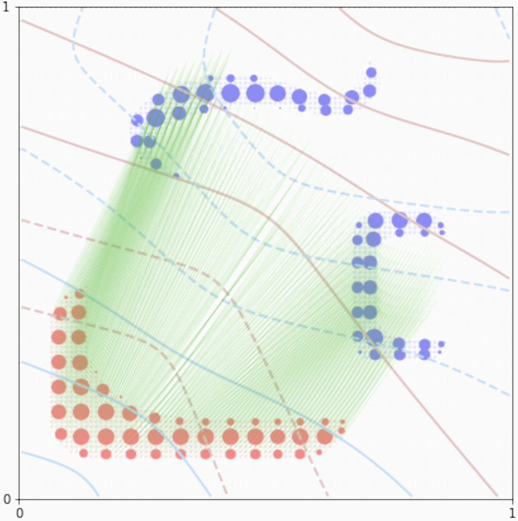

Iteration 3, blur = 2^{-3}

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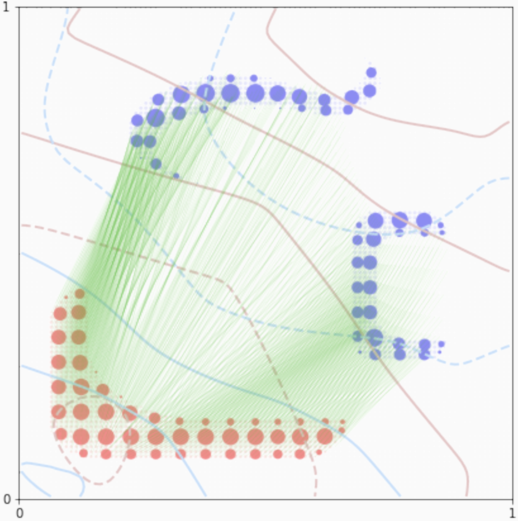

Iteration 4, blur = 2^{-4}

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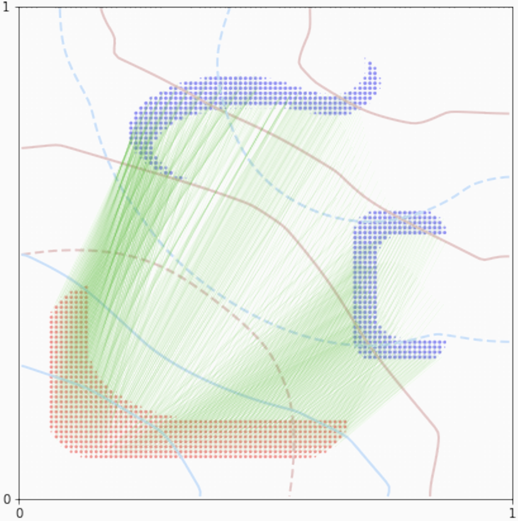

Iteration 5, blur = 2^{-5}

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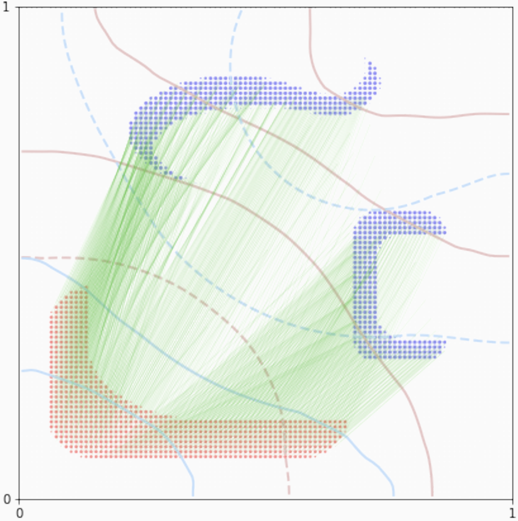

Iteration 6, blur = 2^{-6}

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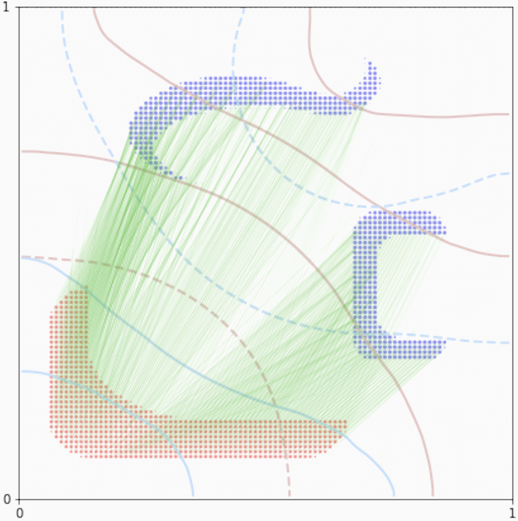

Iteration 7, blur = `.01`

Overview of the last decade

Progresses since [KY94, Cut13]:

+ $O(N \log N)$ instead of $O(N^2)$.

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$\Longrightarrow$ Use the **KeOps** and **GeomLoss** libraries! $\Longleftarrow$

Scaling up to millions of samples on the GPU

Introducing KeOps LazyTensors

$M[\,i\,,\,j\,]$

Array

Coefficients only

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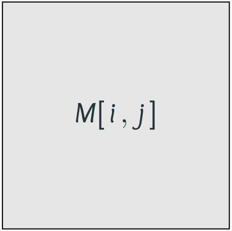

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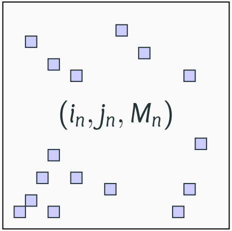
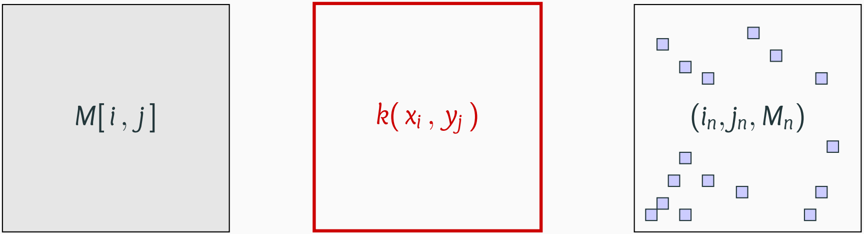


Sparse matrix
Coordinates + coeffs

Introducing KeOps LazyTensors



Array
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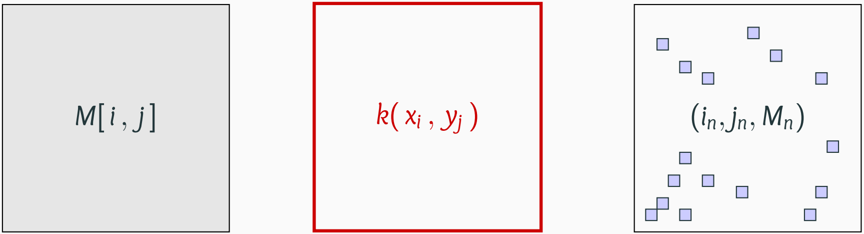
Symbolic LazyTensor
Formula + point clouds

Sparse matrix
Coordinates + coeffs

Introducing KeOps LazyTensors



Array
Coefficients only

Symbolic LazyTensor
Formula + point clouds

Sparse matrix
Coordinates + coeffs

```
pip install pykeops
```

It works!

```
# Large point clouds in [0,1]^3
import torch
x = torch.rand(1000000, 3, requires_grad=True).cuda()
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# Turn our Tensors into KeOps symbolic variables:
from pykeops.torch import LazyTensor
x_i = LazyTensor(x[:,None,:])  # x_i.shape = (1e6, 1, 3)
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# Perform large-scale computations:
D_ij = ((x_i - y_j)**2).sum(dim=2)  # (1e6,2e6,1)
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# Reduction: symbolic LazyTensor -> genuine torch Tensor
a_i = K_ij.sum(dim=1)  # (1e6, 1) torch.cuda.FloatTensor
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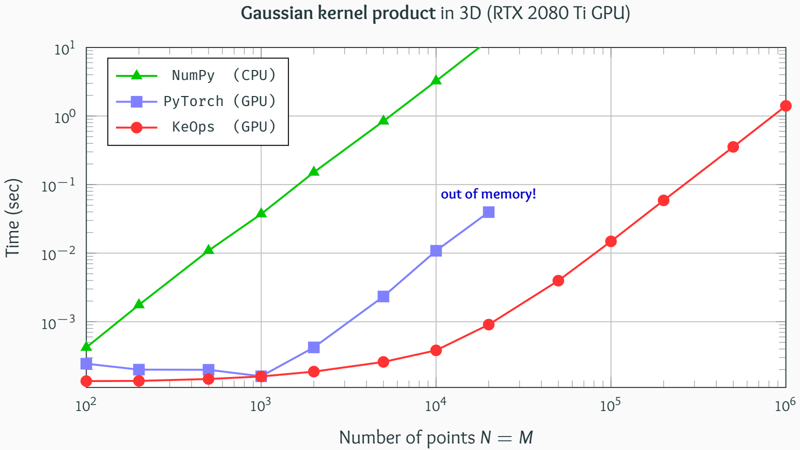
a_i = K_ij.sum(dim=1)  # (1e6, 1) torch.cuda.FloatTensor
g_x = torch.autograd.grad((a_i ** 2).sum(), [x])
```

Scaling up to real data



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- Scikit-learn-like **documentation**:

`www.kernel-operations.io`

Geometric Loss functions for PyTorch

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# Large point clouds in [0,1]^3
import torch
x = torch.rand(100000, 3, requires_grad=True).cuda()
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from geomloss import SamplesLoss  # See also ImagesLoss...
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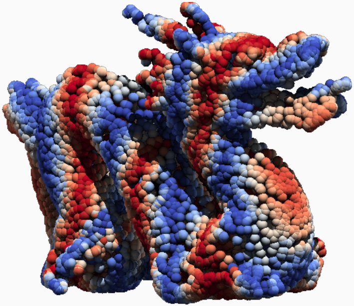
L = loss(x, y)  # By default, use constant weights
# GeomLoss supports autograd, batch processing, etc.
g_x, = torch.autograd.grad(L, [x])
```

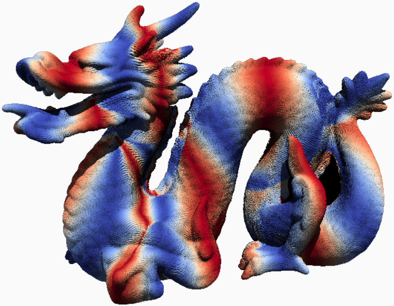
Scaling up optimal transport

Precision controlled by the ratio $\frac{\text{blur}}{\text{diameter}}$.

With a precision of 1%, on a modern gaming GPU – RTX 2080 Ti:



10k points in 30-50ms



100k points in 100-200ms

Conclusion

Wasserstein distance = Multi-dimensional sorting problem ?

The **three regimes** of Optimal Transport:

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- α, β live in **dimension 1**
  $\Longrightarrow$ Simple sorting problem
  $\Longrightarrow$ Quicksort in $\mathbf{O(N \log N)}$.

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- α, β live in dimension **10+**
  $\Longrightarrow$ $C(x_i, y_j)$ has very little structure
  $\Longrightarrow$ Compute all pairs in $\geqslant \mathbf{O}(\mathbf{N}^2)$.

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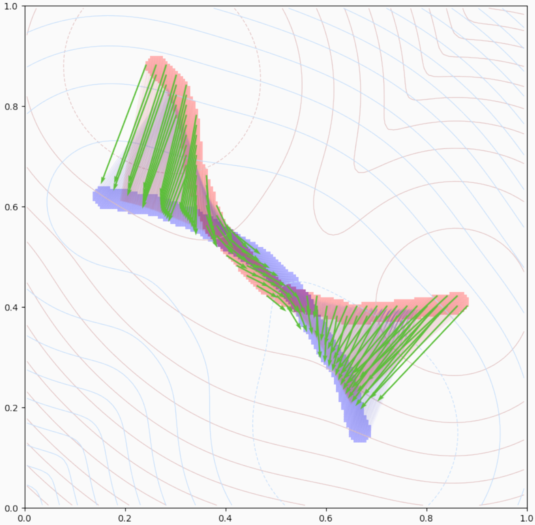
$\Longrightarrow$ Multiscale Sinkhorn algorithm $\simeq$ Multi-dimensional **Quicksort.**

A robust loss function



A high-quality gradient…

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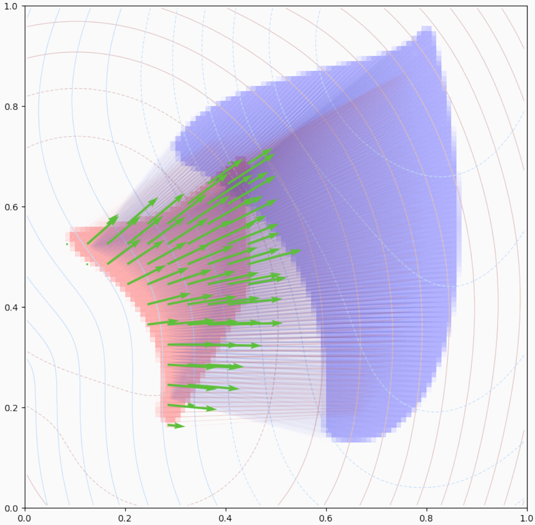

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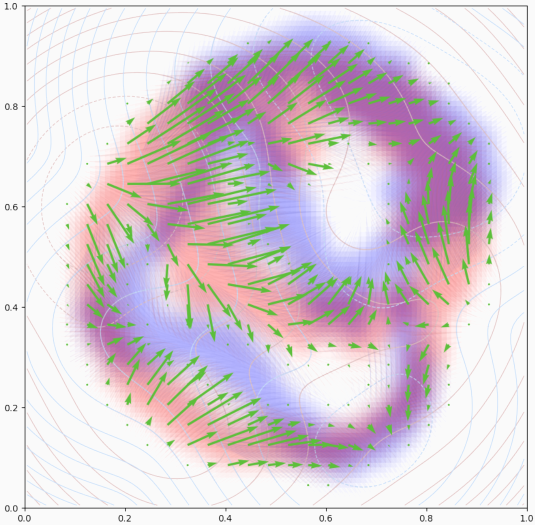
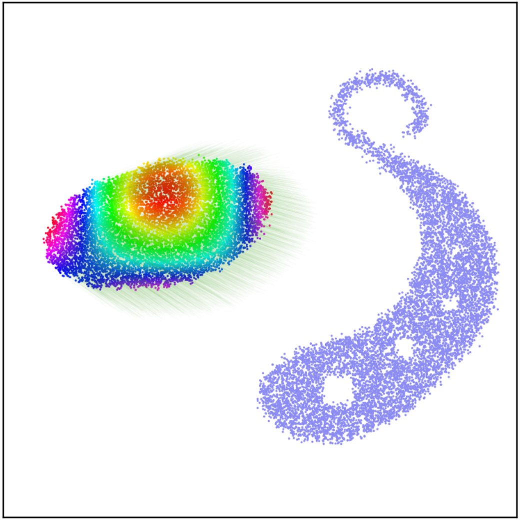


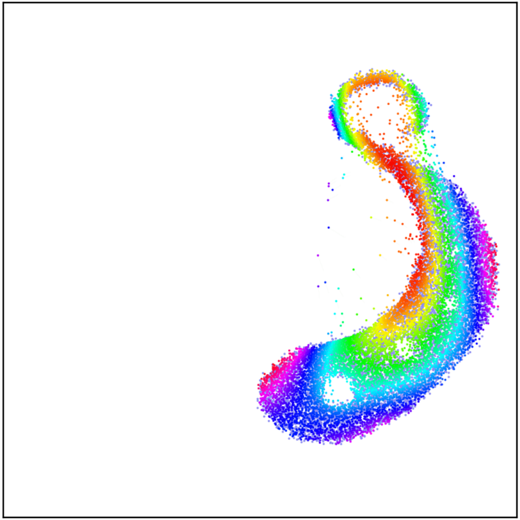
A high-quality gradient... But no preservation of topology!

Gradient descent with OT: cheap'n easy registration?



Iteration 0

Gradient descent with OT: cheap'n easy registration?



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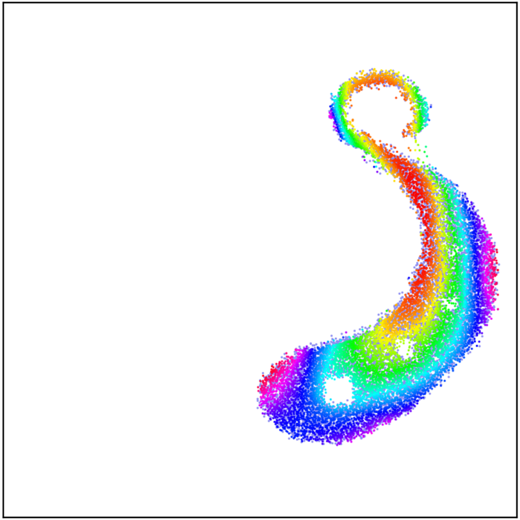
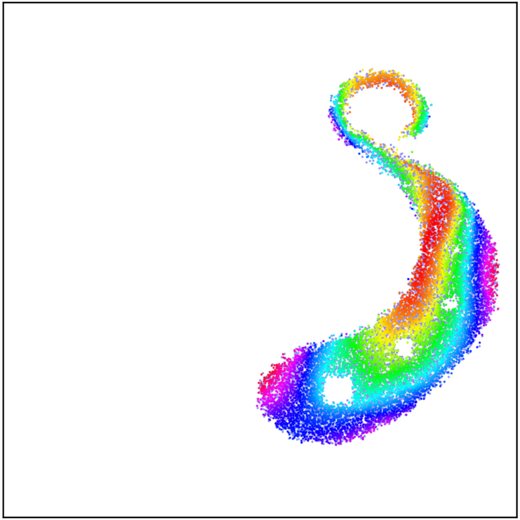


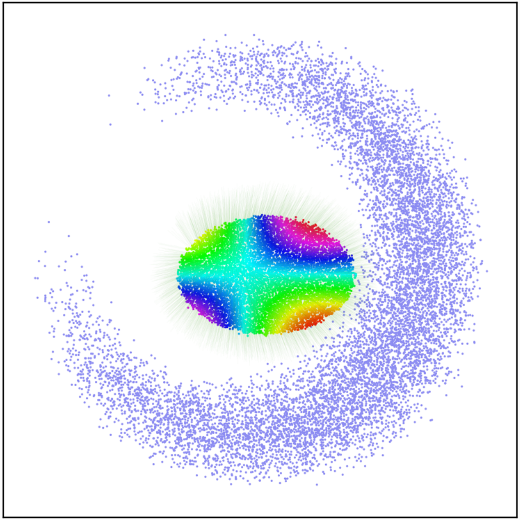
Iteration 2

Gradient descent with OT: cheap'n easy registration?



Iteration 10

Gradient descent with OT: cheap'n easy registration?



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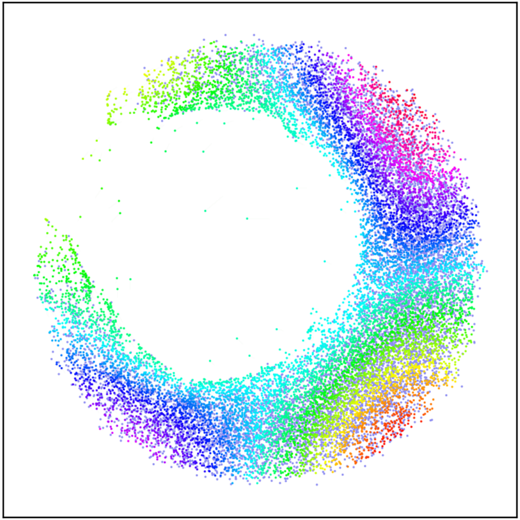

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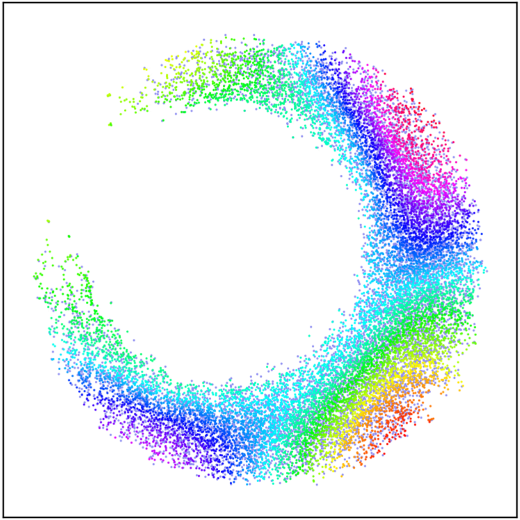

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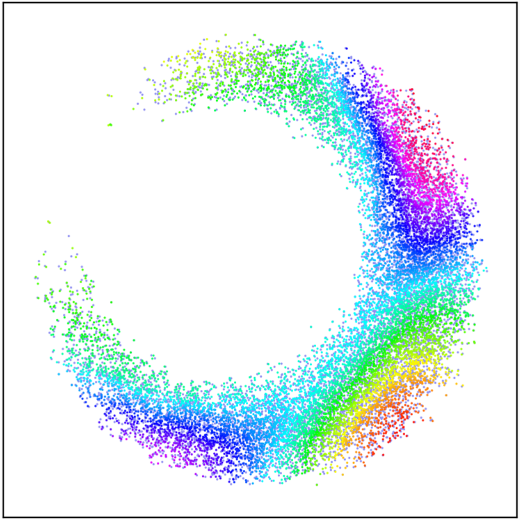

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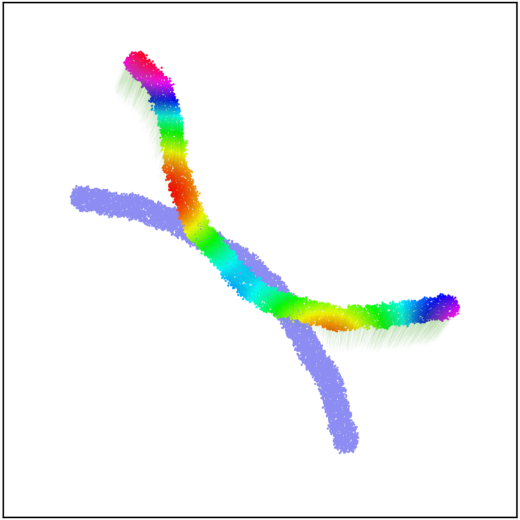

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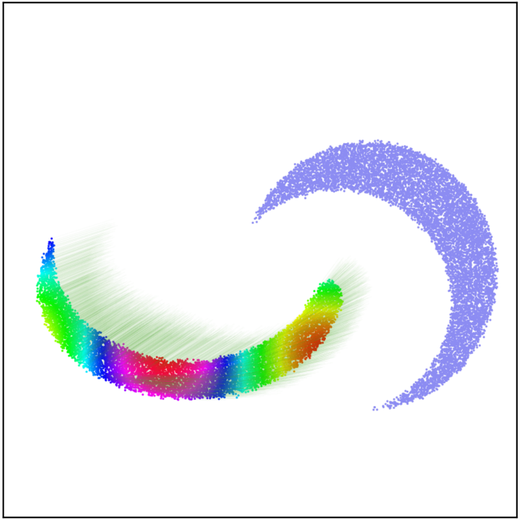

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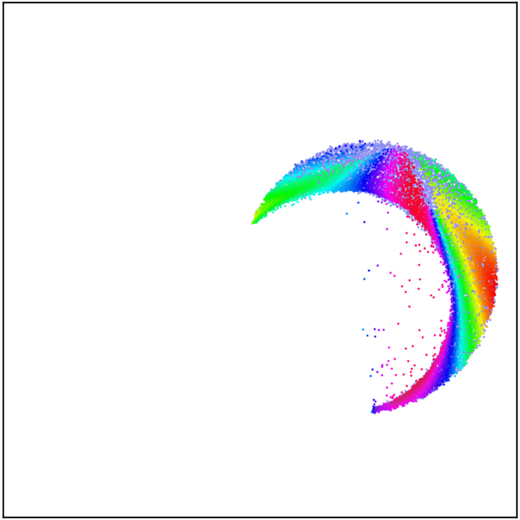

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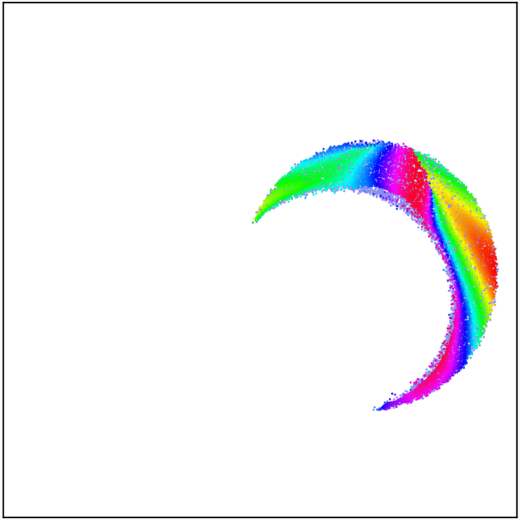

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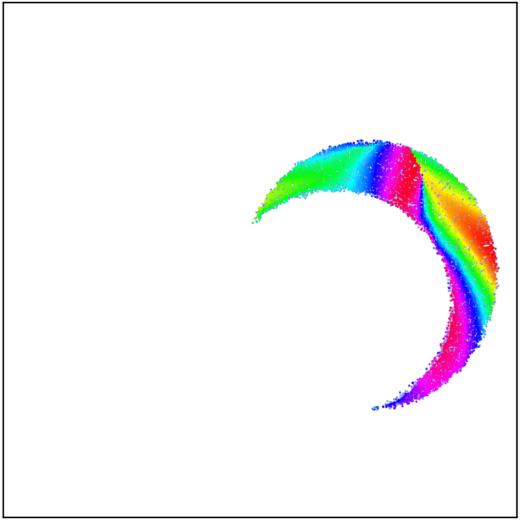

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Affordable geometric barycenters

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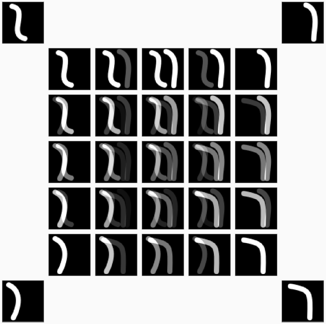

Linear barycenters

$$\text{Loss}(\alpha, \beta) = \|\alpha - \beta\|_{L^2}^2$$

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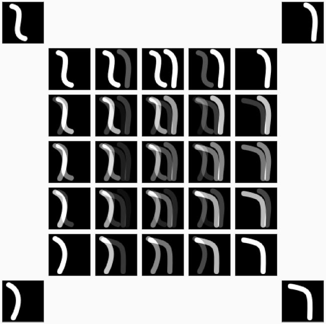
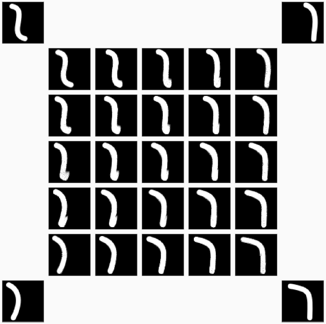


Linear barycenters

$$\text{Loss}(\alpha, \beta) = \|\alpha - \beta\|^2_{L^2}$$



Wasserstein barycenters

$$\text{Loss}(\alpha, \beta) = \text{OT}(\alpha, \beta)$$

Key points

- **Symbolic LazyTensors** are key to performances:
  $\longrightarrow$ KeOps, x30 speed-up vs PyTorch and TF.

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Main reference: my **PhD thesis**.

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For **users**: reliable, efficient `python` toolboxes:

- Fluid mechanics: `github.com/sd-ot/pysdot`
- Machine Learning on the CPU: `pot.readthedocs.io`
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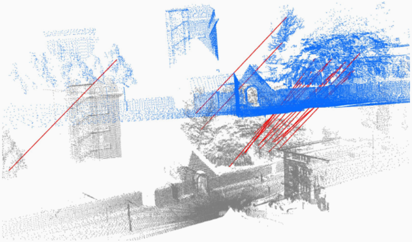
For **us**: new interesting questions:

- Link between S_ε and a **blurred Wasserstein** distance?
- What about **graphs**?

Thank you for your attention.

Any questions ?

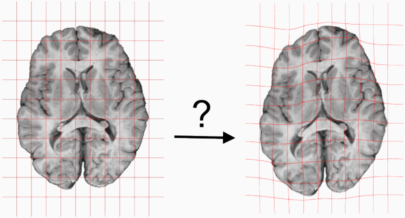
First setting: processing of point clouds



From the documentation of the Point Cloud Library.

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

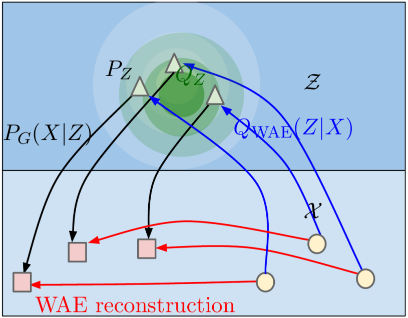
Second setting: medical imaging



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,
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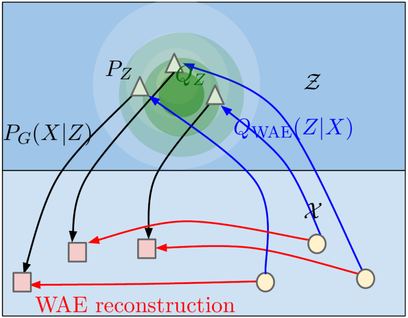

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Which **Loss** function should we use?

Dual norms - link with the GANs literature

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

$$\text{look for } \theta^* = \arg\min_{\theta} \max_{f \in B} \langle \alpha(\theta) - \beta , f \rangle$$

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- $B = \{\, \| f \|_\infty \leqslant 1 \,\} \implies$ Loss = TV norm:
  - zero geometry
  - **too many** test functions

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- $B = \{ \| f \|_\infty \leqslant 1 \} \implies \text{Loss} = \text{TV norm:}$
    - zero geometry
    - **too many** test functions
- $B = \{ \| f \|_2^2 + \| \nabla f \|_2^2 + \cdots \leqslant 1 \} \implies \text{Loss} = \text{kernel norm:}$
    - may saturate at infinity
    - **screening** artifacts

Dual norms - link with the GANs literature

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

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