Geometric data analysis, beyond convolutions

Jean Feydy

King's College London – December 2019

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

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Quick CV:

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

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$\Longrightarrow$ Looking for contacts in London!

The medical imaging pipeline [Ptr19, EPW+11]

Sensor data

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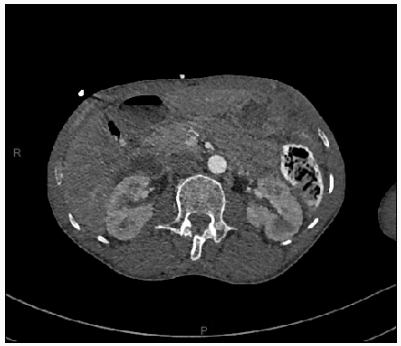

Raw image

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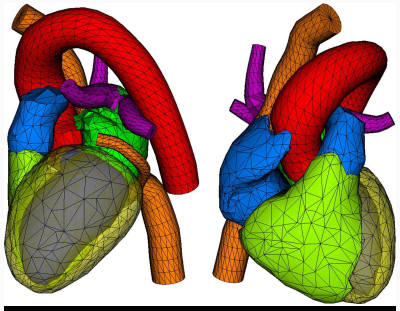

High-level description

Raw image

Sensor data

Computational anatomy

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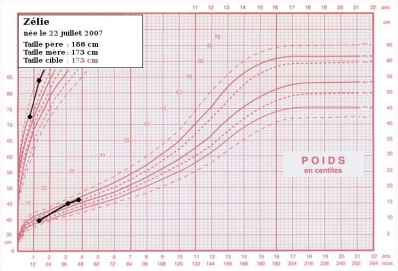

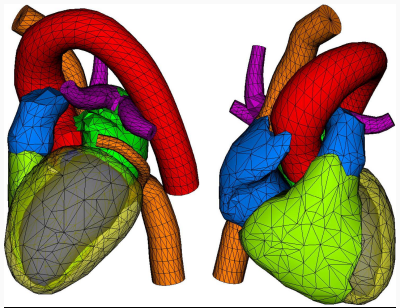

Valuable information

Statistics

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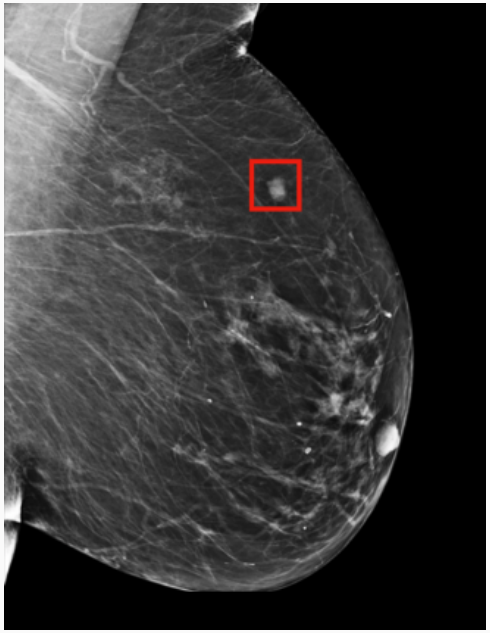
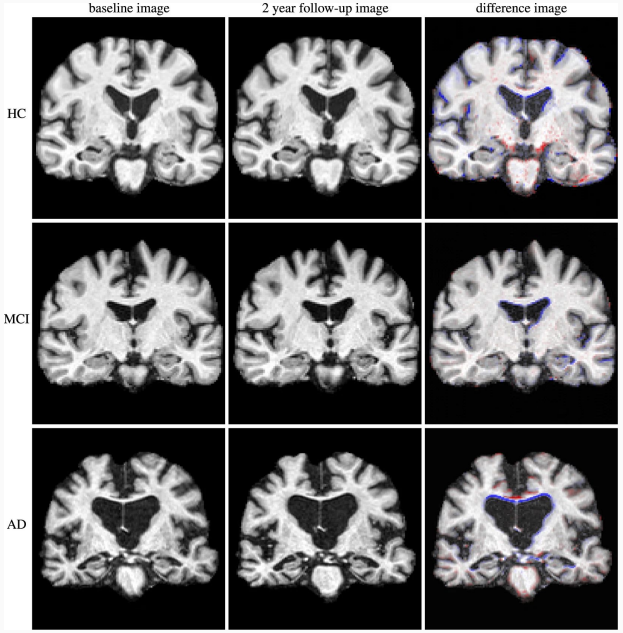
Computational anatomy [CSG19, LSG+18, CMN14]

Three main problems:



Spot patterns

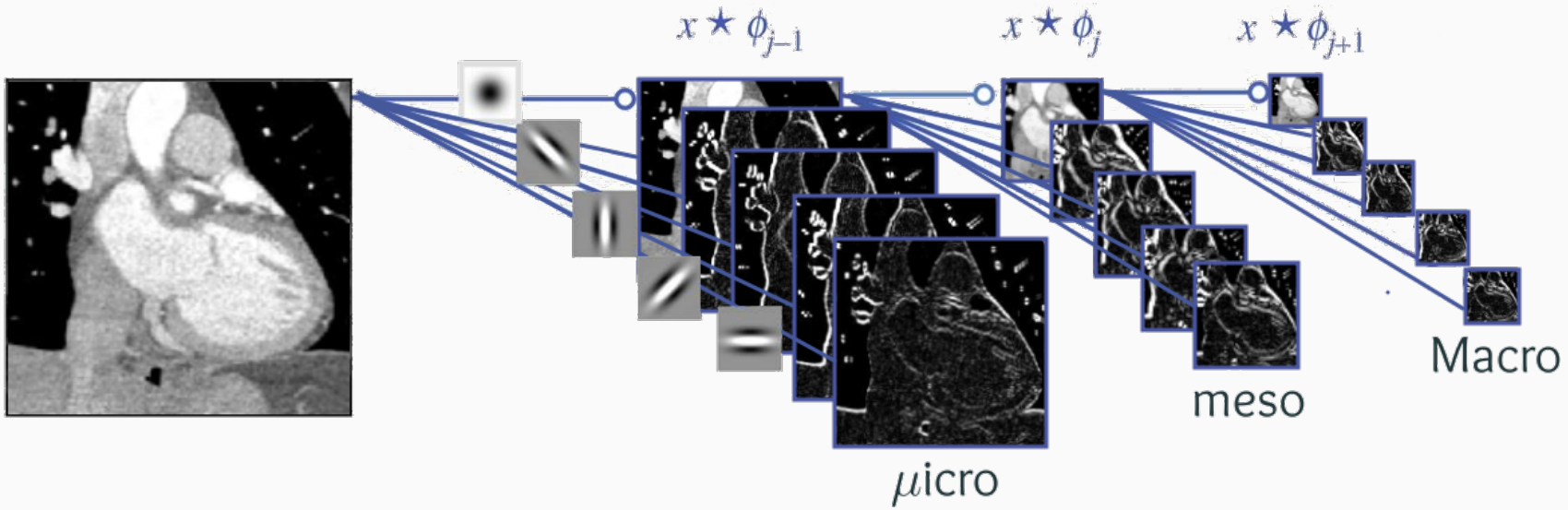


Analyze variations

Fit models

2010-2020: the deep learning revolution [Mal16, PMC11, WZTF17]

Explicit wavelet transform



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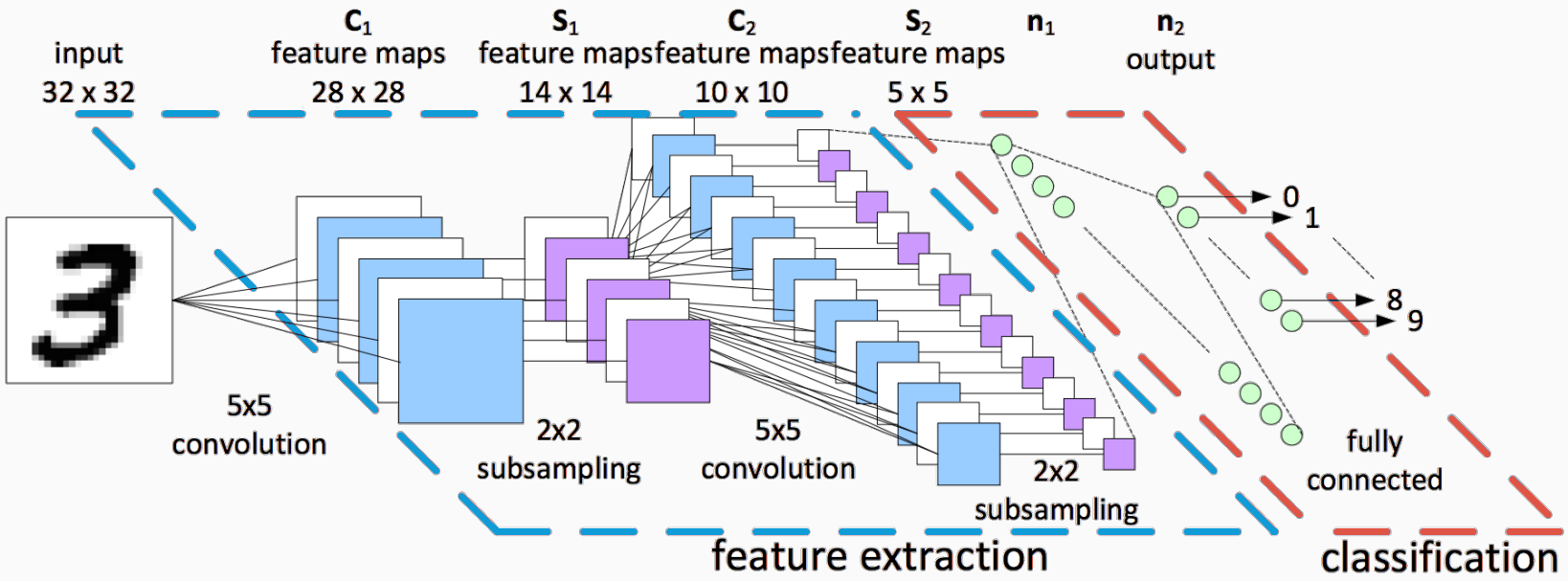
Explicit wavelet transform $\longrightarrow$ **data-driven** CNN



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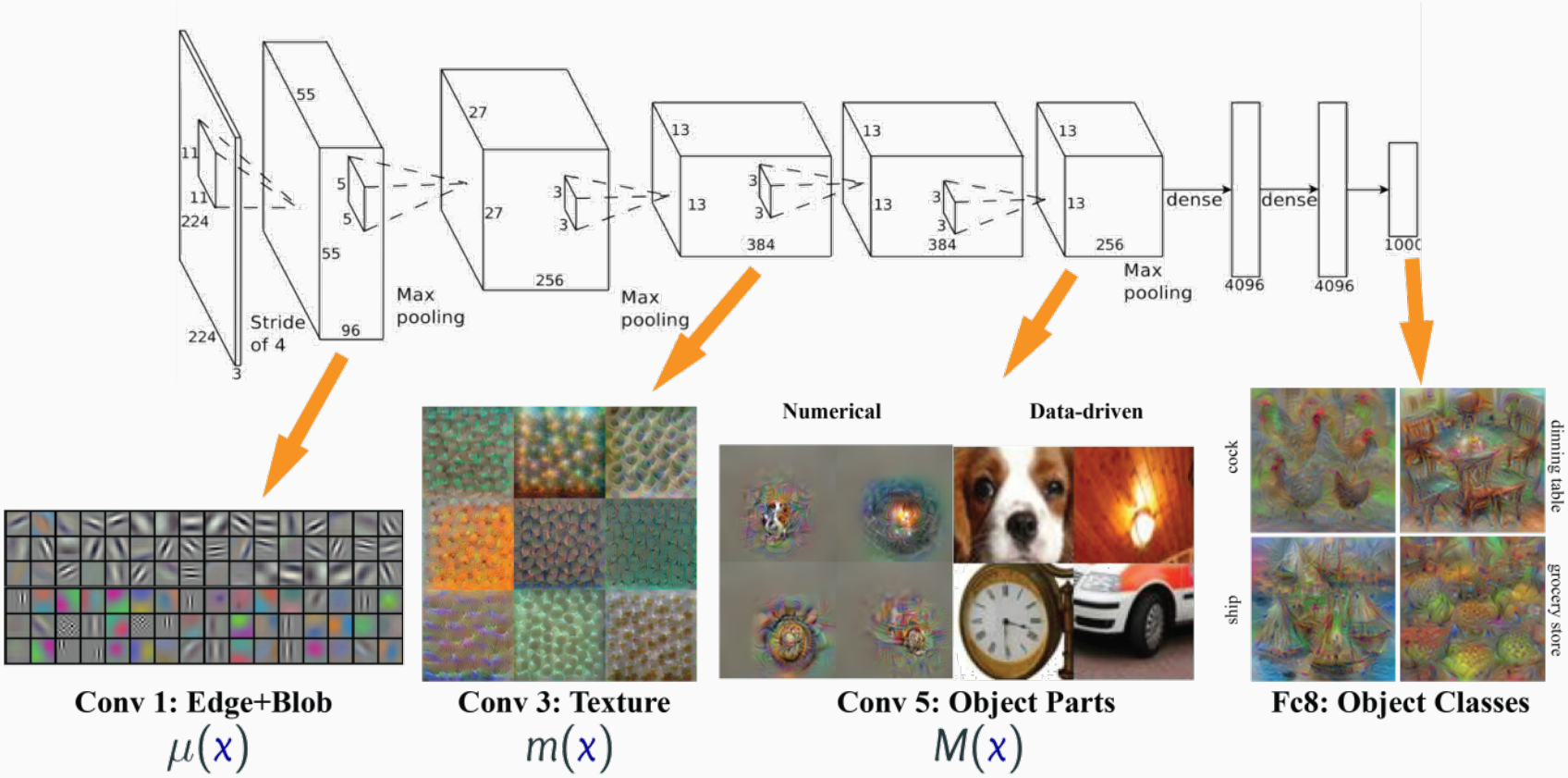


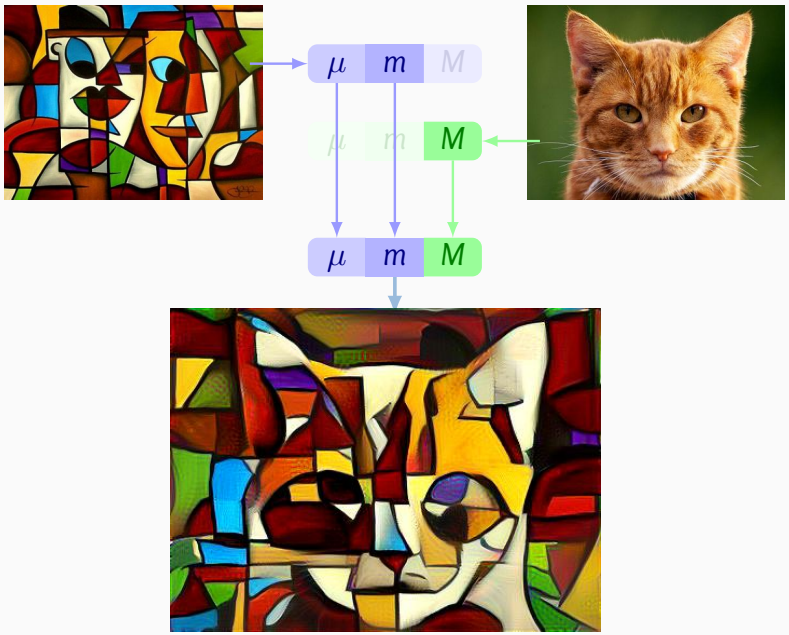
Conv 1: Edge+Blob $\mu(x)$

Conv 3: Texture $m(x)$

Conv 5: Object Parts $M(x)$

Fc8: Object Classes

(Wavelets $\rightarrow$ CNNs) = improvement for... [NN16, Ola18]



Texture processing

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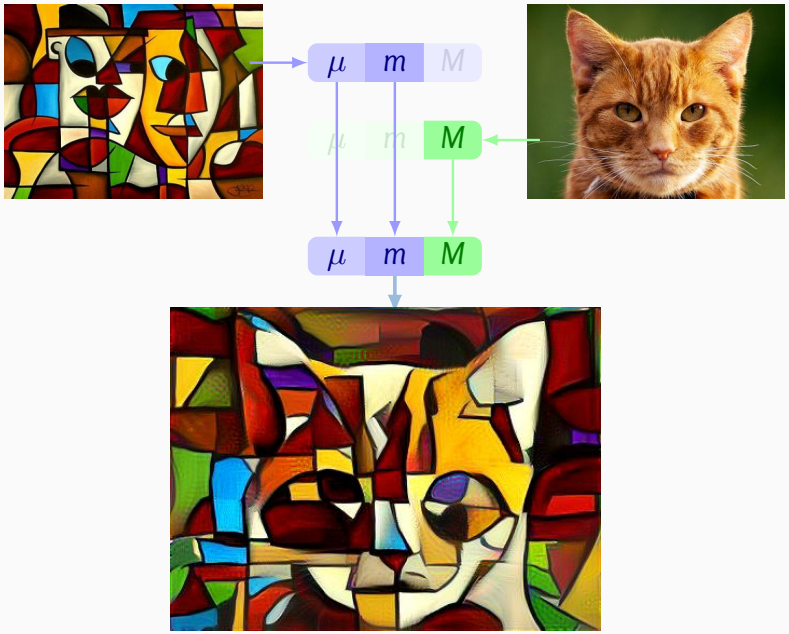

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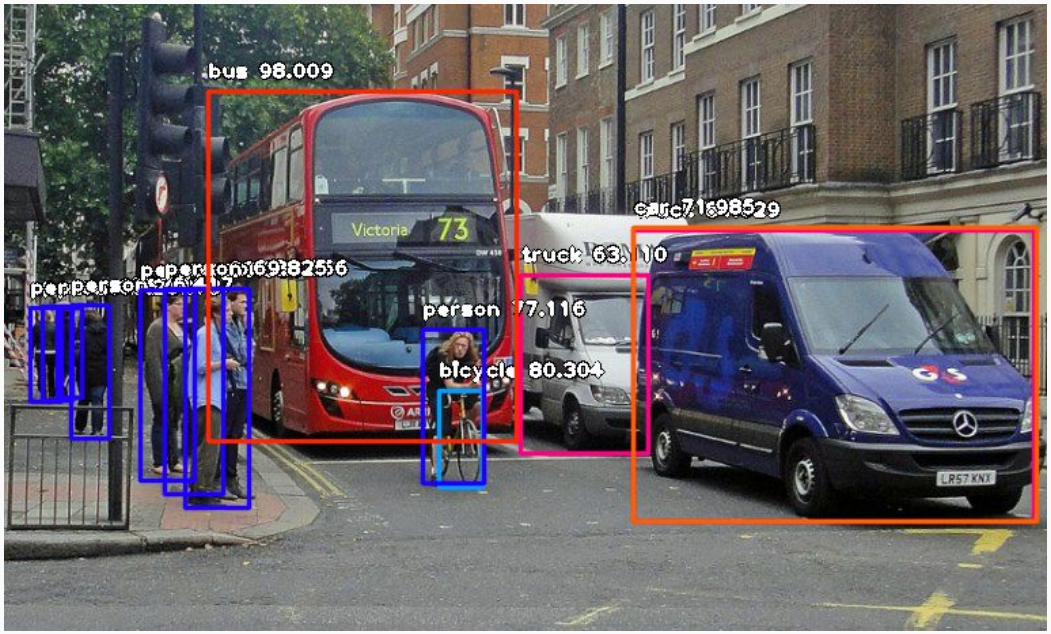
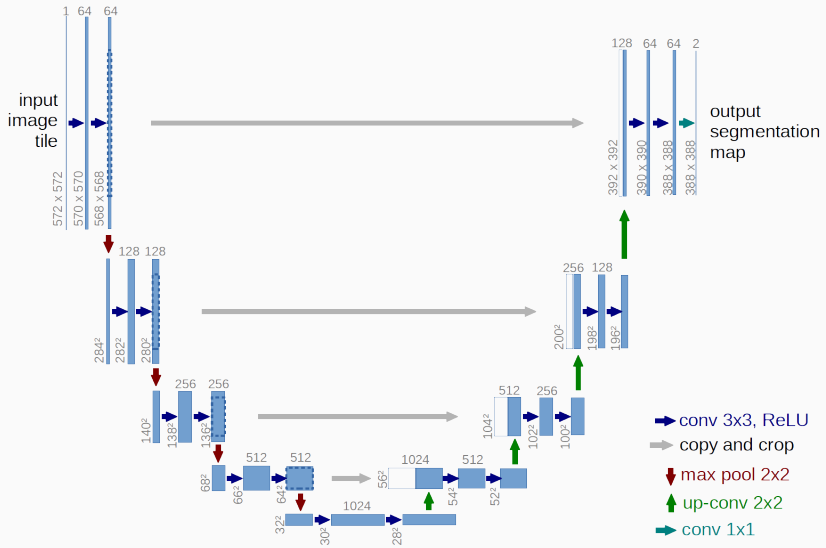
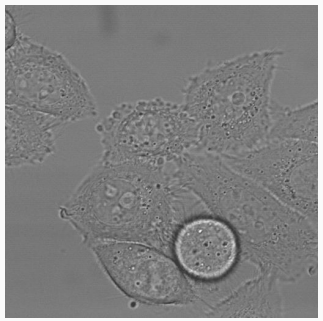
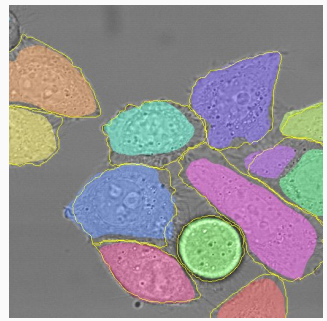


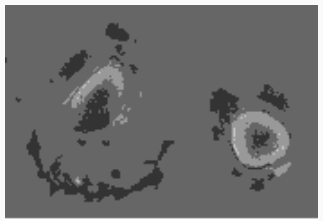
Feature detection

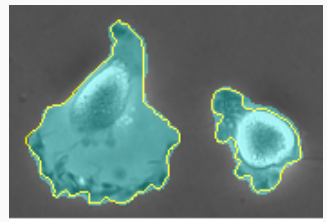
Segmentation with U-nets [RFB15]









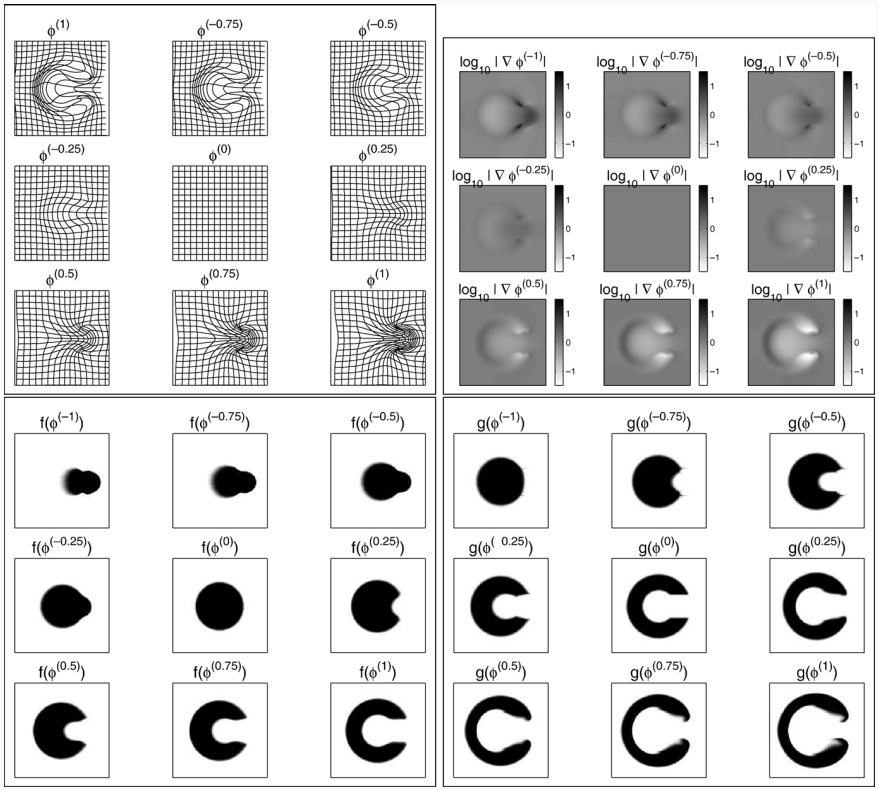


Architecture

Input

Output

Limitations of CNNs [Ash07, Gla05]



Advection $\neq$ Convolution

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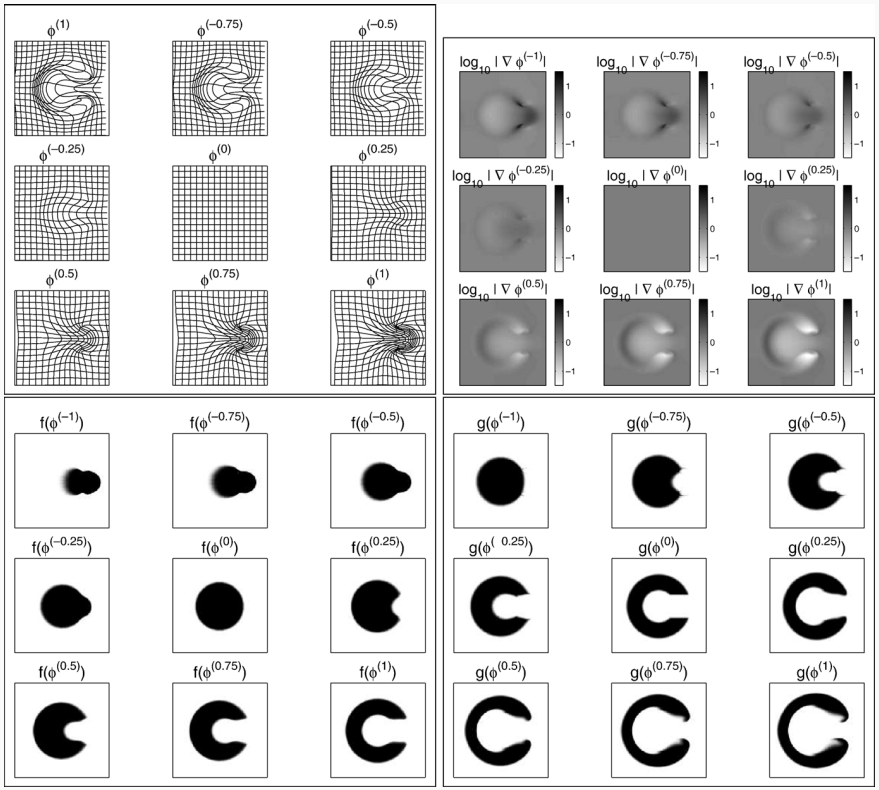

Advection ≠ Convolution

Mesh deformation

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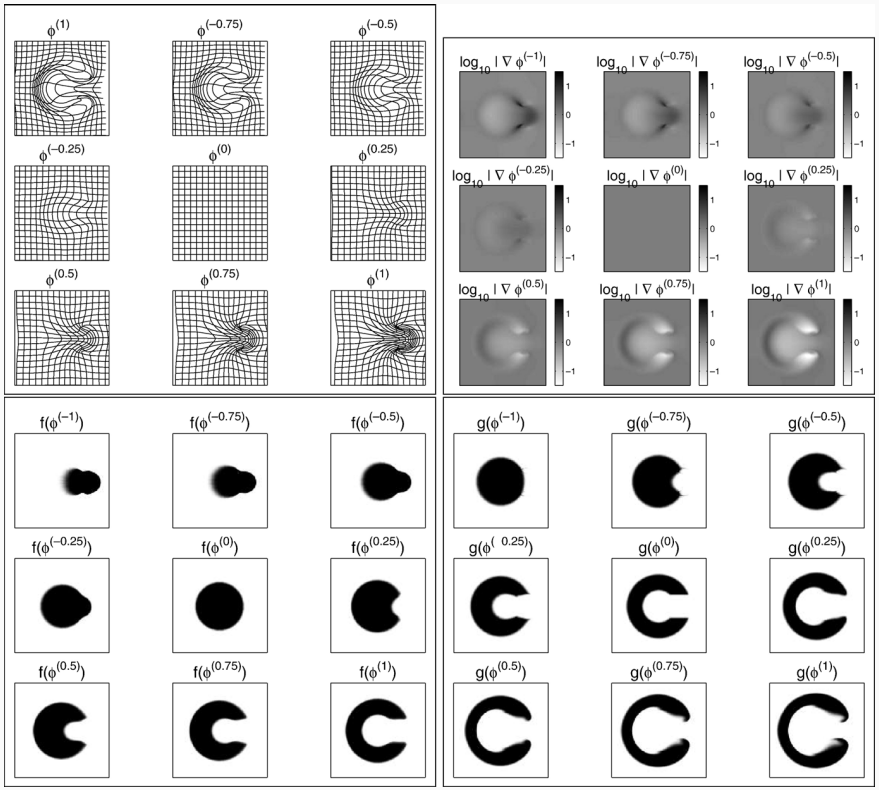

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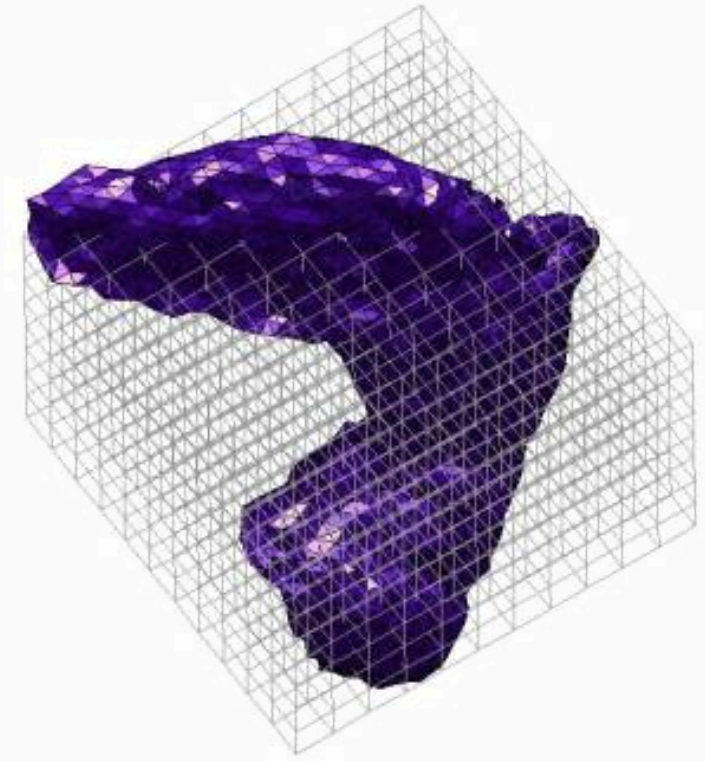

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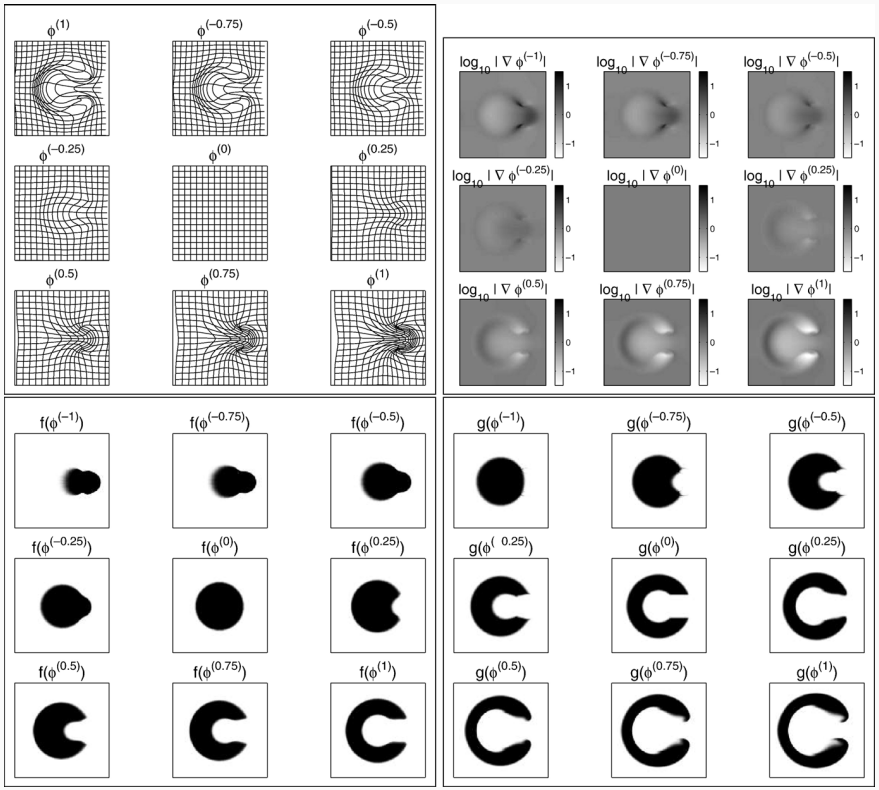

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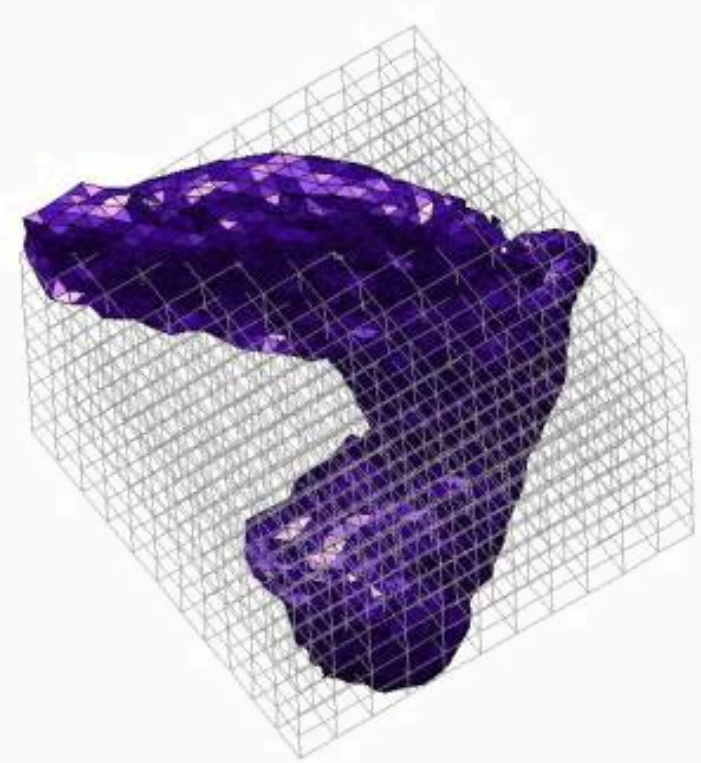

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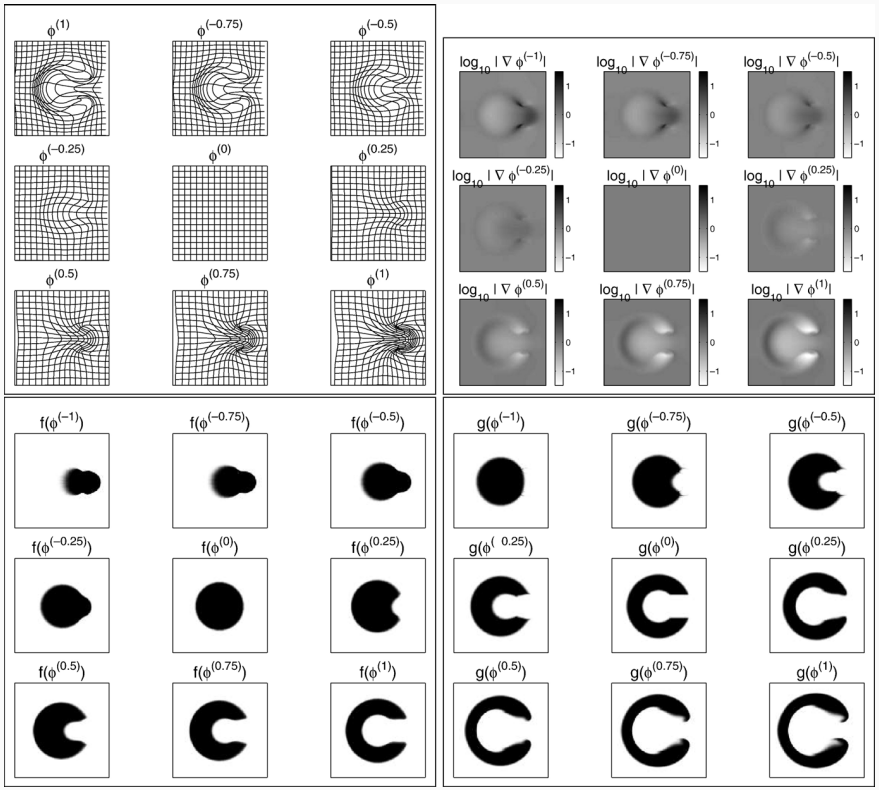

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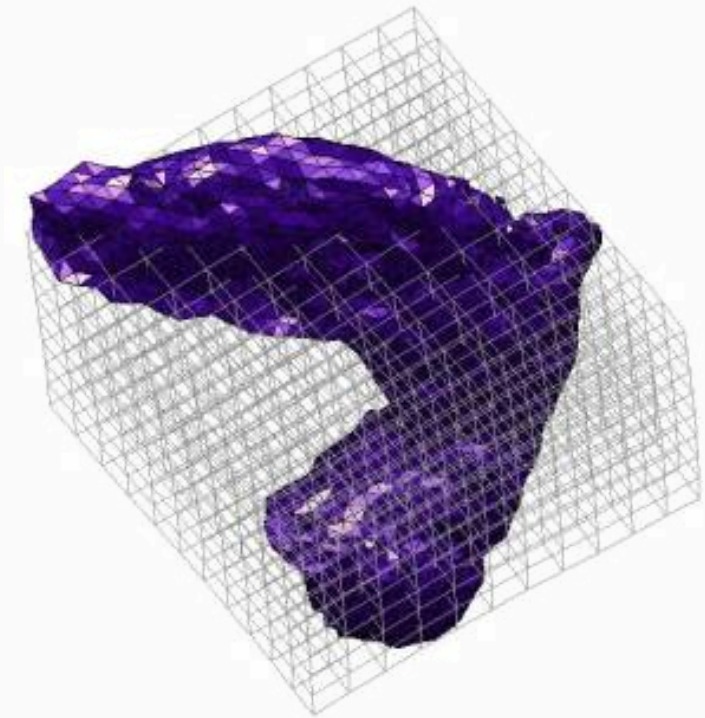

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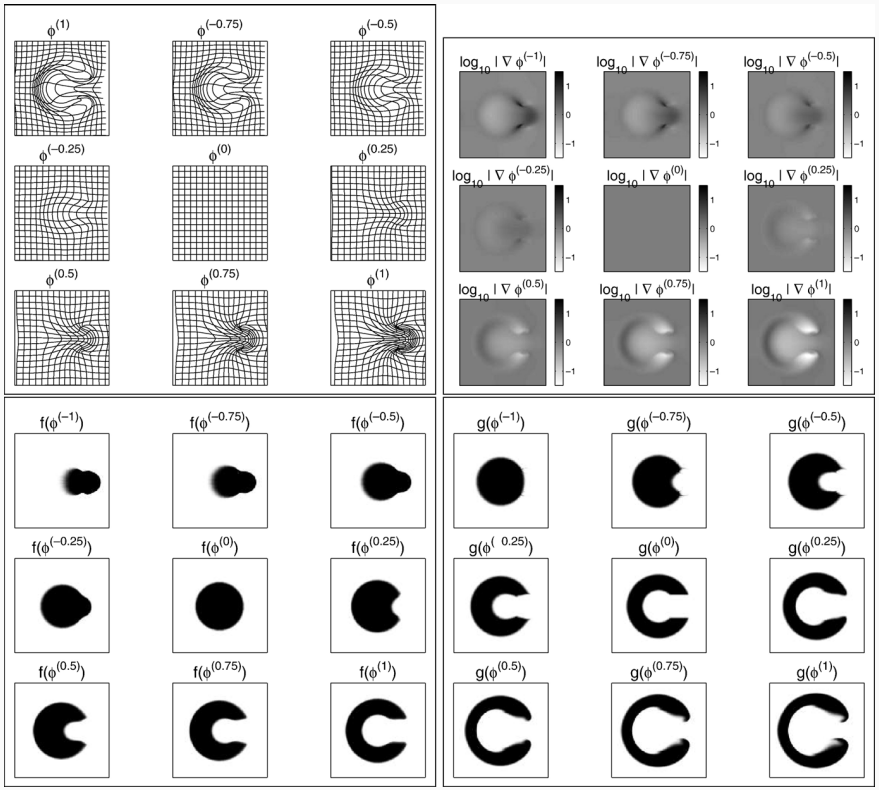

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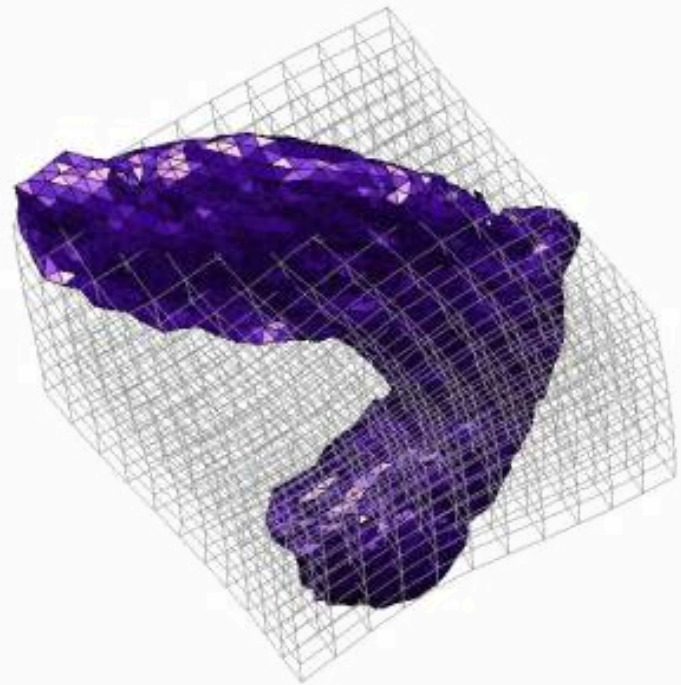

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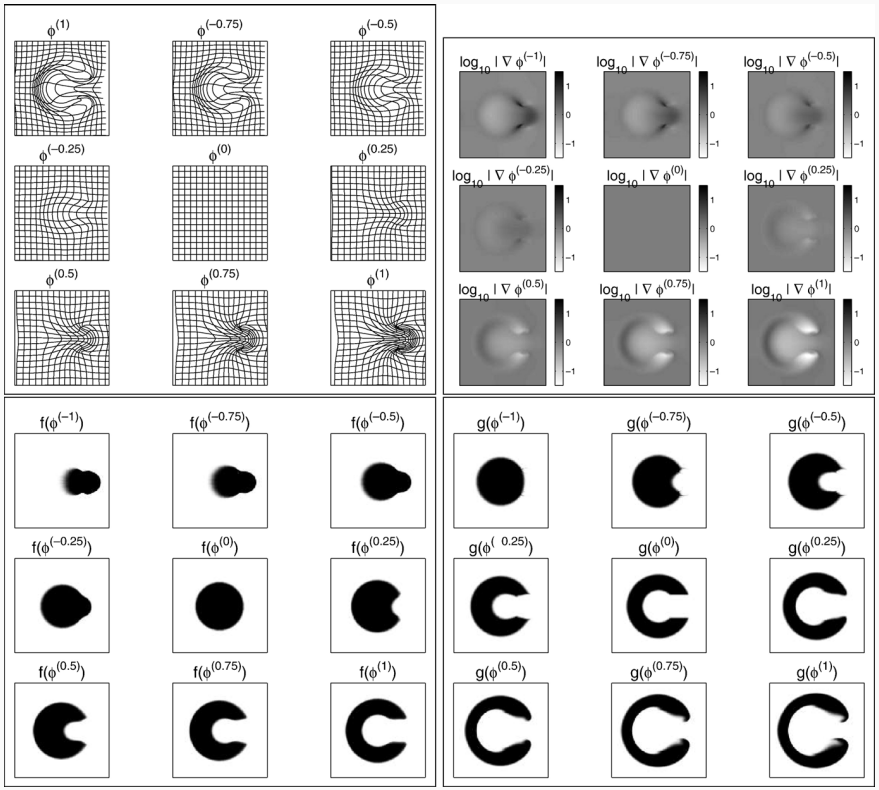

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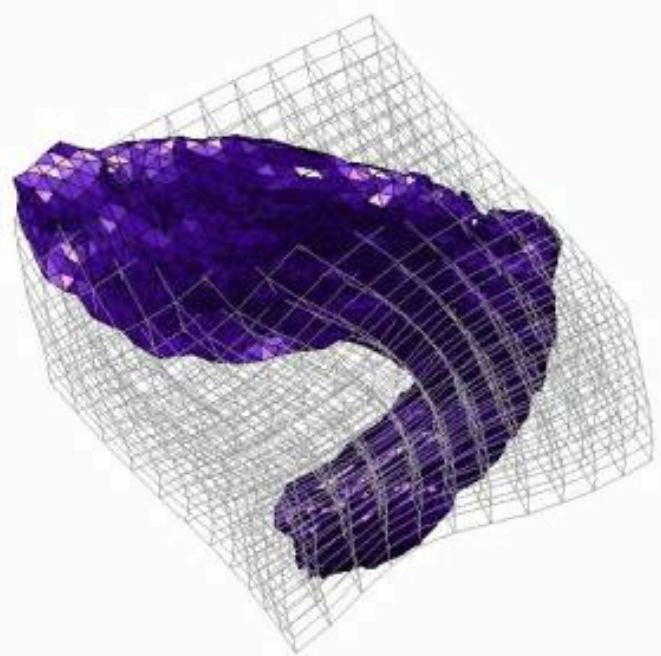

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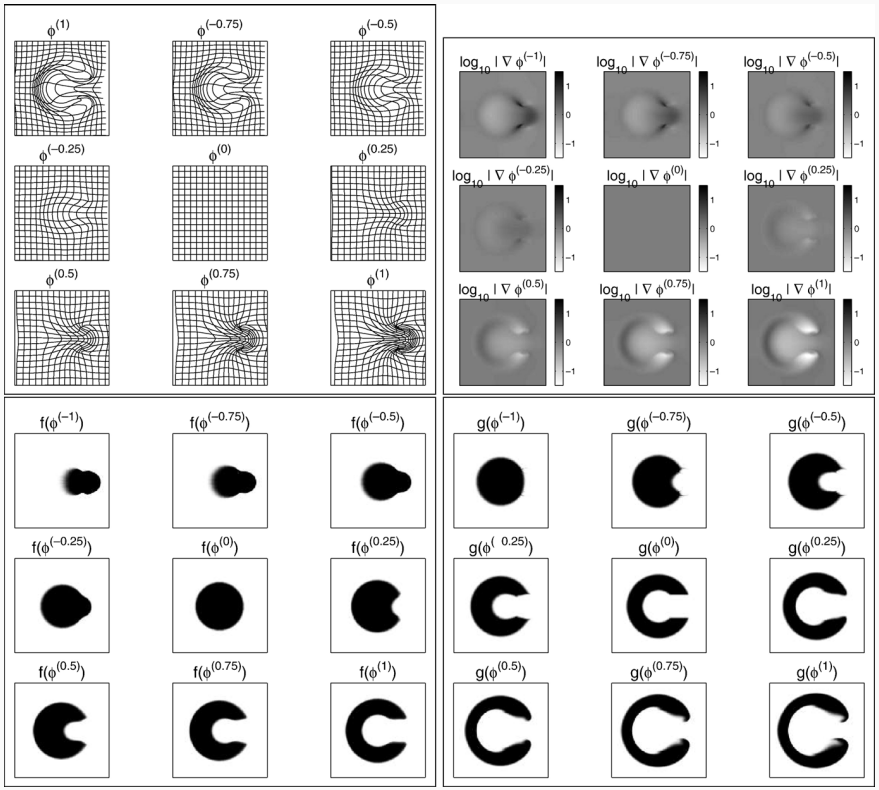

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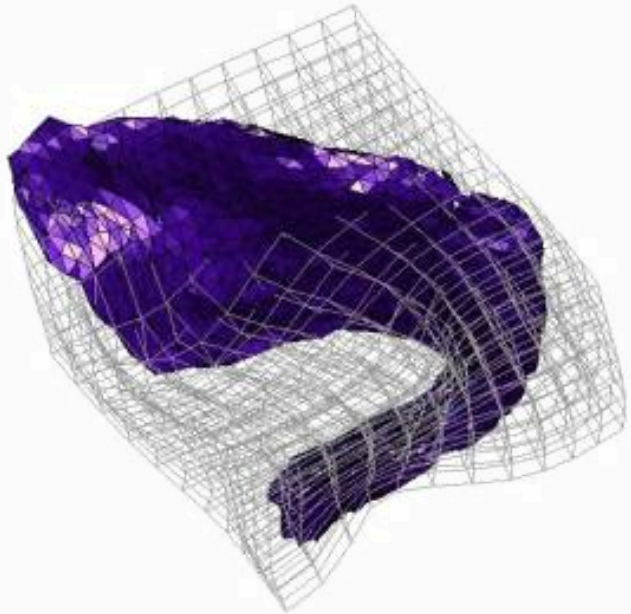

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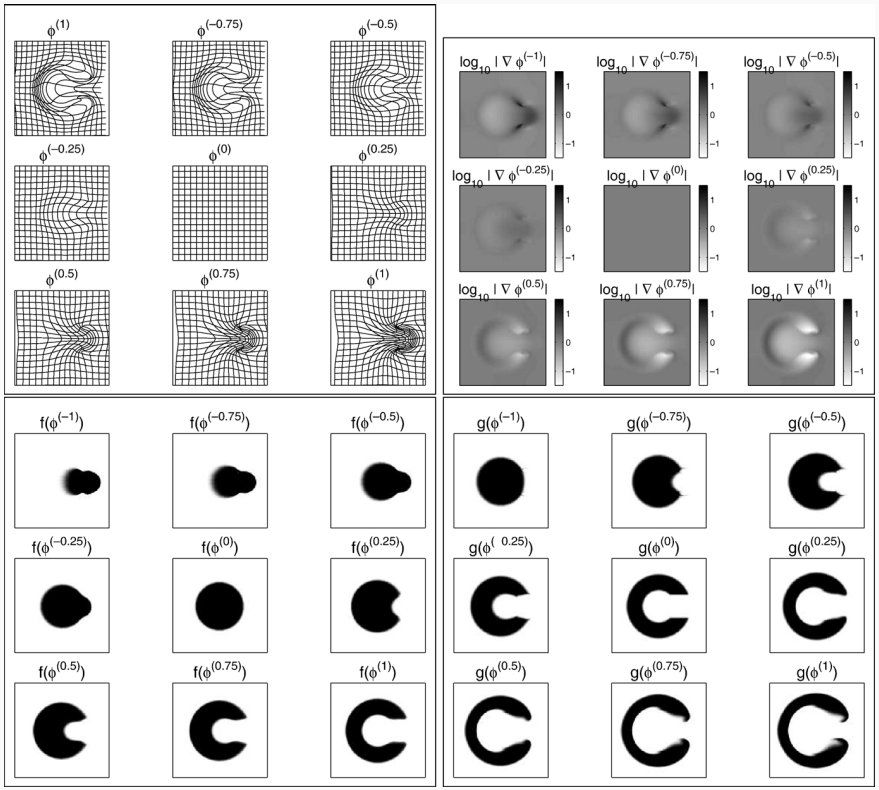

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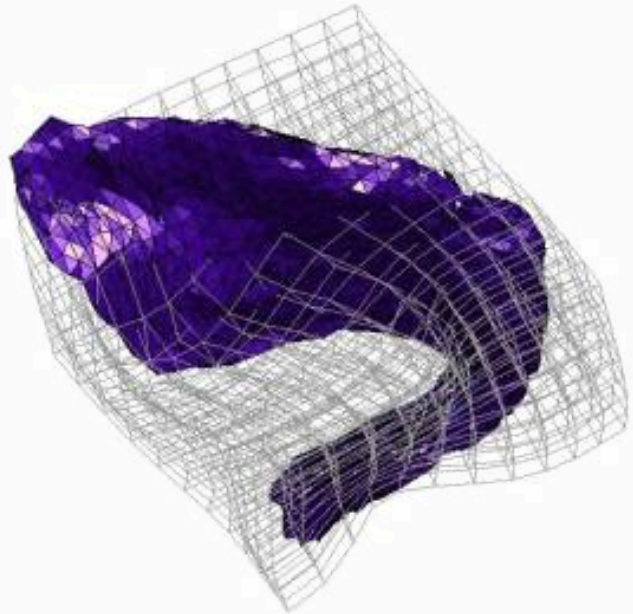

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$\Longrightarrow$ Geometry is easier with **coordinates:** point clouds and meshes.

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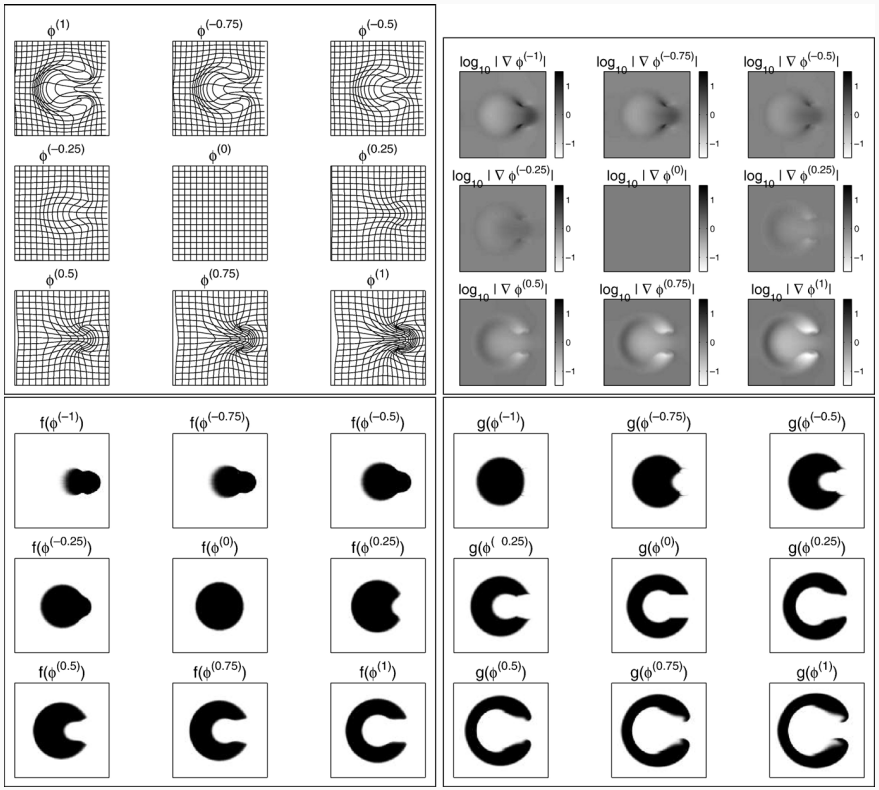

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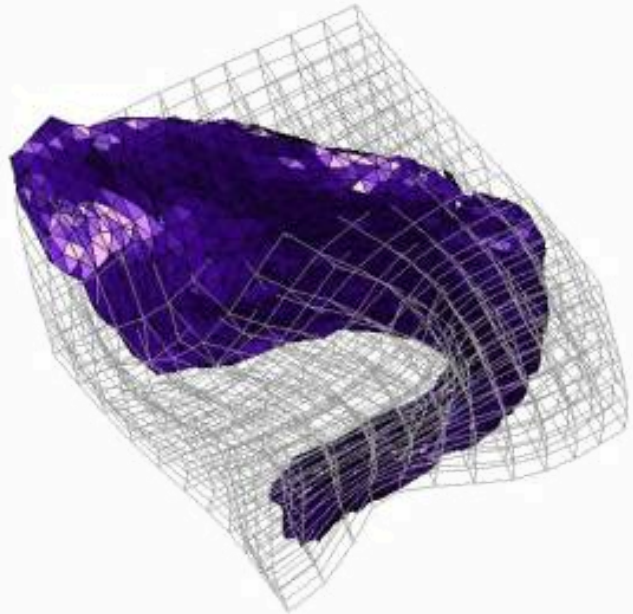

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Problem: not supported well by TensorFlow and PyTorch.

Geometry's back on the menu!

Today, we'll discuss:

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- **Efficient** GPU implementations
  $\longrightarrow$ KeOps extension for PyTorch, NumPy, Matlab, R.

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- **Geometric** loss functions
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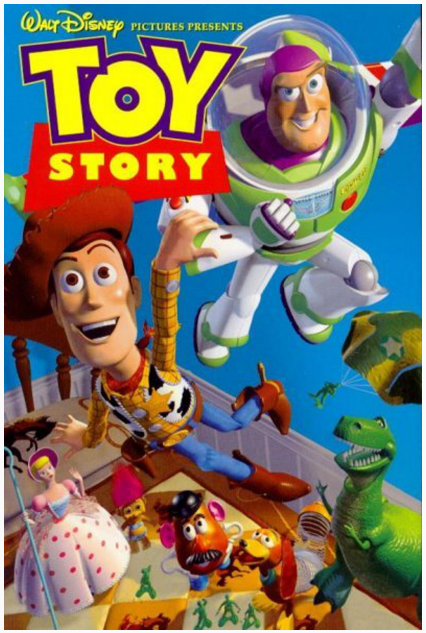
- **Robust** deformation architectures
  $\longrightarrow$ After the break :–)

Combining graphics and deep learning

What is a GPU?

Nvidia RTX 2080 Ti = **4,352 cores**, 11Gb RAM for **~1,500$.**

Designed for graphics: 1 GFlop $\simeq$ 1 $



1995

Today

Deep learning frameworks: unlocking GPUs for research

Theano (RIP), TensorFlow and PyTorch combine:

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$\Longrightarrow$ Ideally suited for research!

PyTorch, in practice

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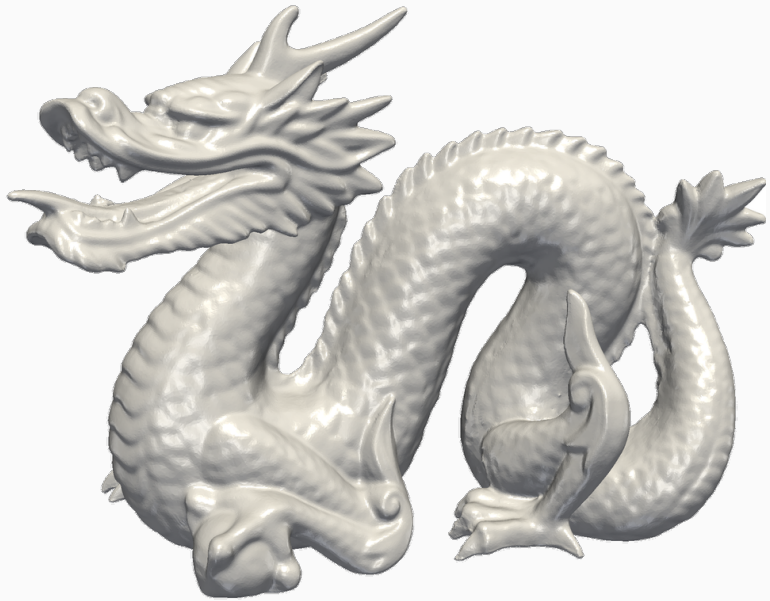
```
RuntimeError: cuda runtime error (2) : out of memory at
/opt/conda/.../THCStorage.cu:66
```

Memory overflow with 10k points? We should do better. [CL96]

11k triangles



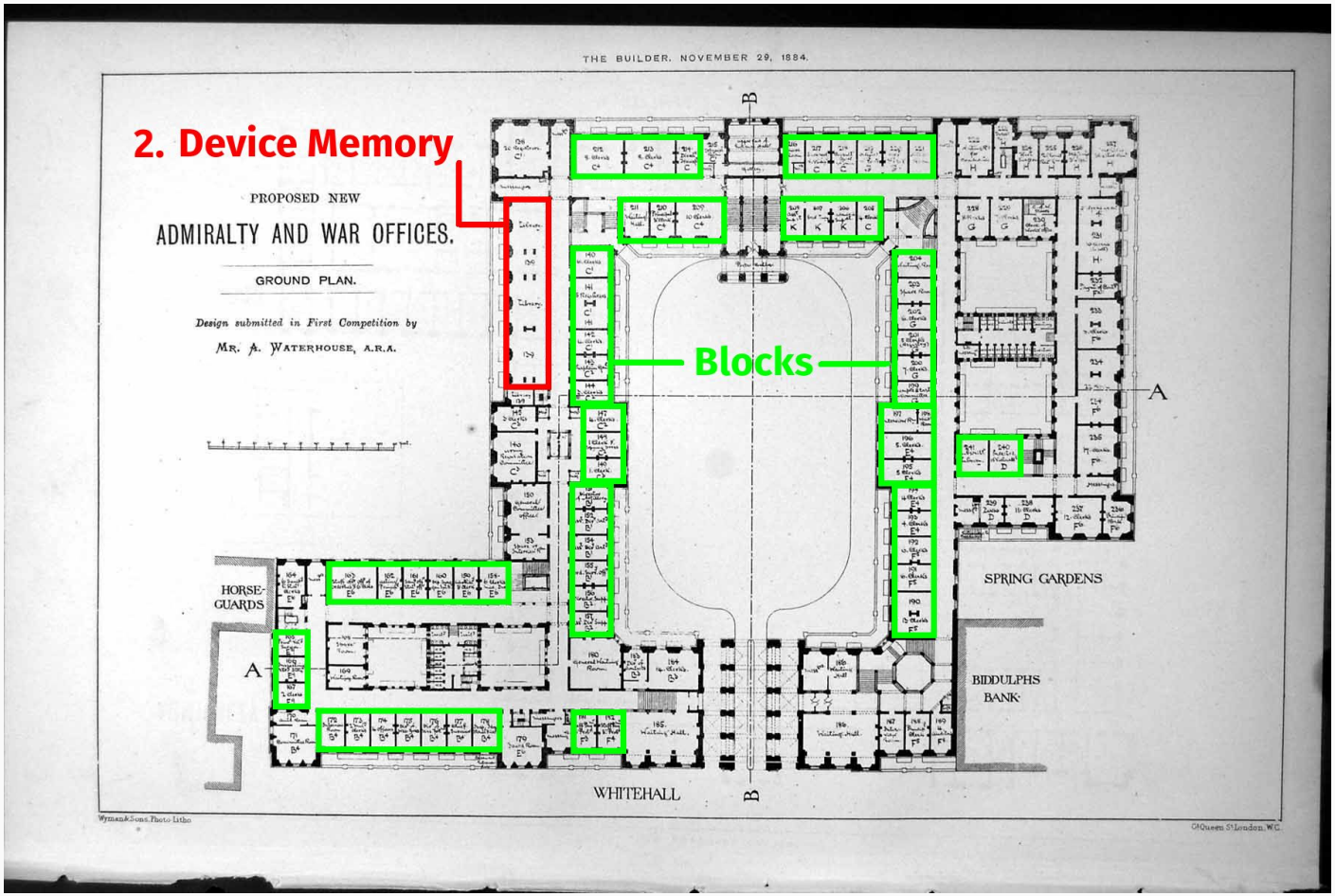
871k triangles

What a GPU really looks like

Turing architecture.

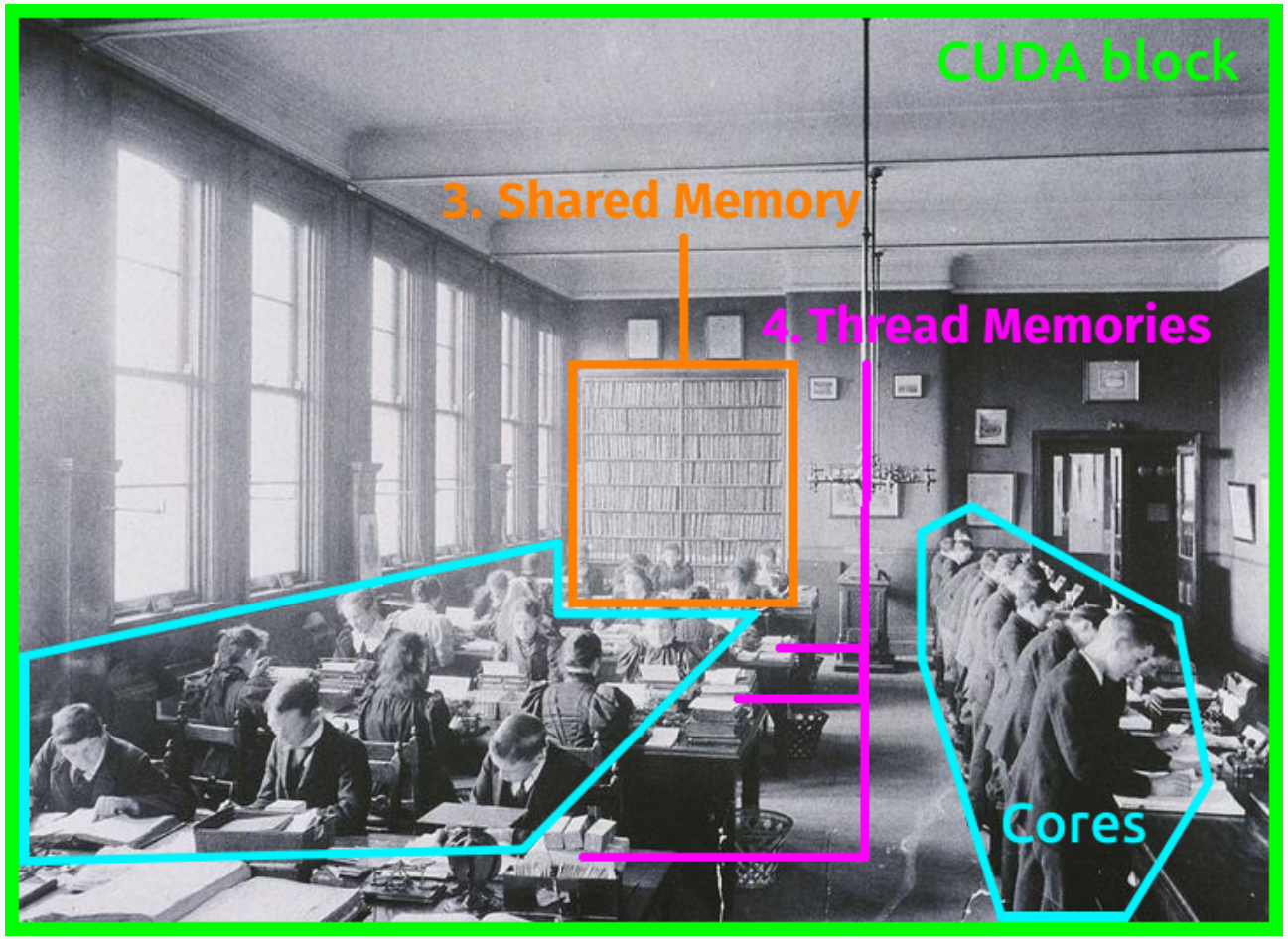
What a GPU really looks like

The Admiralty and War Offices, built in 1884.



What a GPU really looks like

Inside view of a CUDA block.



Memory management is key

Rules of CUDA programming:

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PyTorch and TF variables are always stored in the **Device** mem.

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- 4 layers of **memory** (Host, Device, Block, Thread).
- **Shared Block buffer** (~128 Kb) is 50x faster than Device mem.

PyTorch and TF variables are always stored in the **Device** mem.
Explicit C++ implementations for:

- Convolutions.
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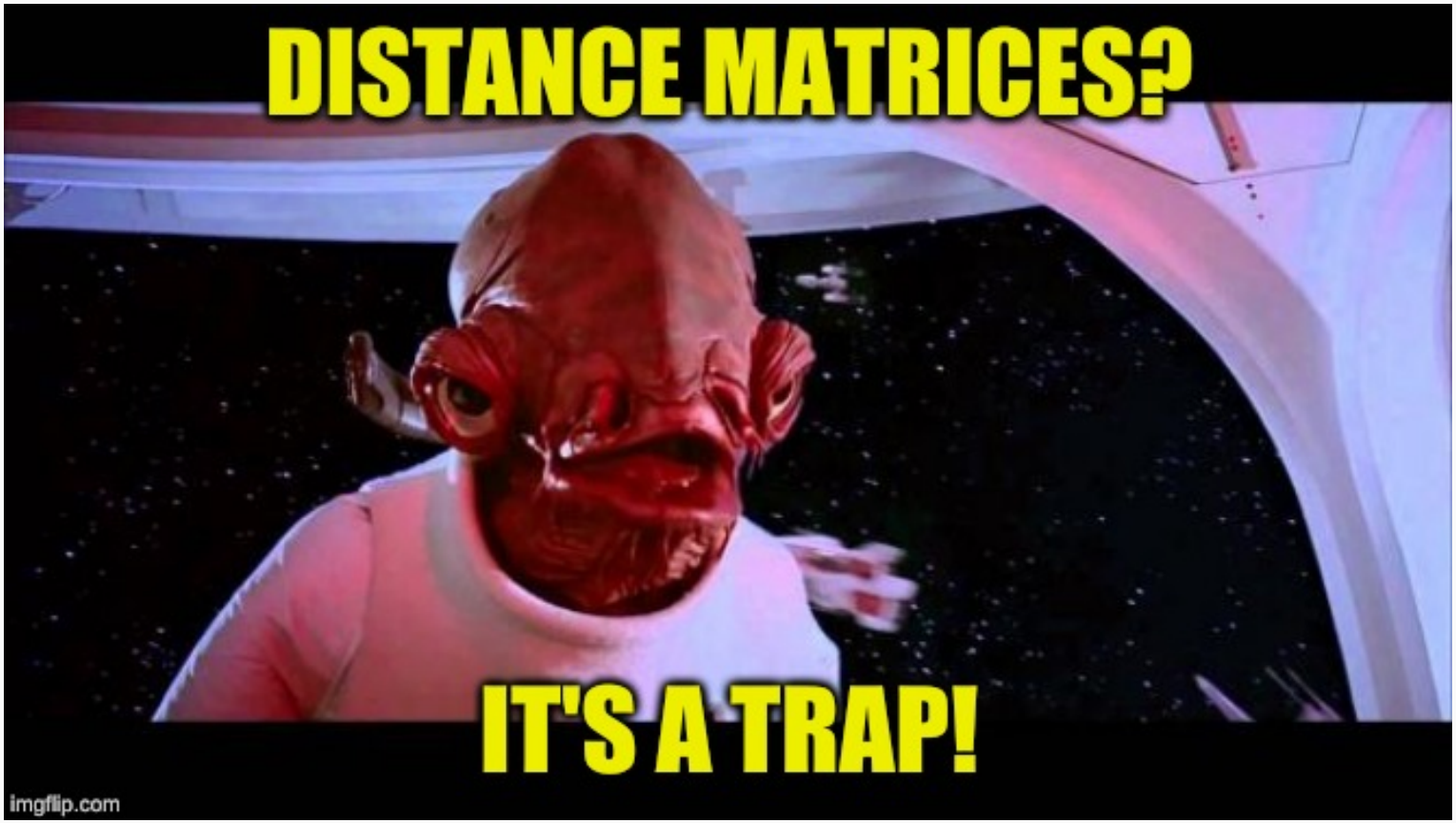
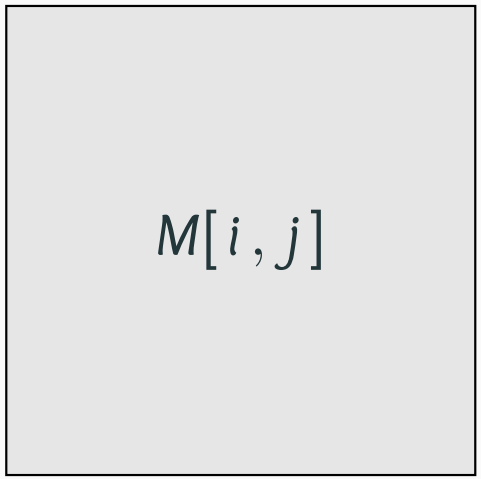
$\Longrightarrow$ We need to do the same!

Keep in mind...



Introducing KeOps LazyTensors



Array

Coefficients only

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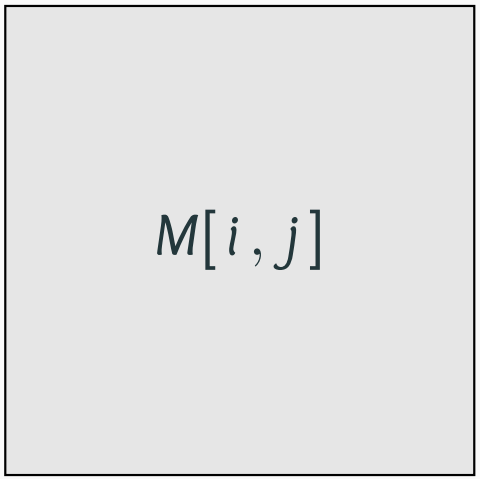

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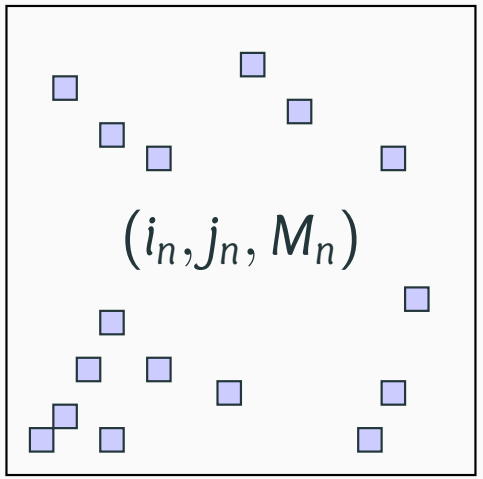

Sparse matrix

Coordinates + coeffs

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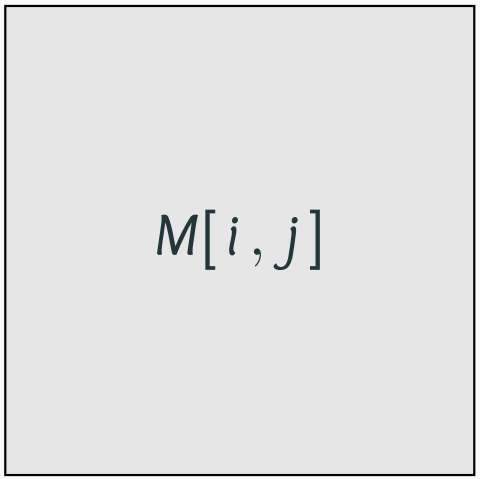

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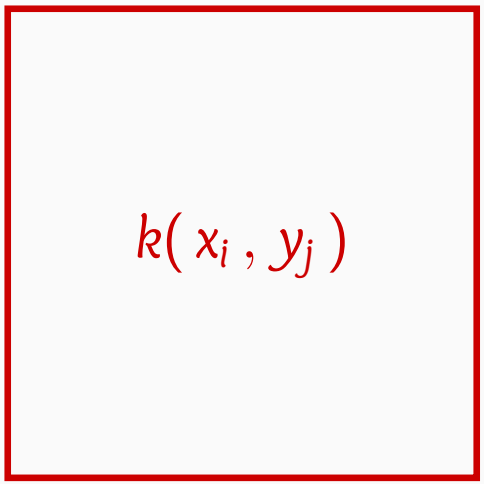
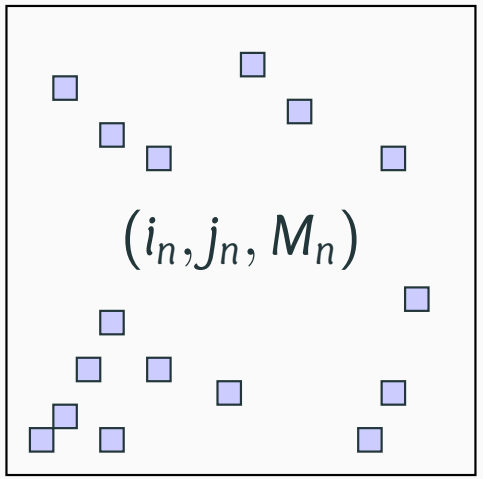


Symbolic LazyTensor

Formula + point clouds



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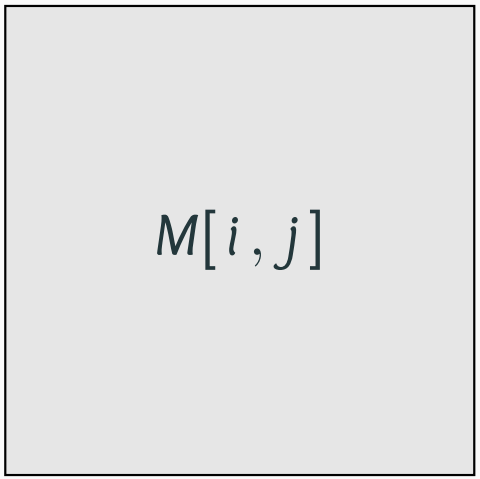

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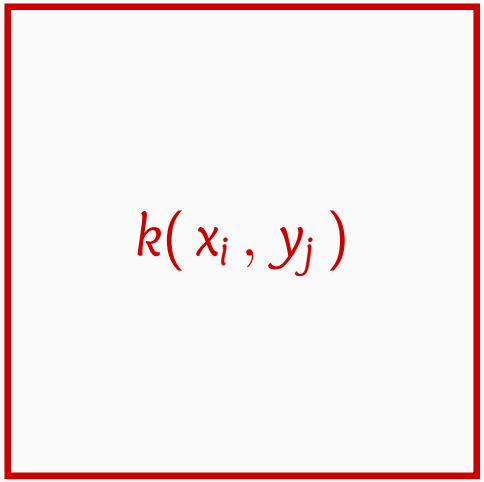

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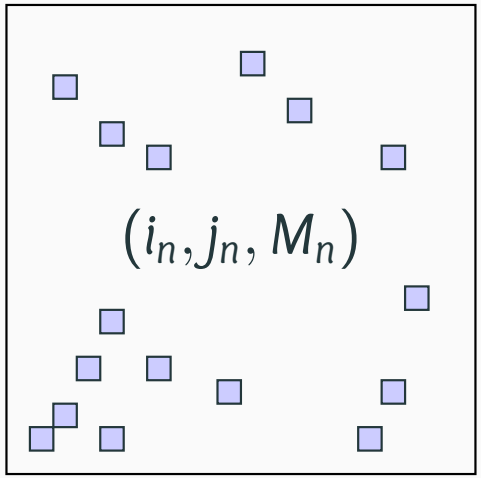

Sparse matrix

Coordinates + coeffs

```
pip install pykeops
```

It works!

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# Large point clouds in [0,1]^3
import torch
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g_x = torch.autograd.grad((a_i ** 2).sum(), [x])
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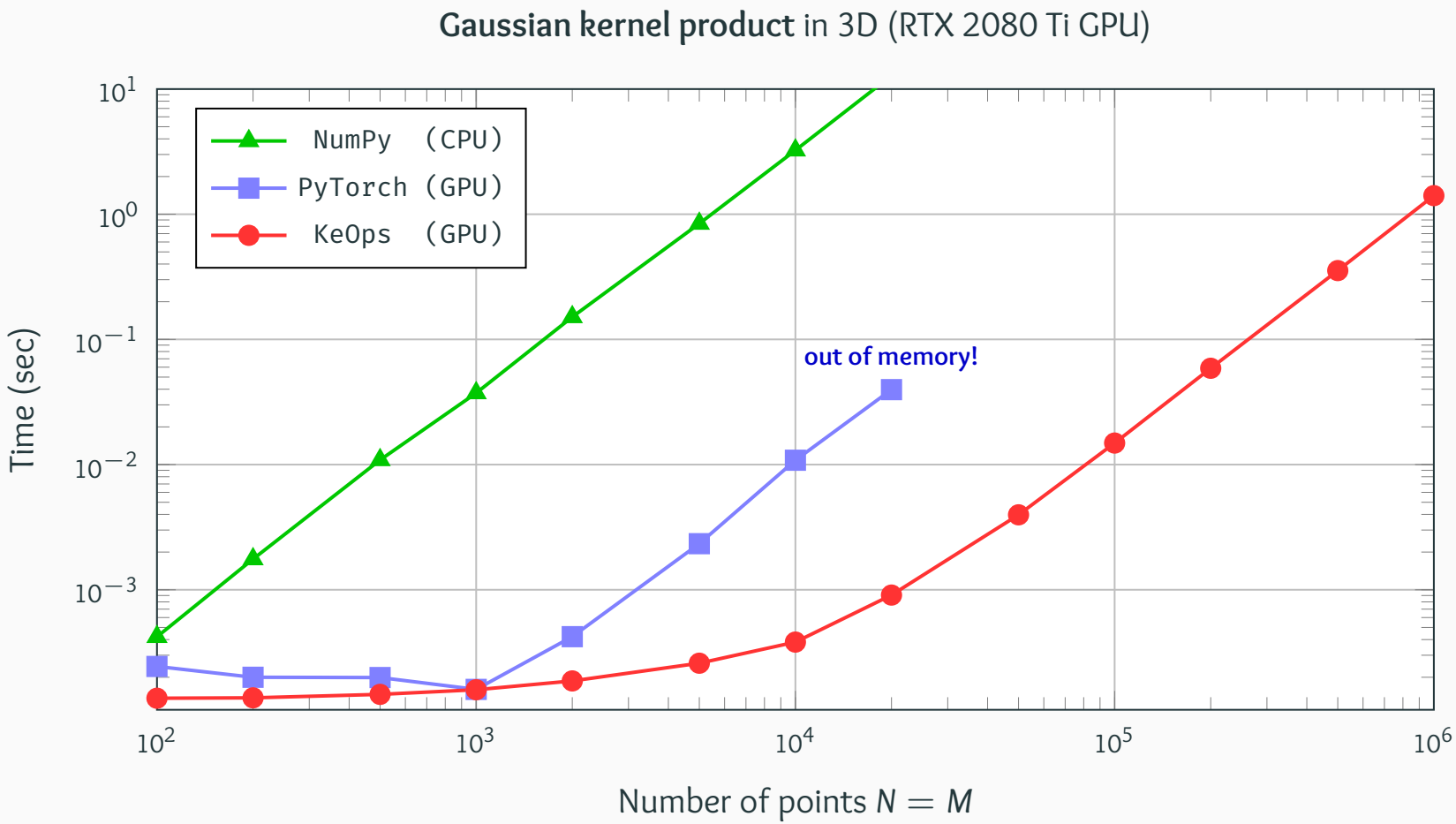
Scaling up to real data



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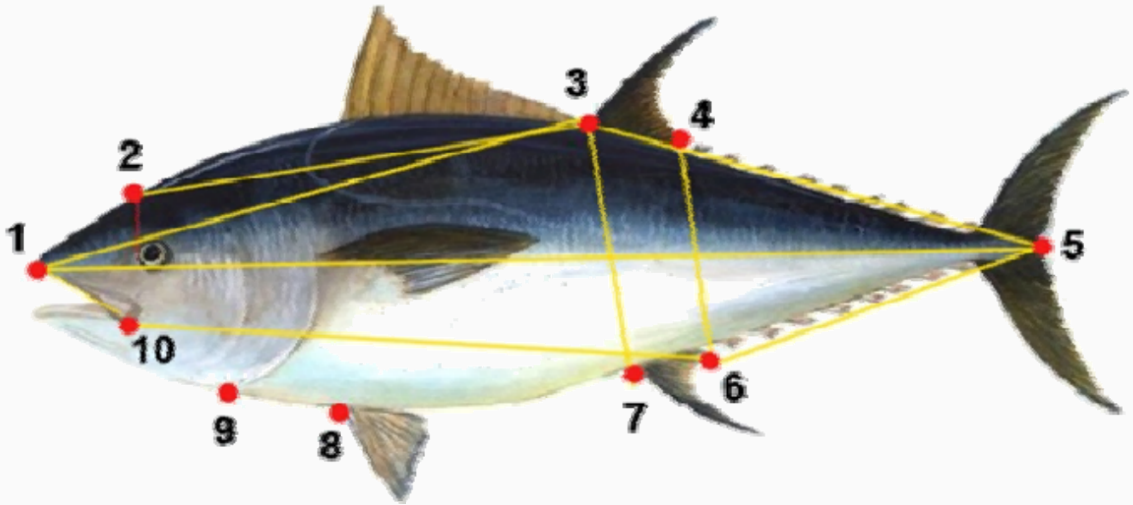
- Scikit-learn-like **documentation**:

`www.kernel-operations.io`

Geometric loss functions

Life is easy when you have landmarks...



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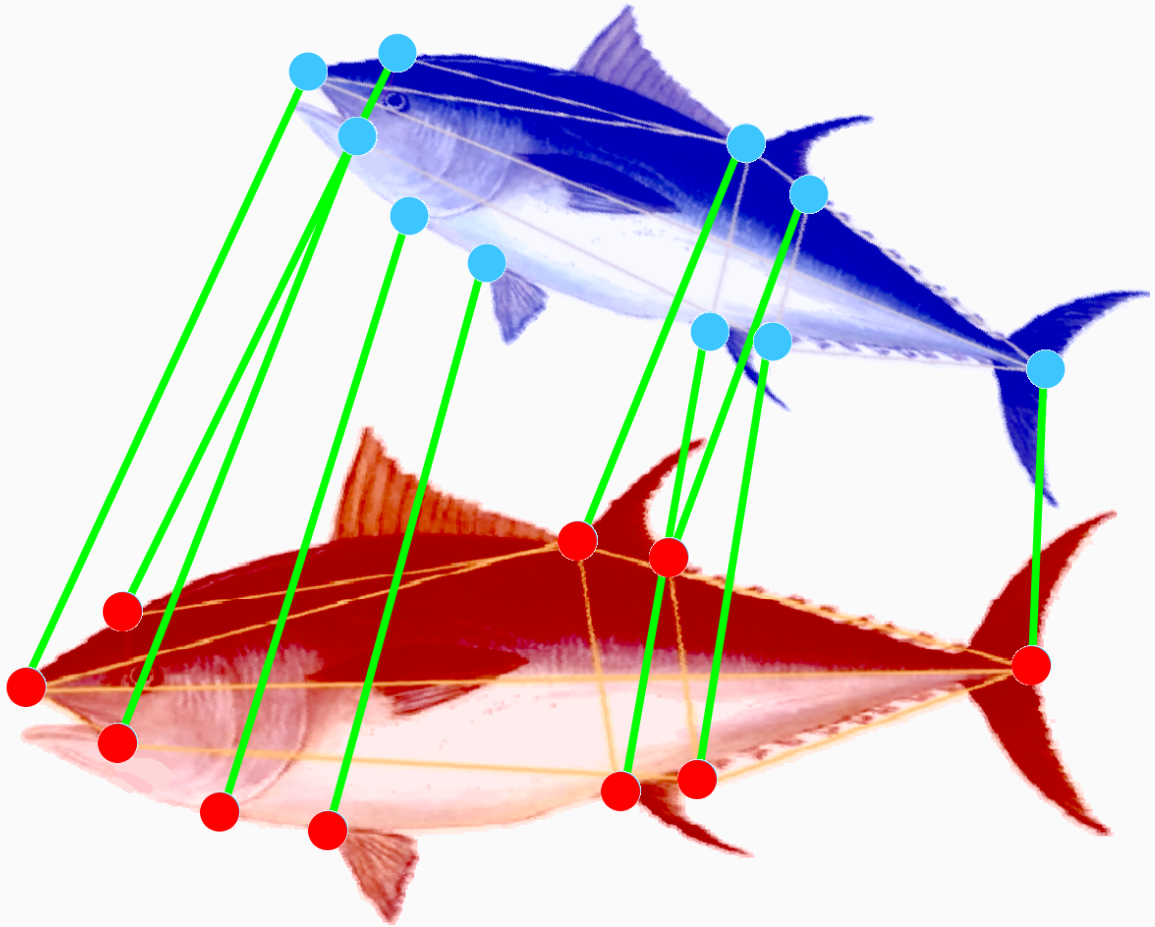

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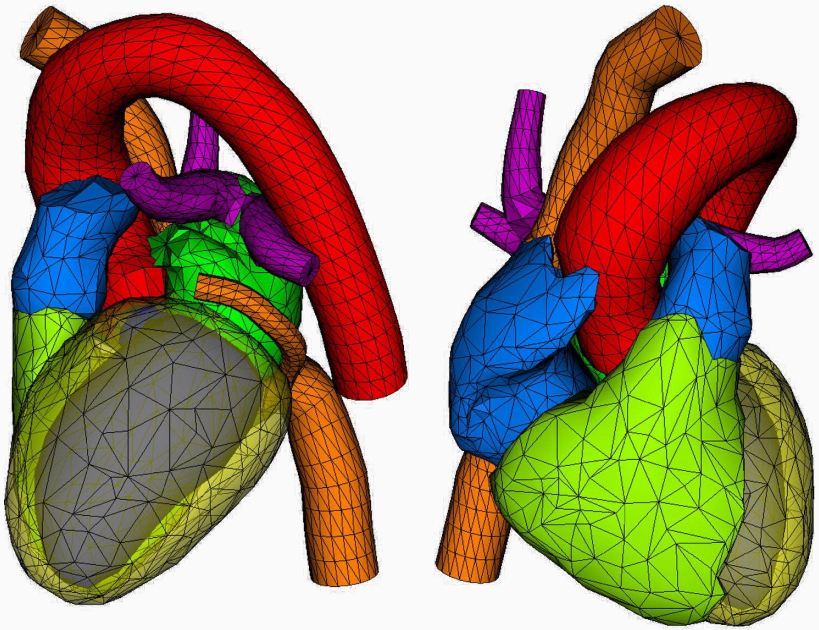
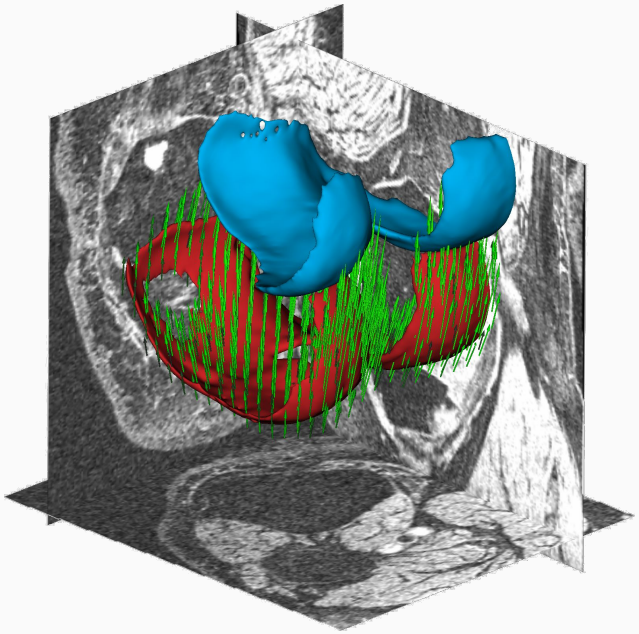
Unfortunately, medical data is often unlabeled [EPW+11]



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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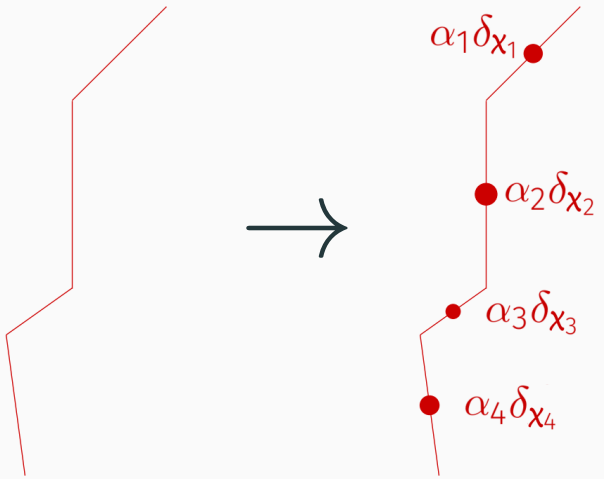

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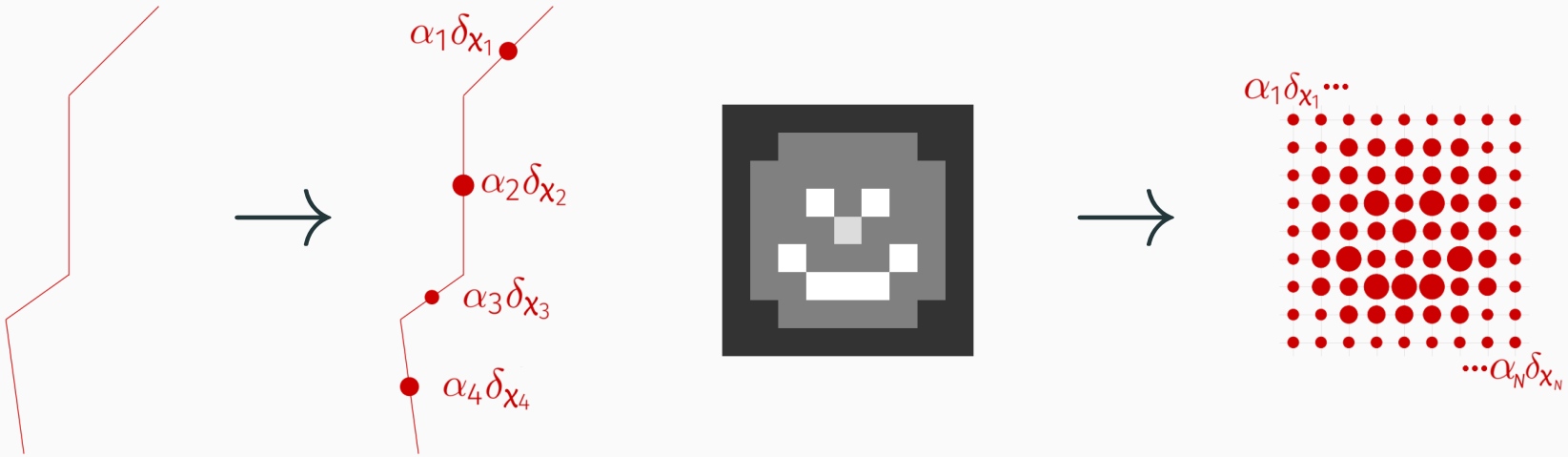
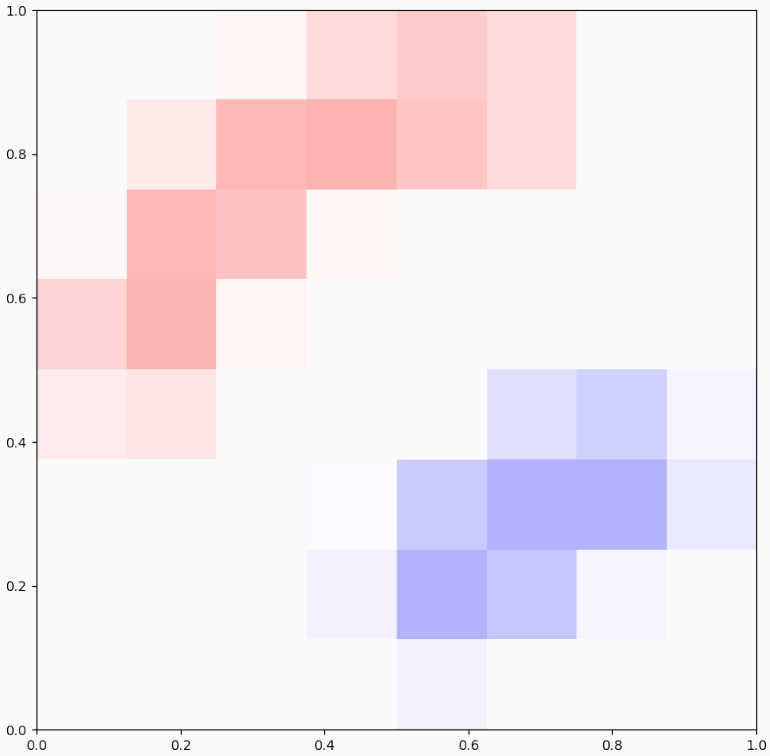


A baseline setting: density registration



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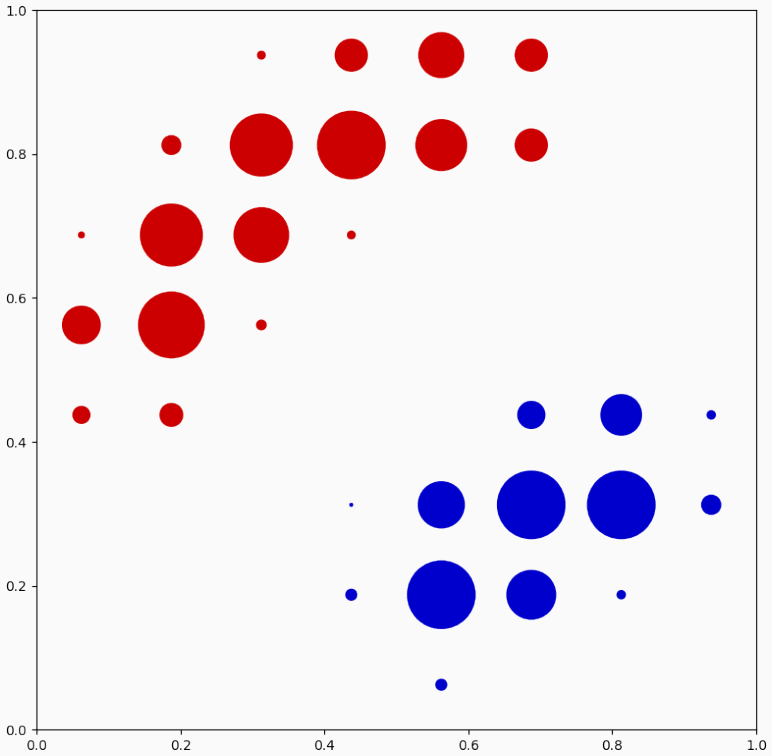

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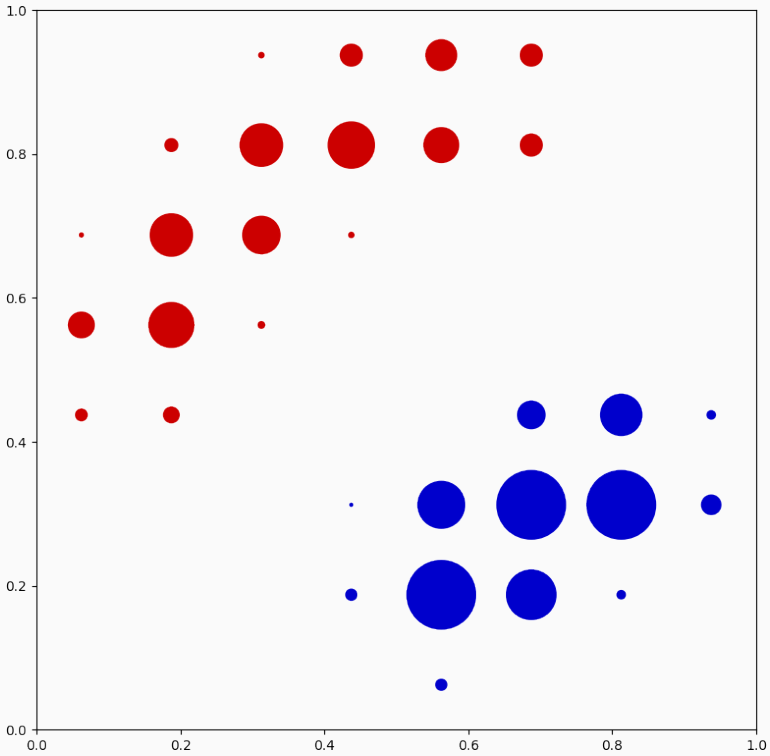

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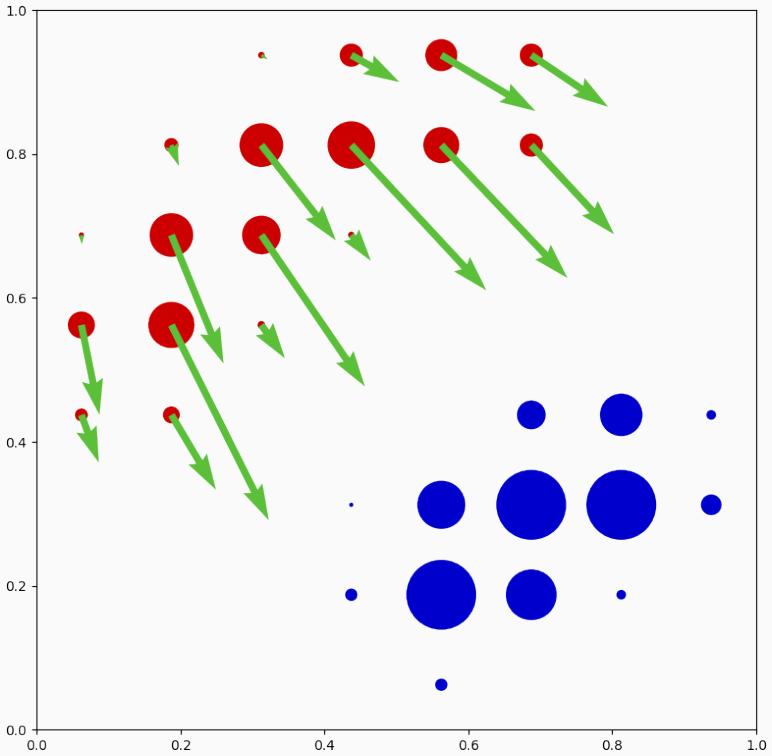

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Display $v_i = -\frac{1}{\alpha_i} \nabla_{x_i} \mathrm{Loss}(\alpha, \beta)$.

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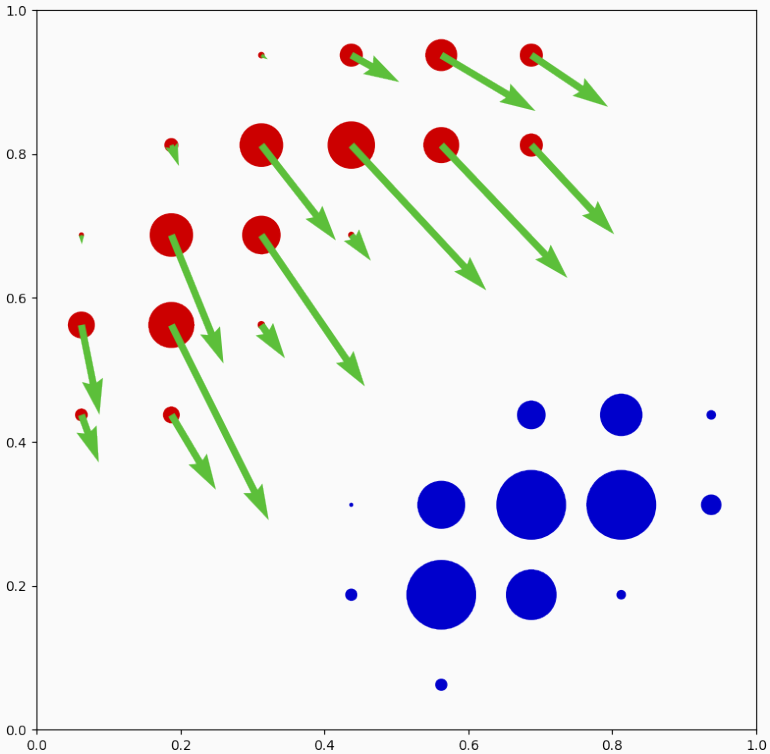

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Seamless extensions to:

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

Simple loss functions

- **Chamfer** distance $\simeq$ soft-**Hausdorff**:
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  $$\text{Loss}(\alpha, \beta) \;=\; \tfrac{1}{2}\|g \star (\alpha - \beta)\|^2_{L^2(\mathbb{R}^D)} \;=\; \tfrac{1}{2}\langle\, \alpha - \beta \,,\, k \star (\alpha - \beta)\,\rangle$$

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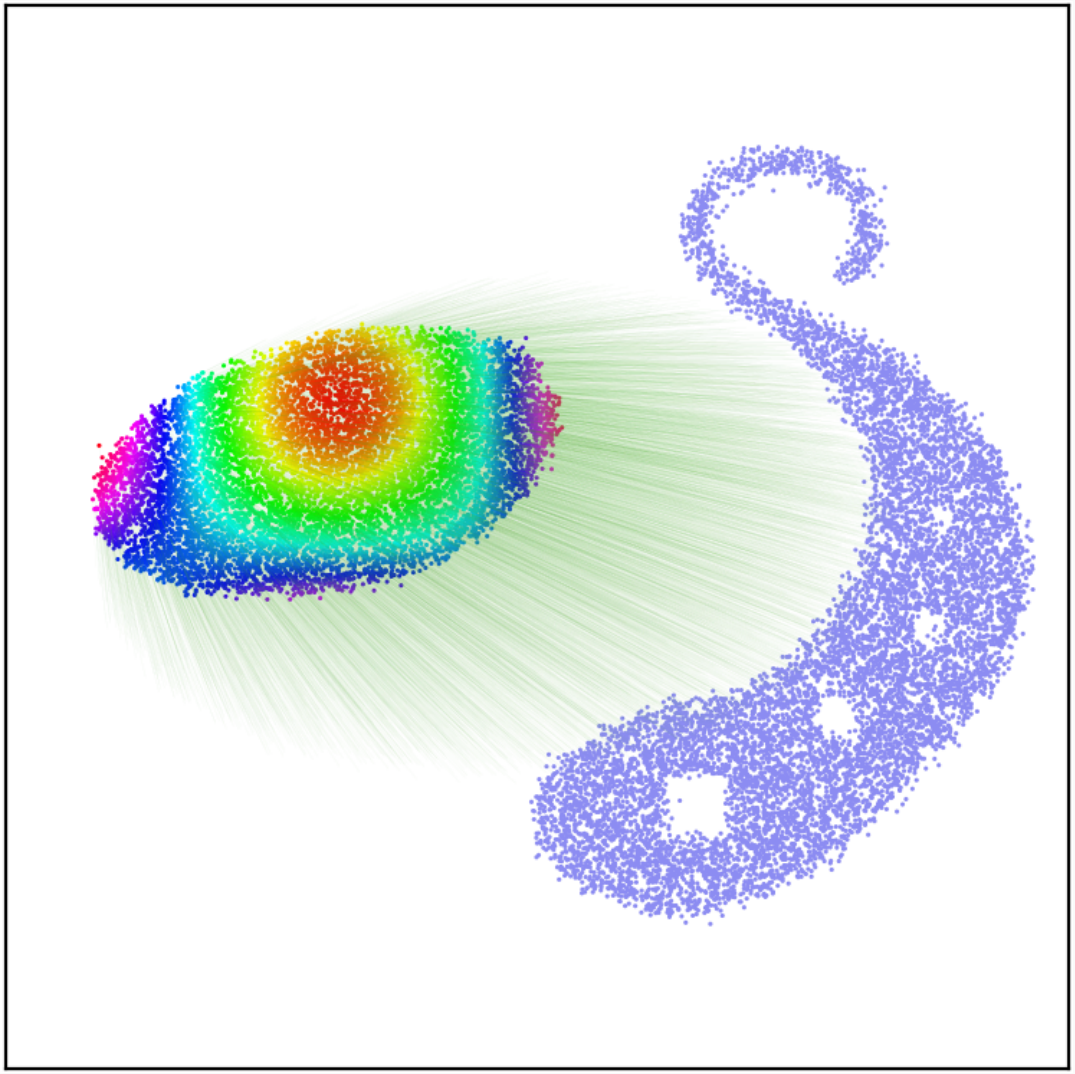
- Example: the Energy Distance, $k(x,y) = -\|x-y\|$:

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

Gradient flow as a toy registration problem



$t = .00$

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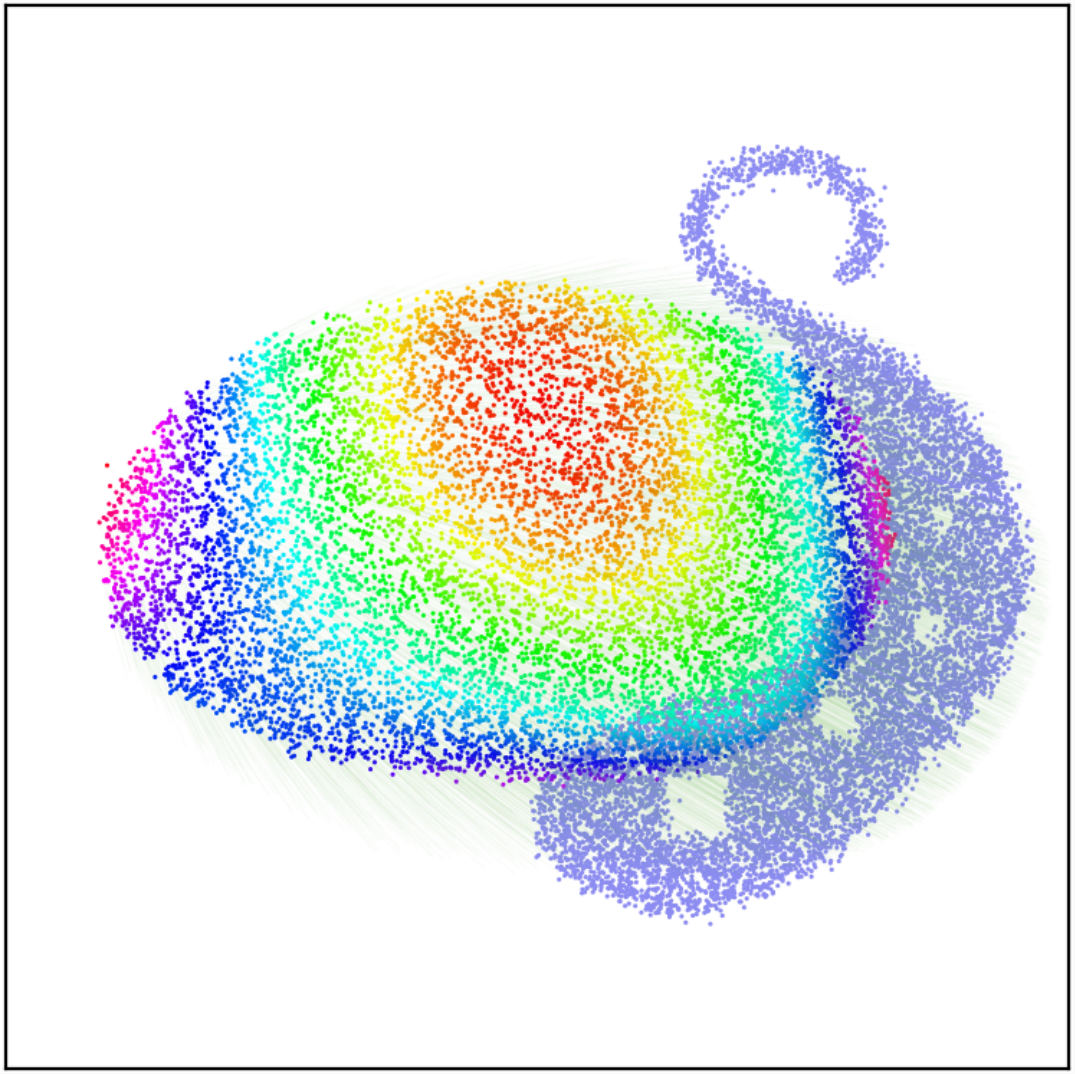

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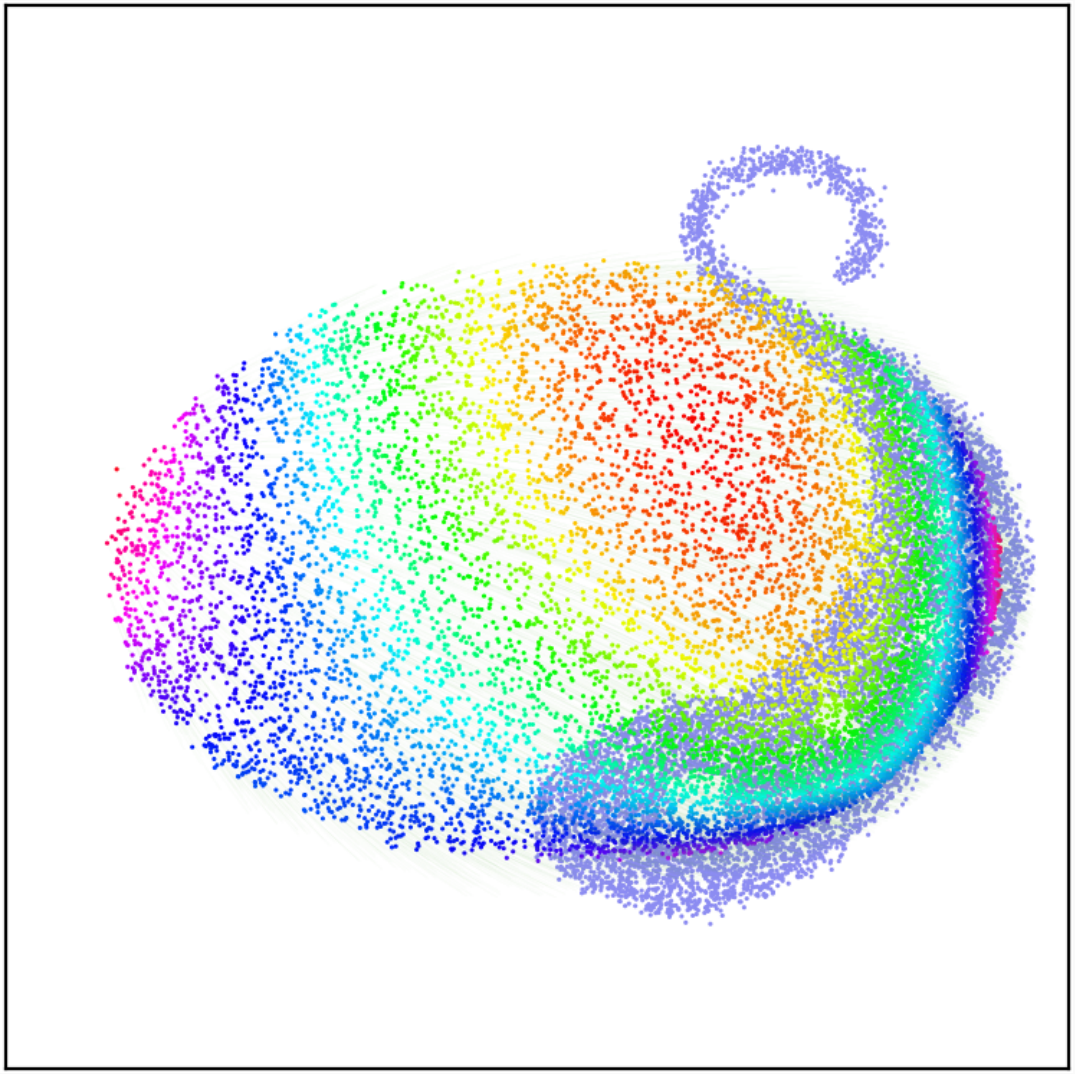
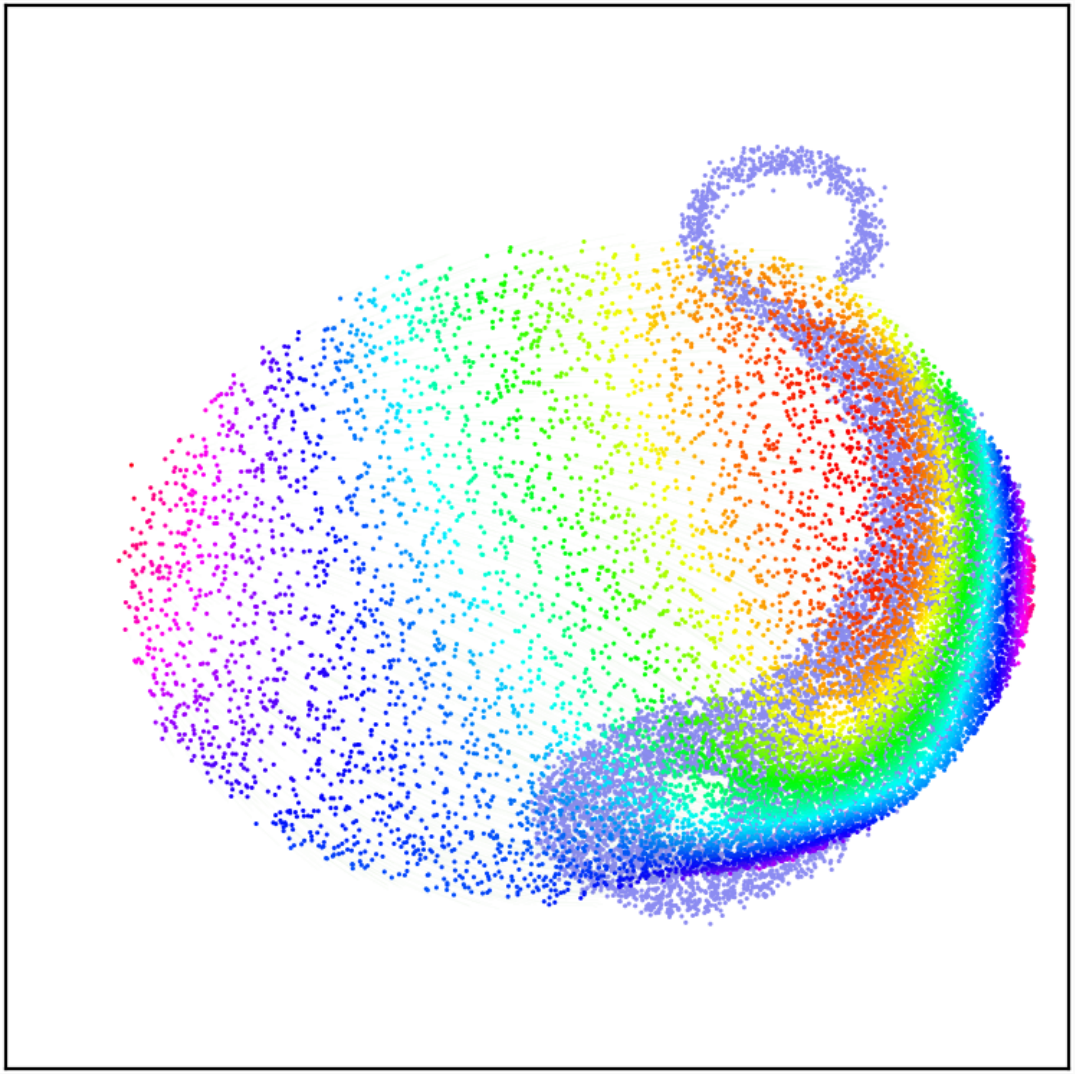


$t = .50$

Gradient flow as a toy registration problem



$t = 1.00$

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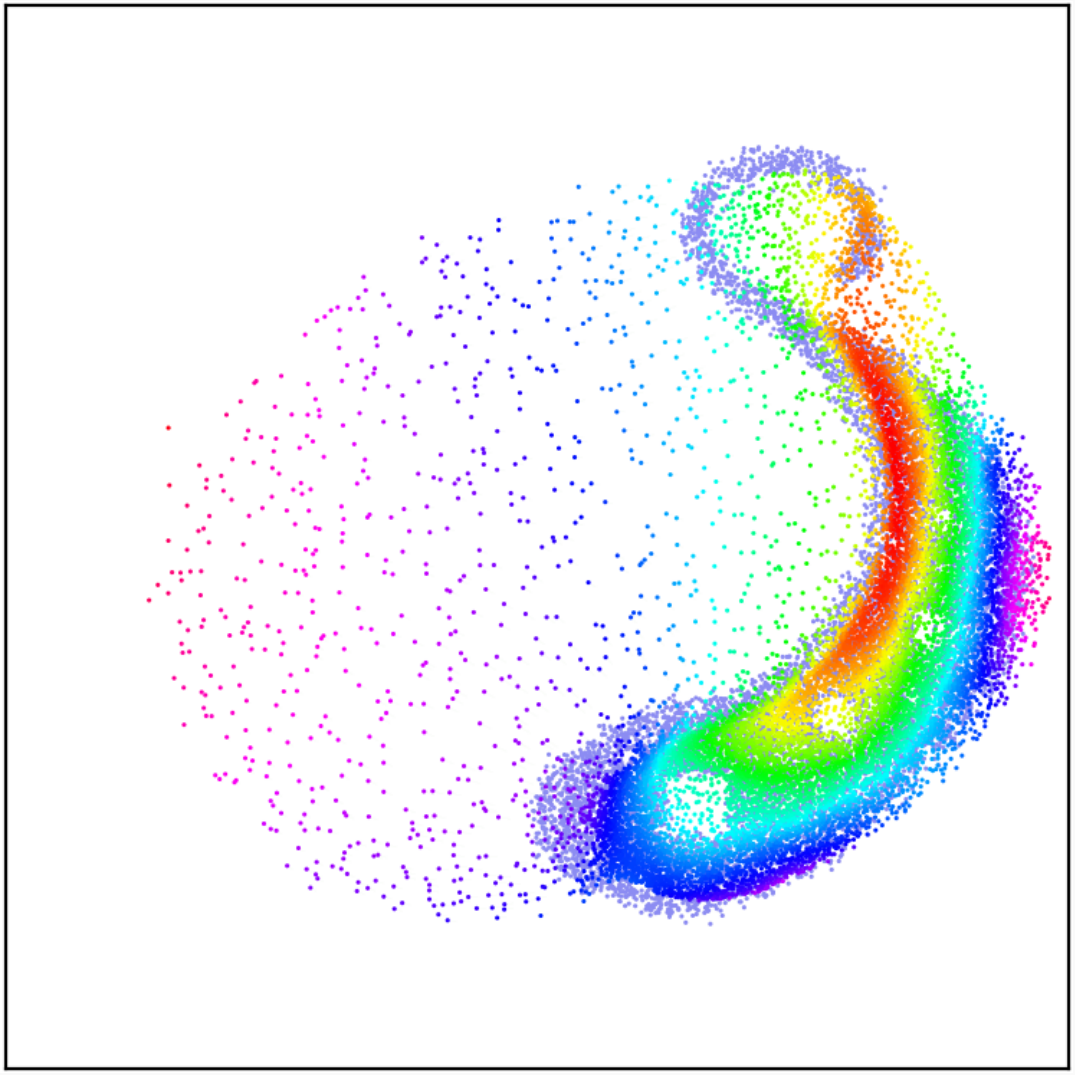
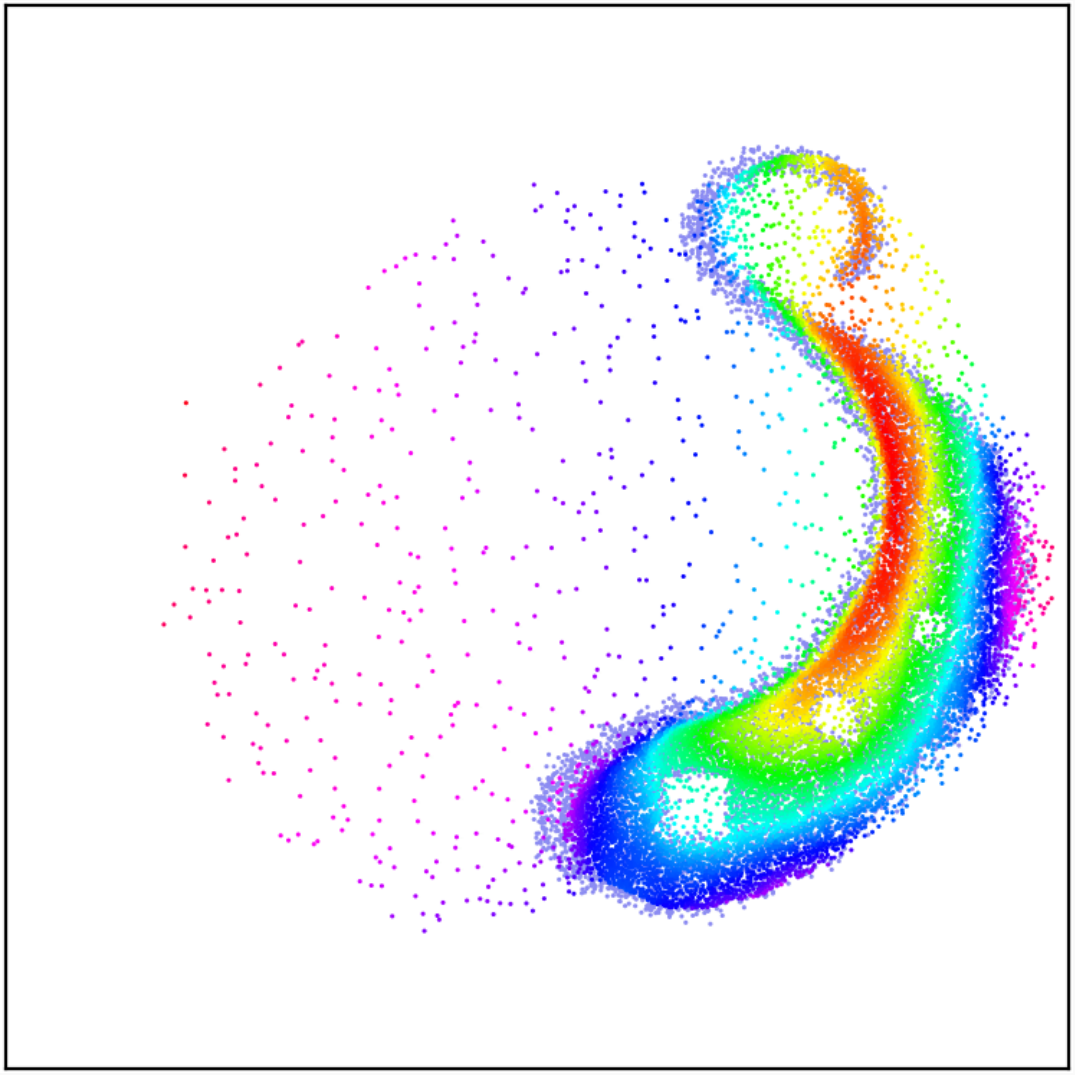


$t = 5.00$

Gradient flow as a toy registration problem



$t = 10.00$

The Wasserstein distance

We need **clean gradients**, without artifacts.

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Simple toy example in 1D :

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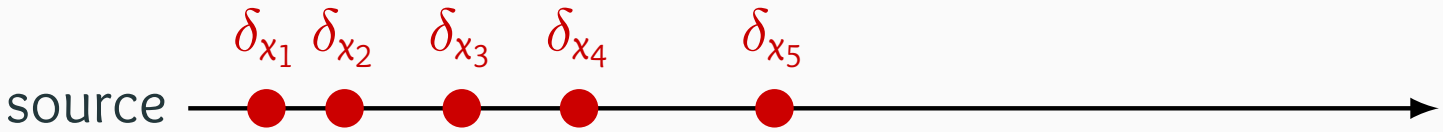

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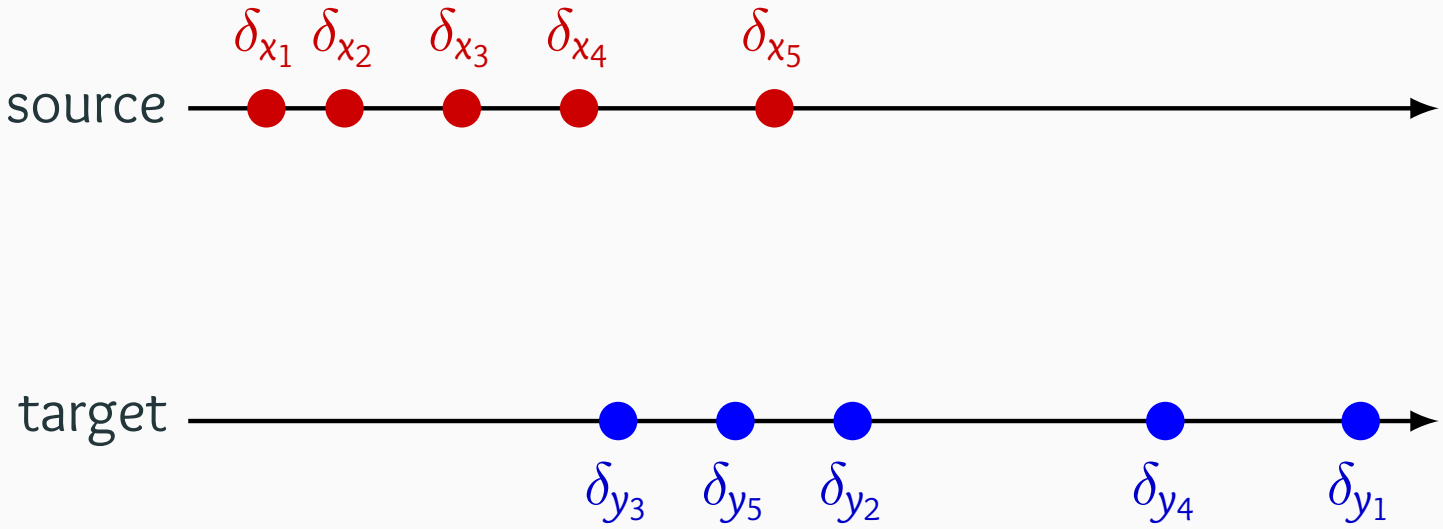

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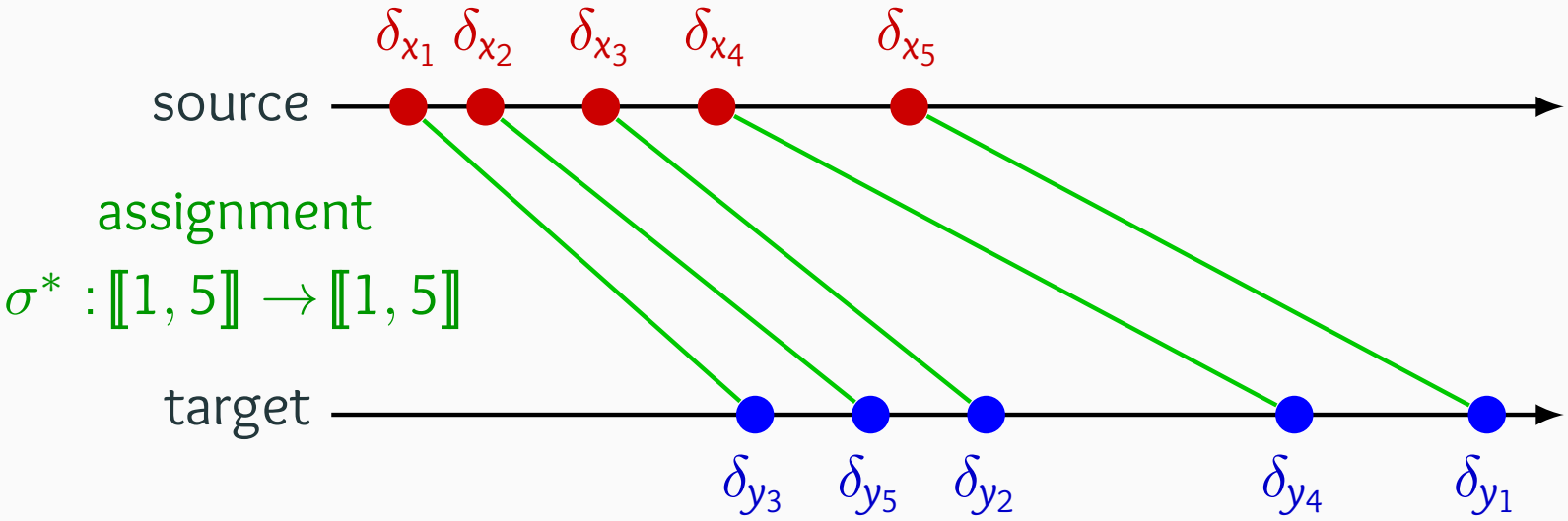

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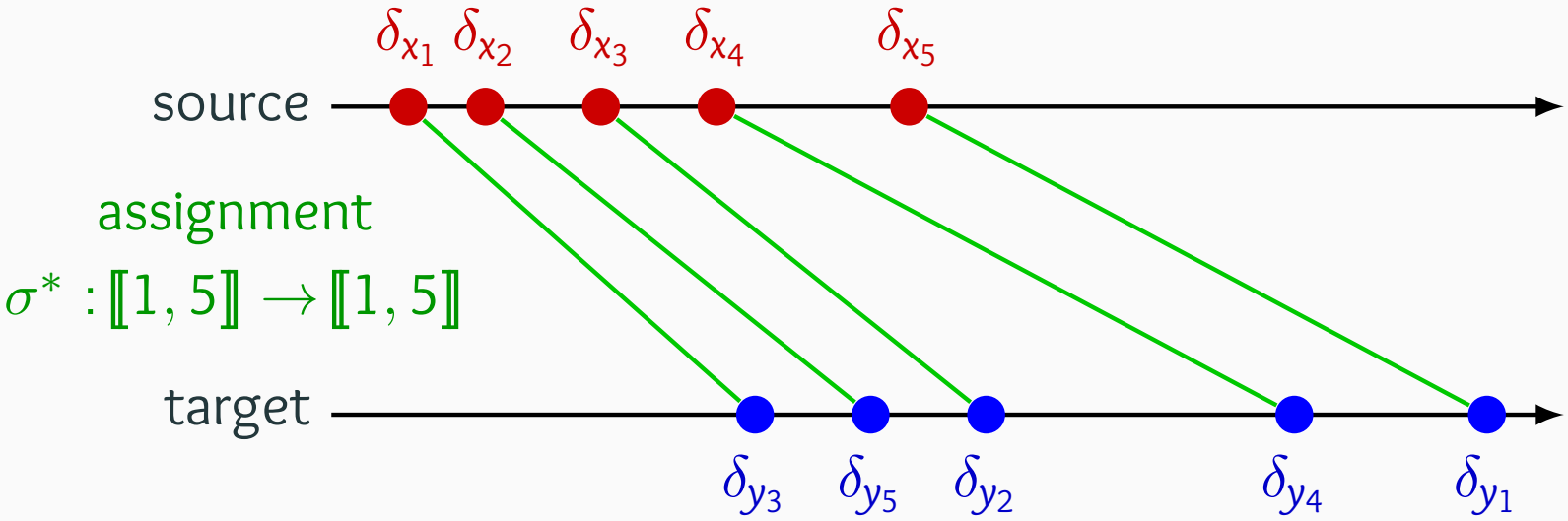

$$\mathrm{OT}(\alpha, \beta) = \frac{1}{2N} \sum_{i=1}^{N} |x_i - y_{\sigma^*(i)}|^2$$

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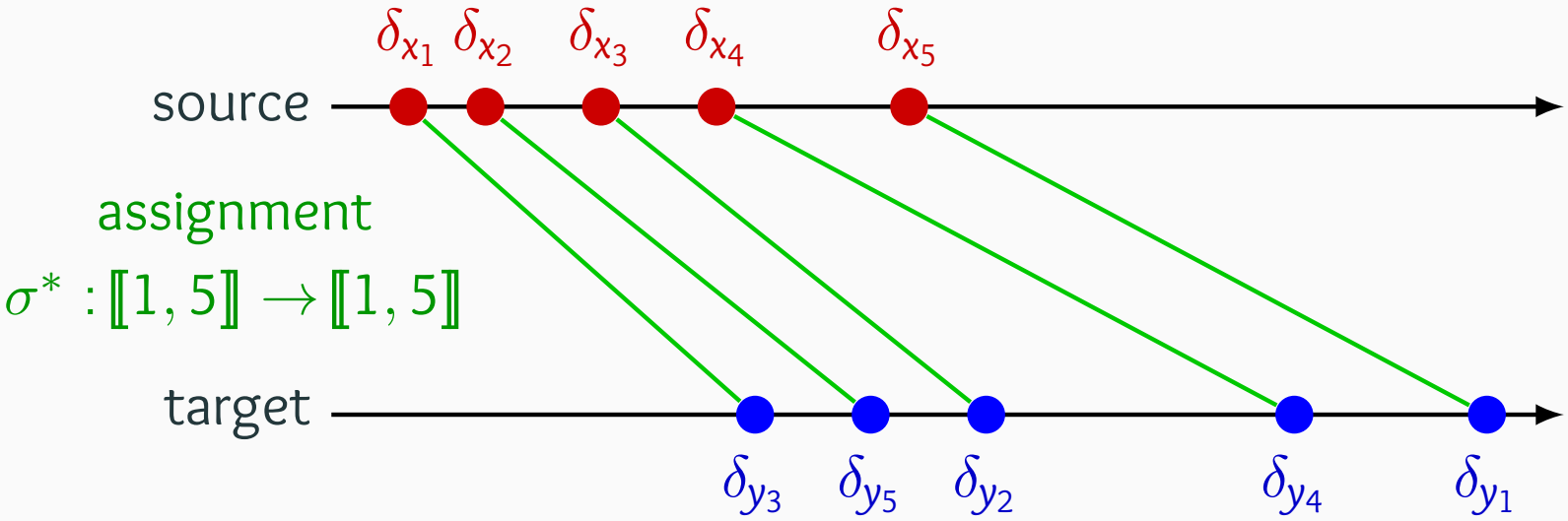
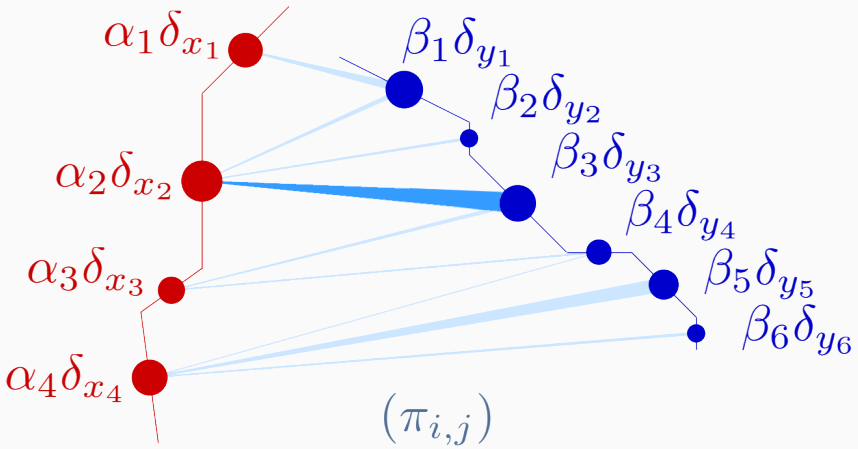
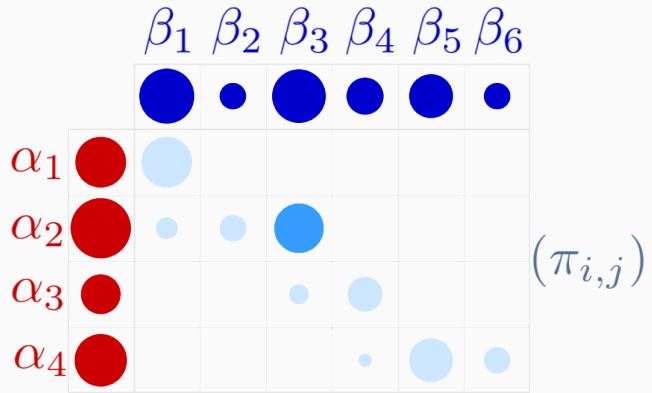
Simple toy example in 1D :



$$\mathrm{OT}(\alpha,\beta) \;=\; \frac{1}{2N}\sum_{i=1}^{N} |x_i - y_{\sigma^*(i)}|^2 \;=\; \min_{\sigma\in\mathcal{S}_N} \frac{1}{2N}\sum_{i=1}^{N} |x_i - y_{\sigma(i)}|^2$$

Optimal transport generalizes sorting to D $>$ 1





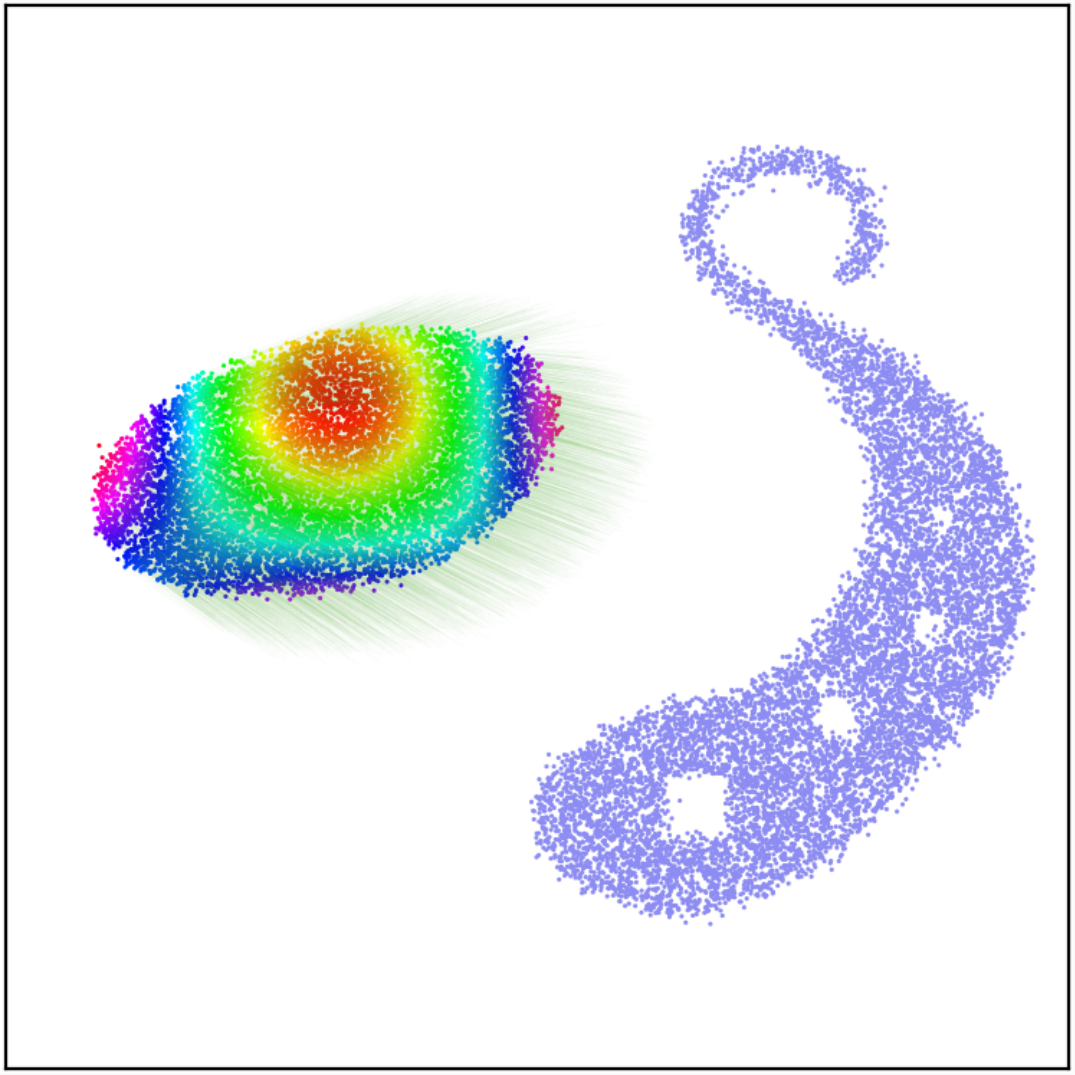
Minimize over N-by-M matrices (transport plans) π :

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

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

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

Wasserstein gradients are homogeneous



$t = .00$

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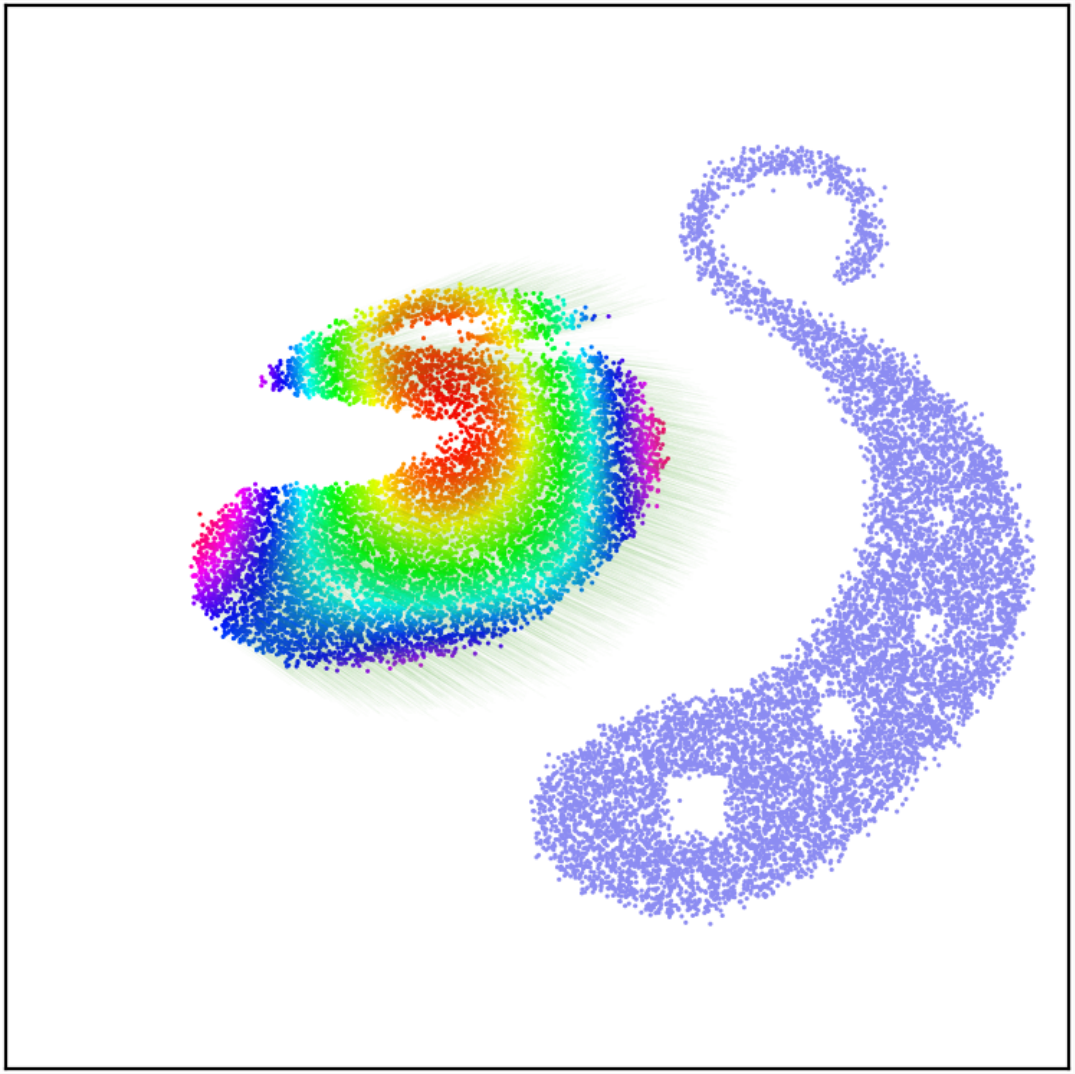

$t = .25$

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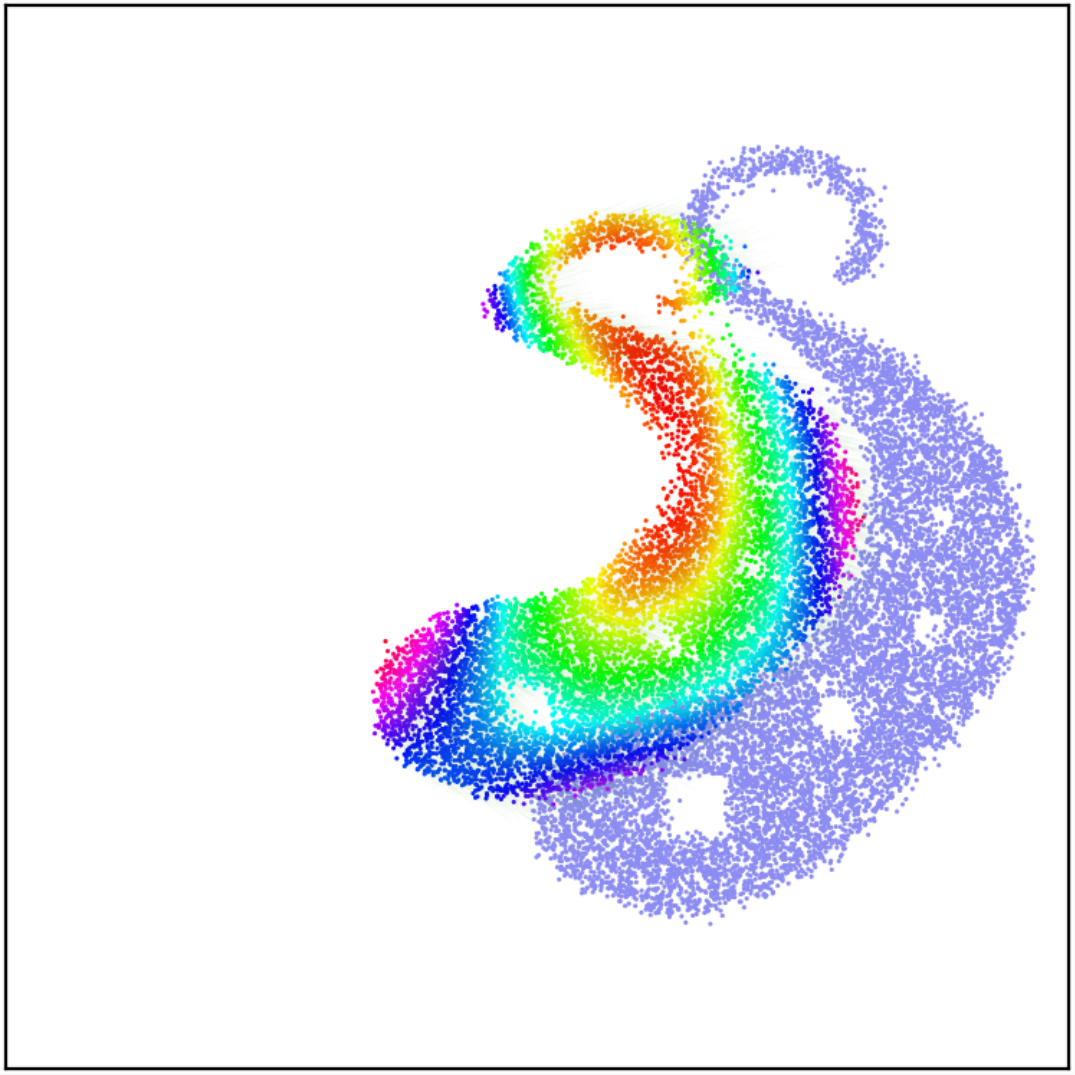

$t = 1.00$

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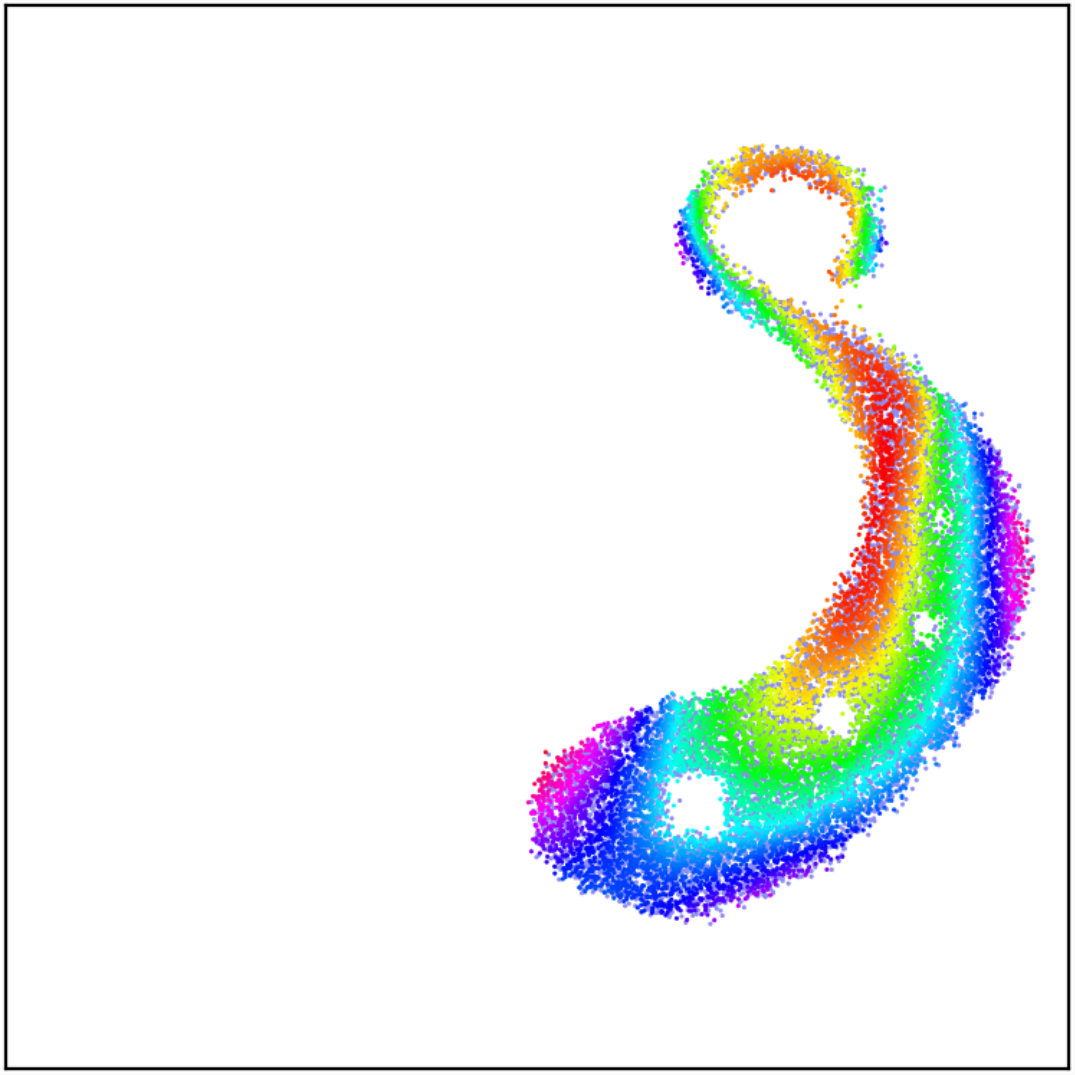

$t = 5.00$

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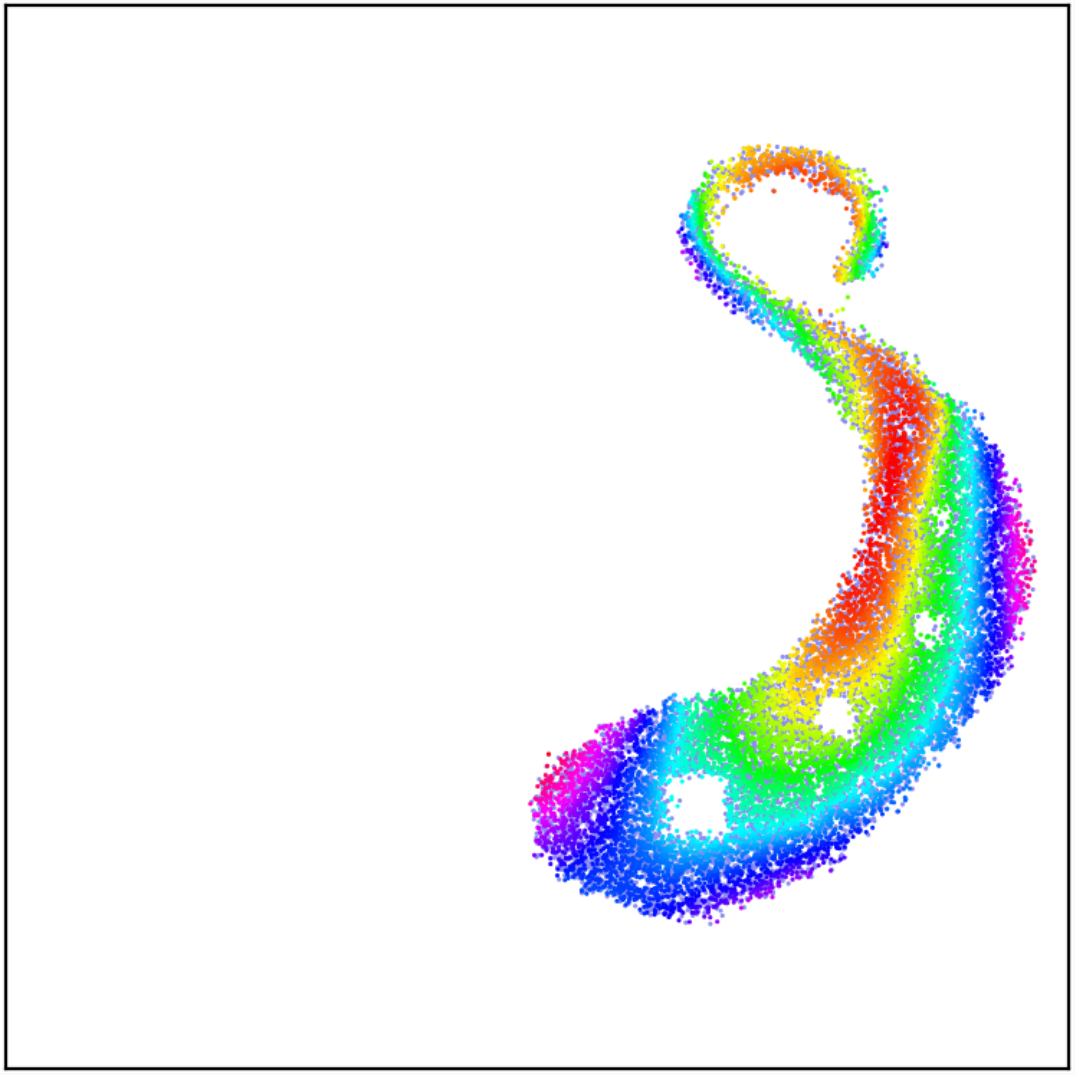

$t = 10.00$

Key properties [Bre91]

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

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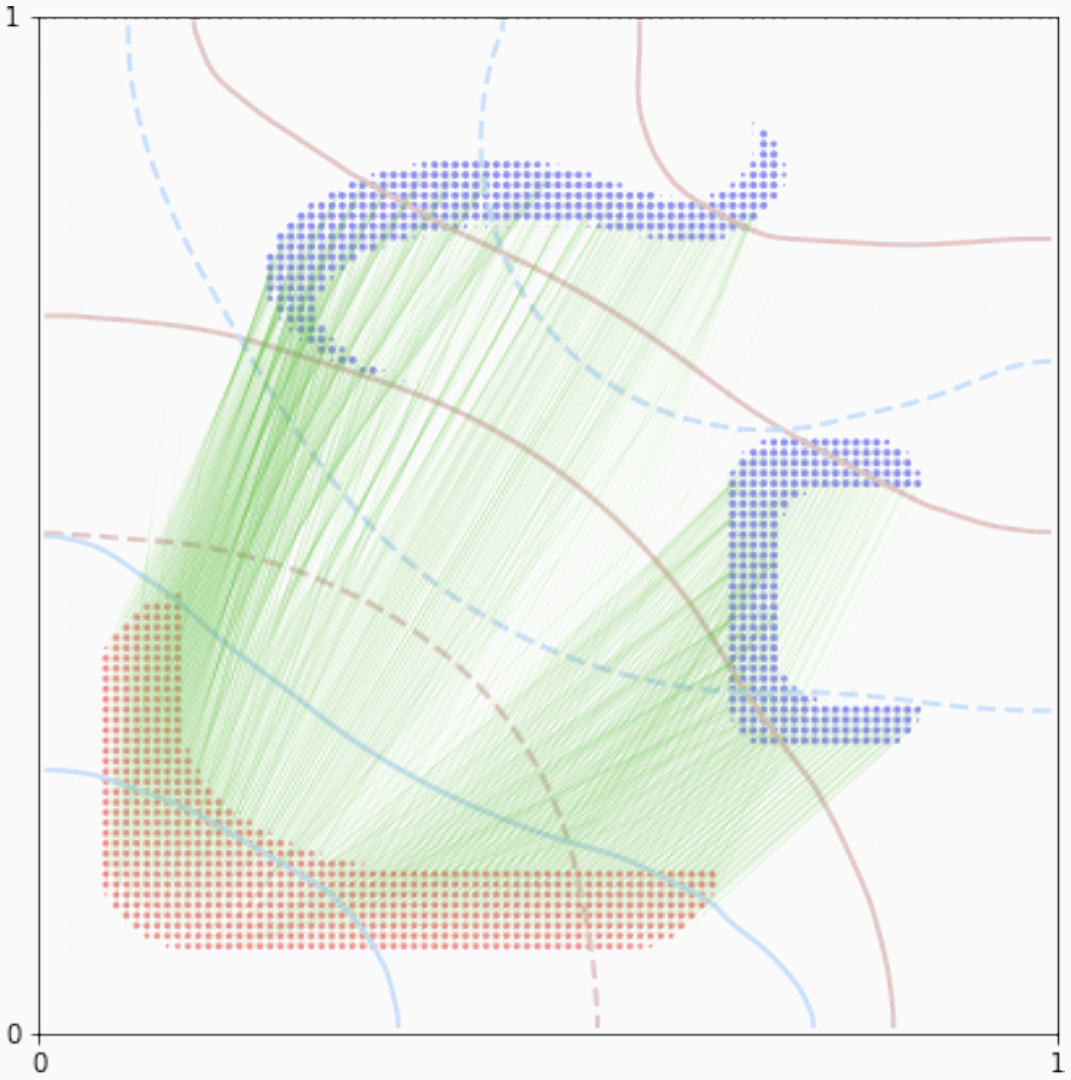
$\Longrightarrow$ Generalized **QuickSort** algorithm.

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



OT plan in 2D.

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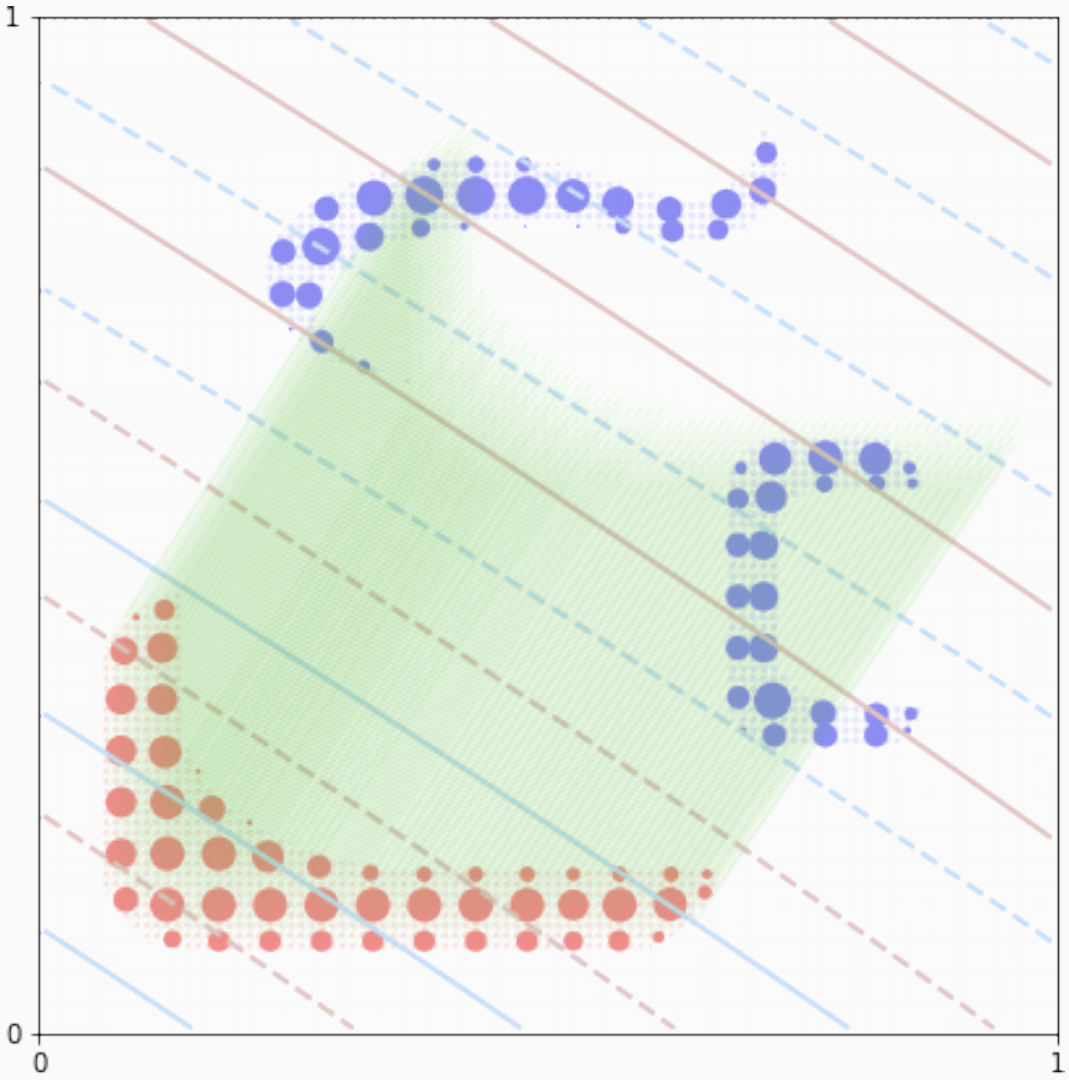

Iteration 0, blur = 2^0

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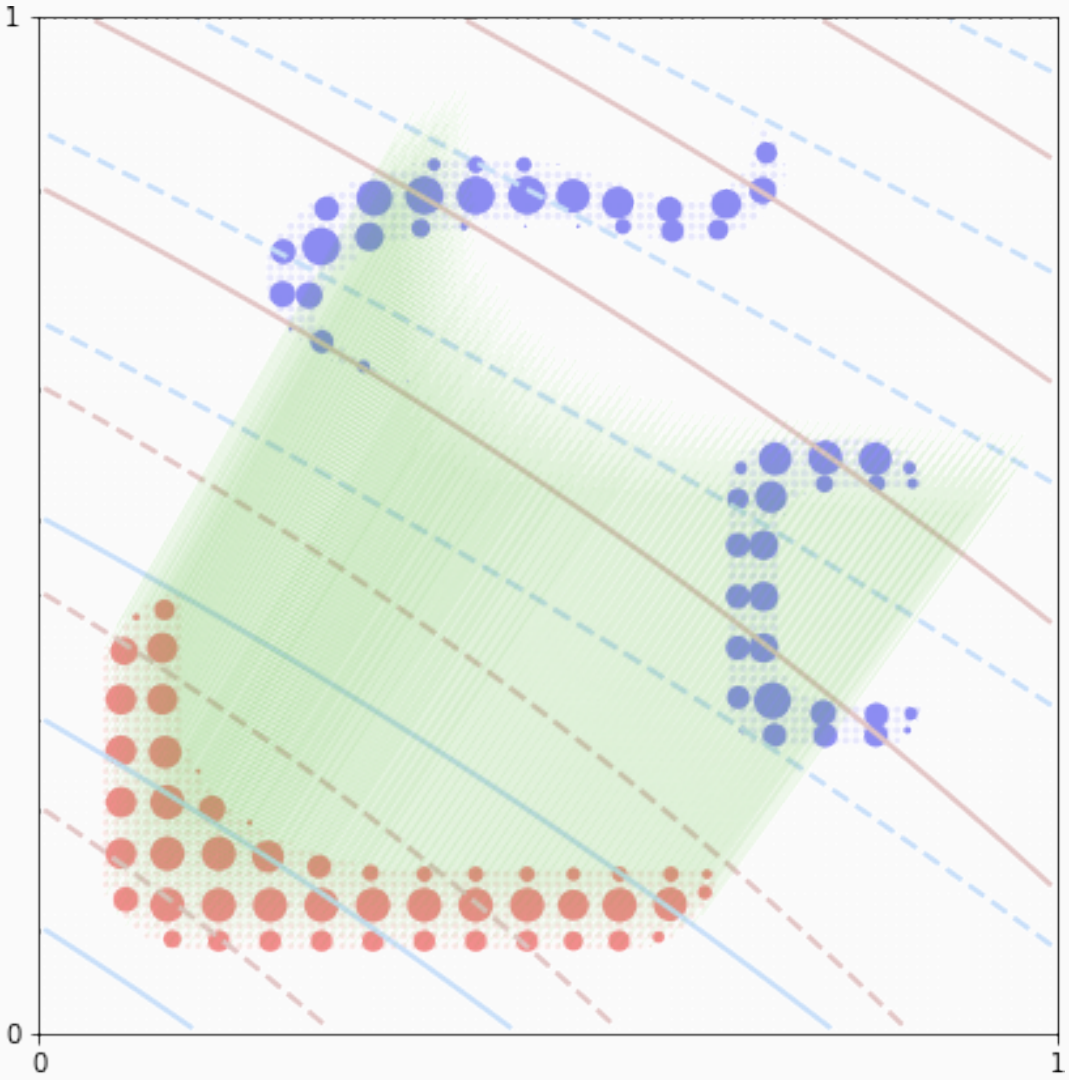

Iteration 1, blur = 2^{-1}

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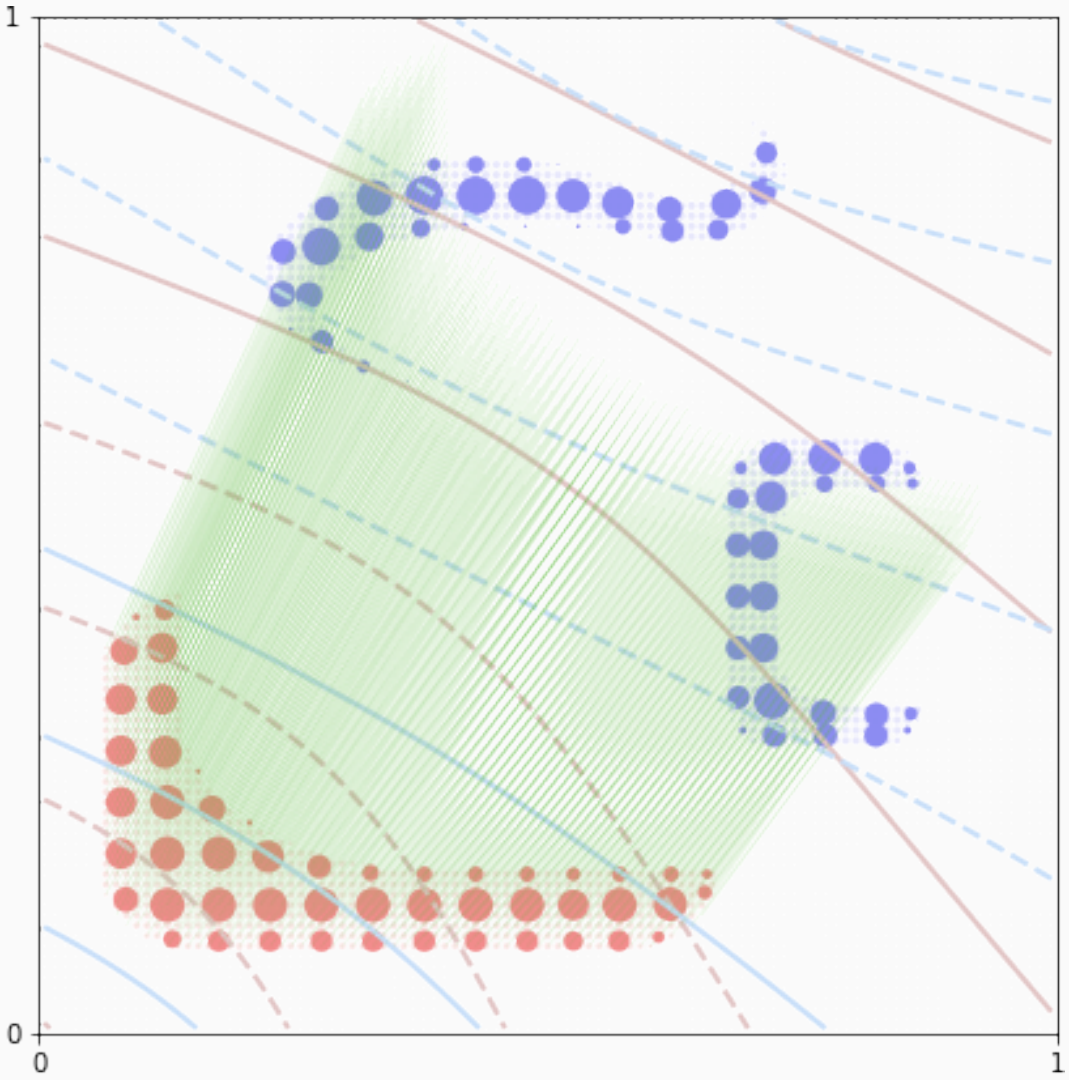

Iteration 2, blur = 2^{-2}

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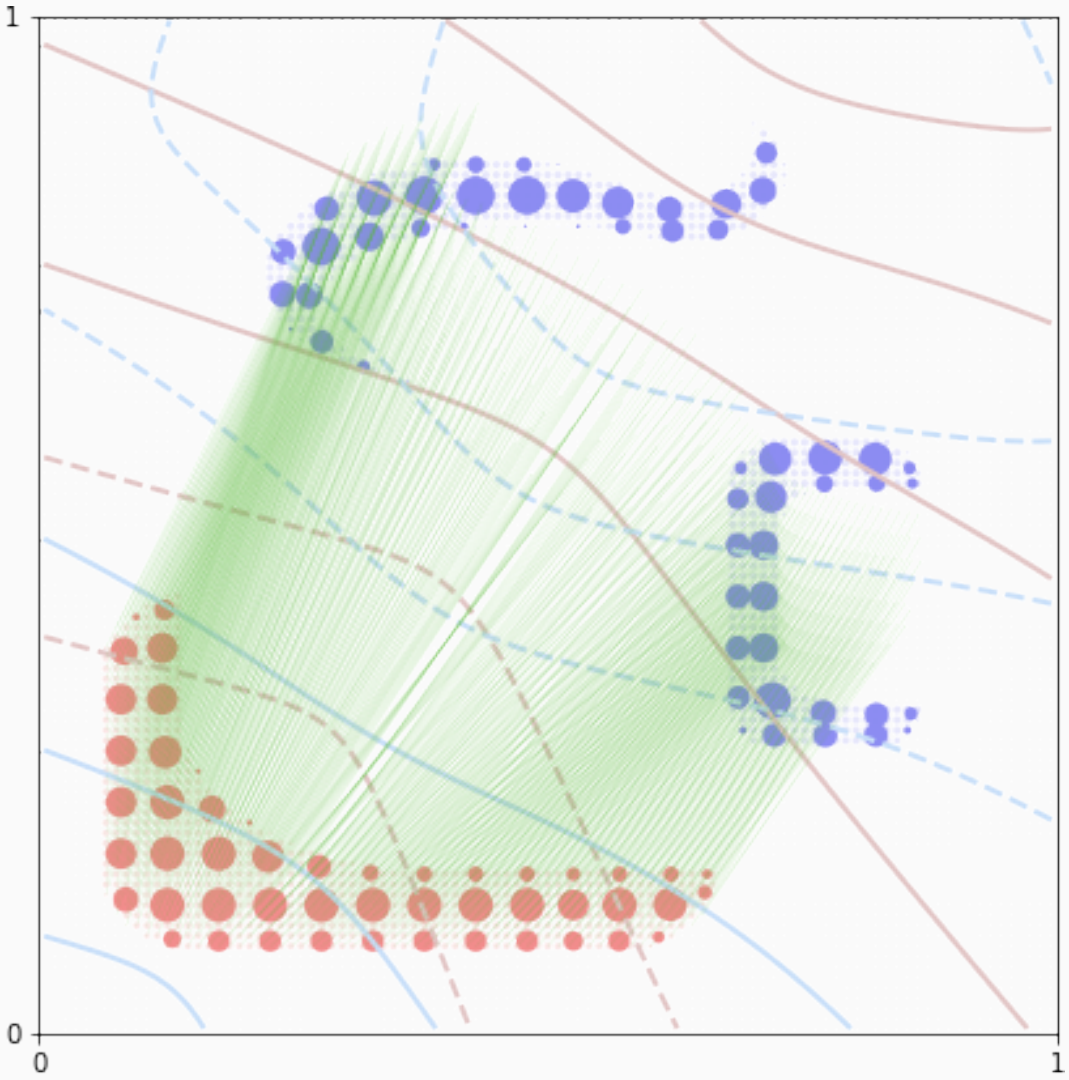

Iteration 3, blur = 2^{-3}

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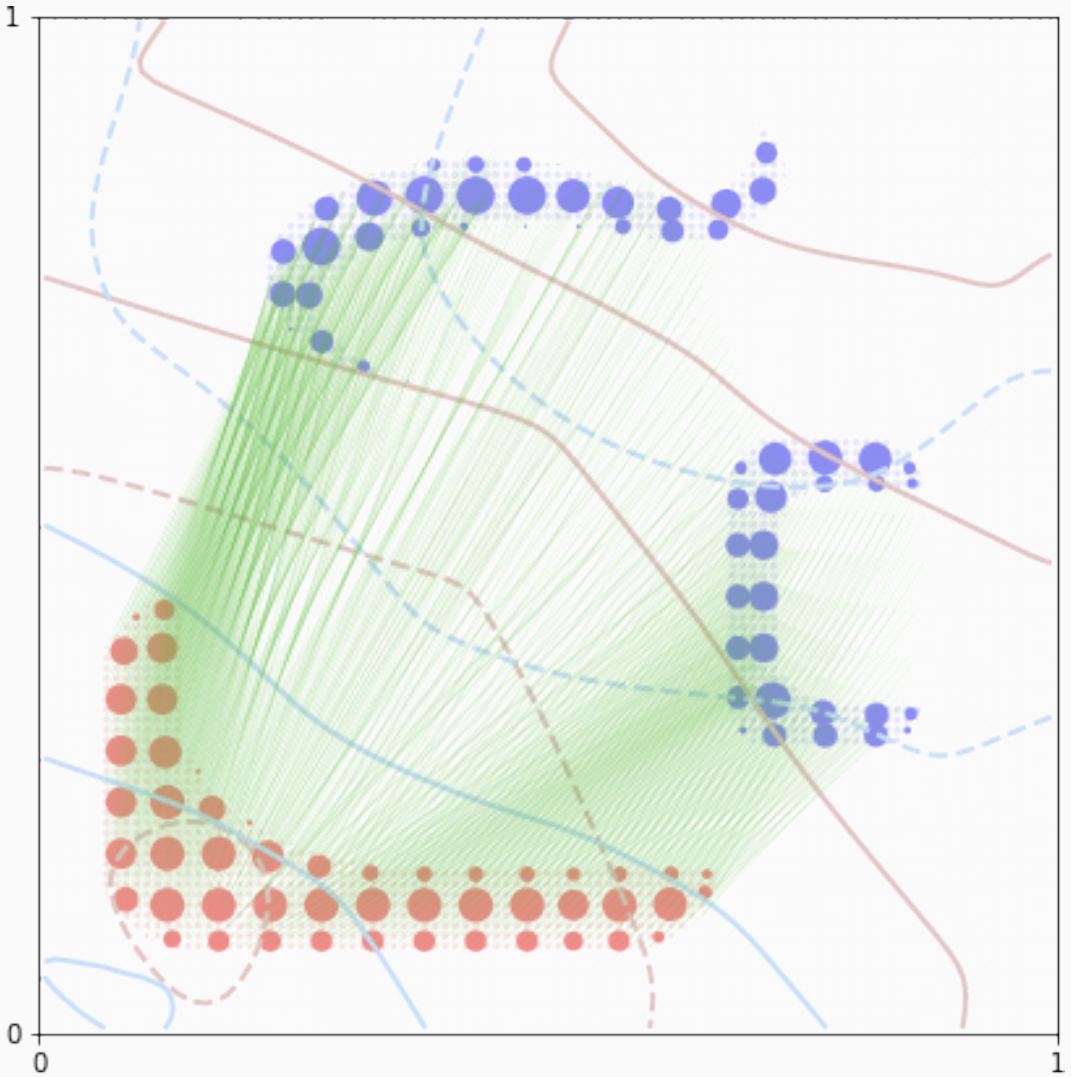

Iteration 4, blur = 2^{-4}

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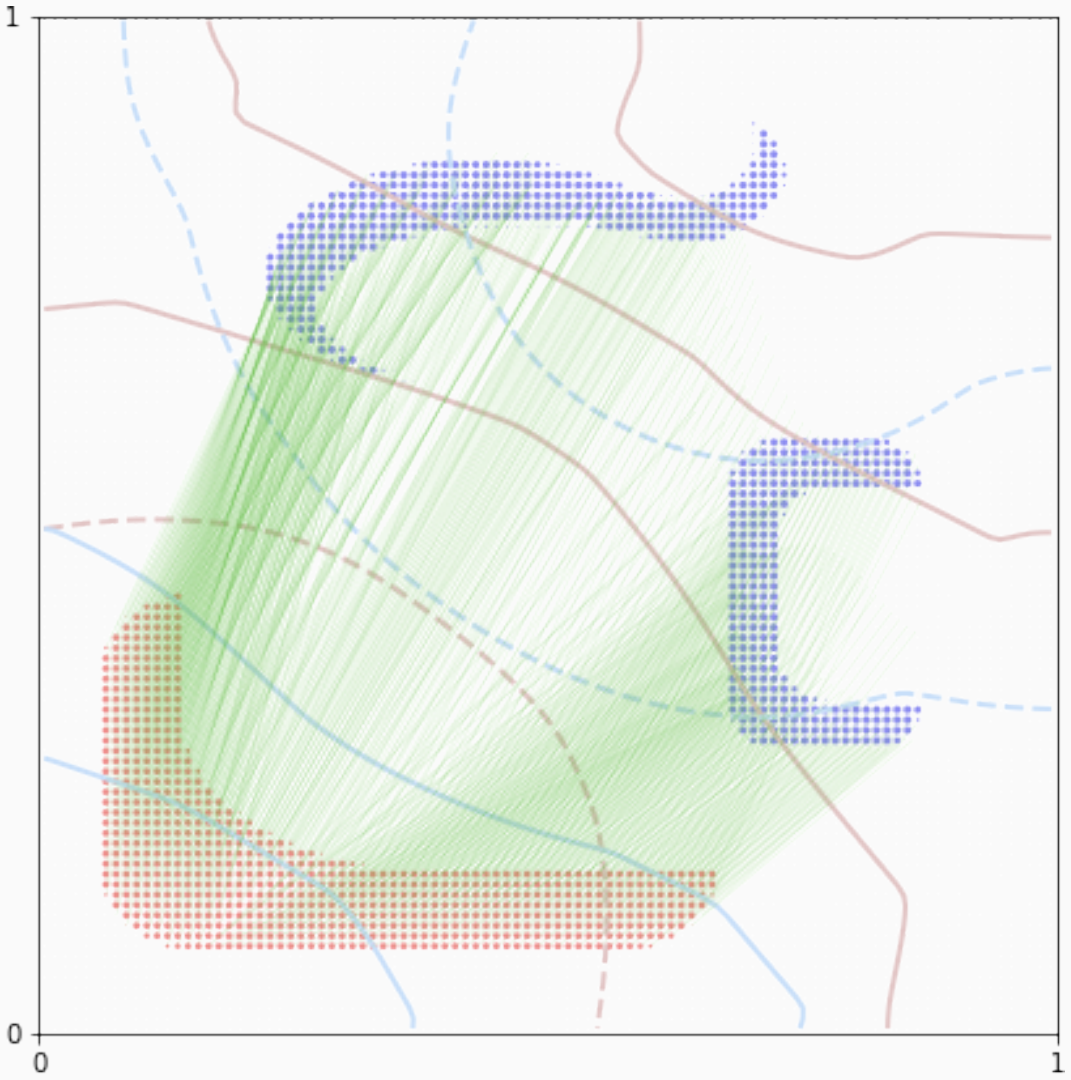

Iteration 5, blur = 2^{-5}

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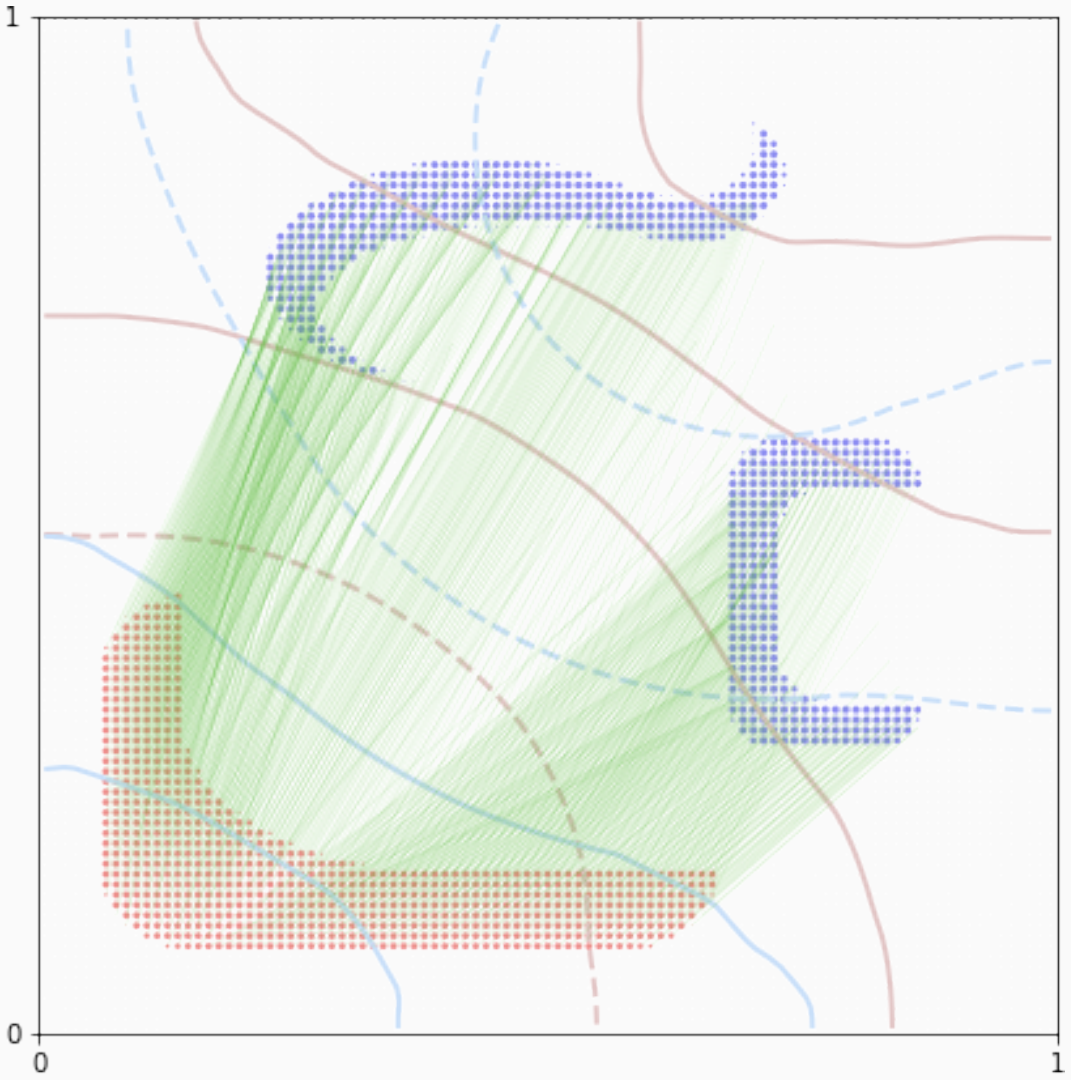

Iteration 6, blur = 2^{-6}

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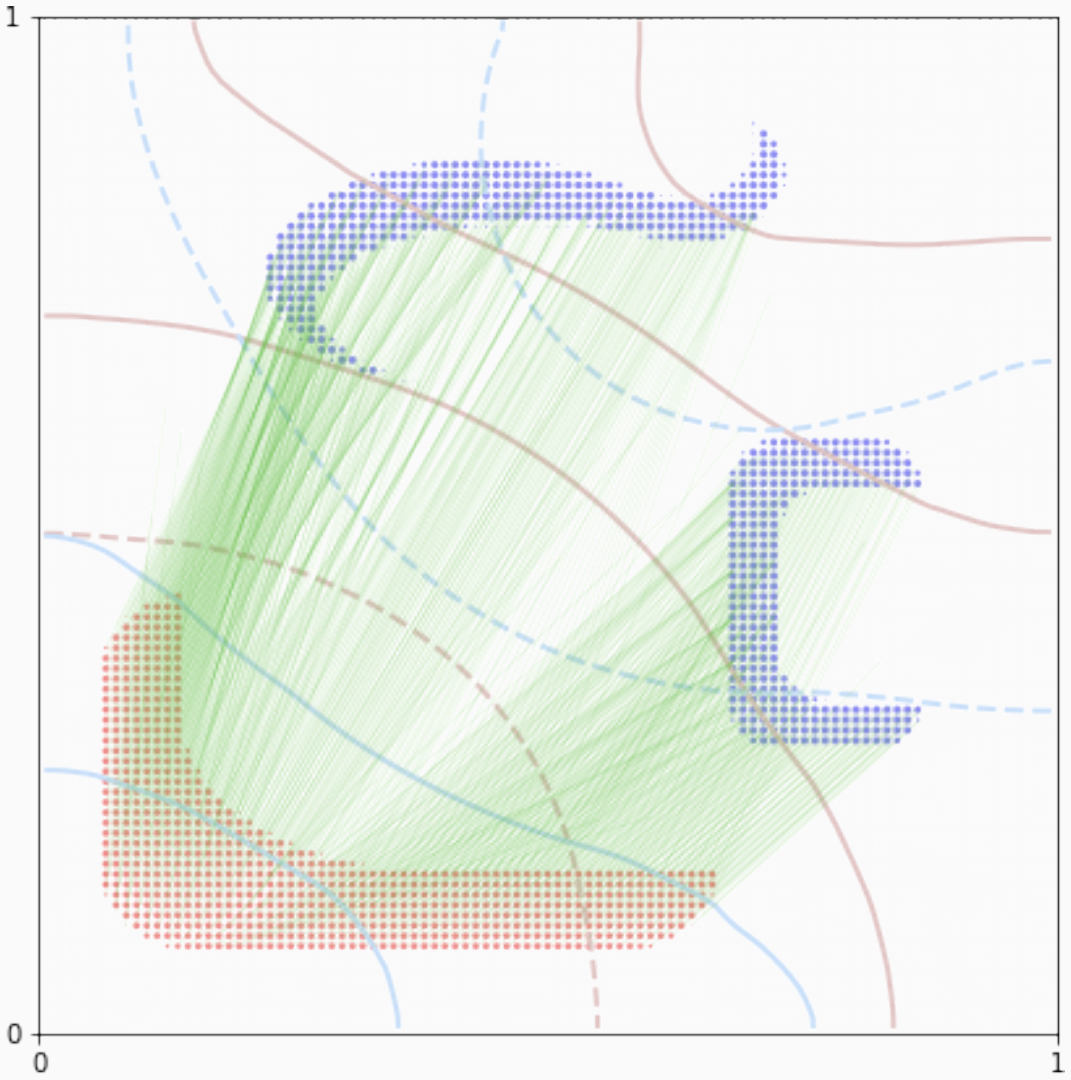

Iteration 7, blur = `.01`

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 **GeomLoss** library!

Geometric Loss functions for PyTorch

Our website: `www.kernel-operations.io/geomloss`

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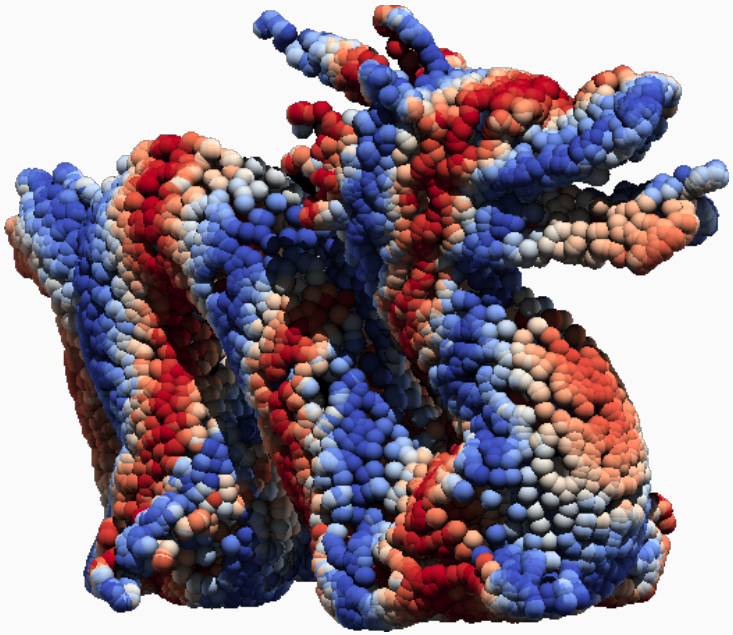
# GeomLoss supports autograd, batch processing, etc.
g_x, = torch.autograd.grad(L, [x])
```

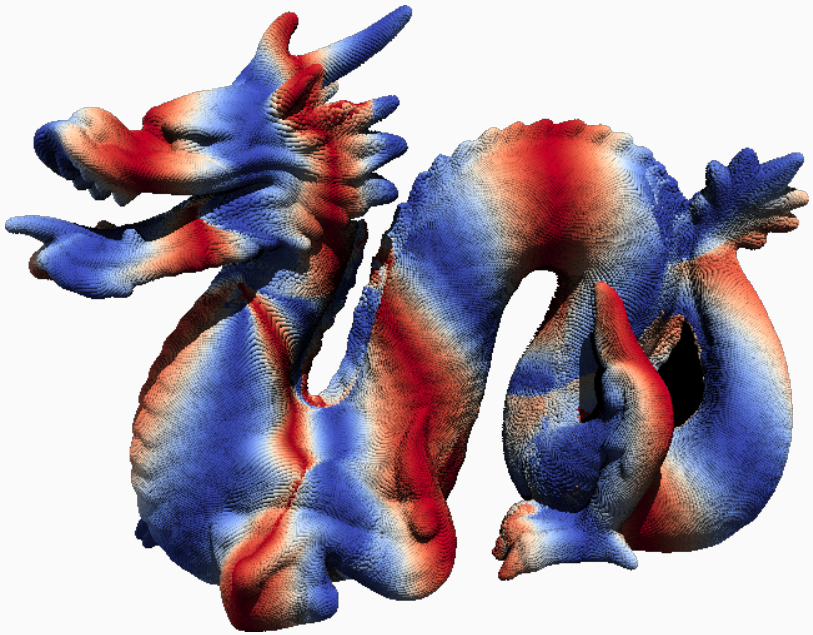
Scaling up optimal transport

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

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



10k points in 30-50ms



100k points in 100-200ms

Affordable geometric barycenters

$$\text{Barycenter } \alpha^* = \arg\min_{\alpha} \sum_{i=1}^{N} \lambda_i \, \text{Loss}(\, \alpha \,,\, \beta_i \,) \,.$$

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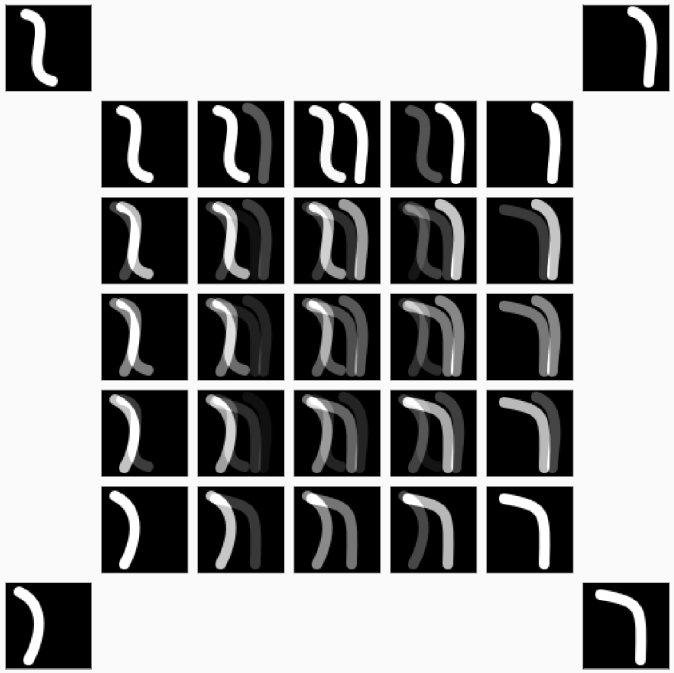

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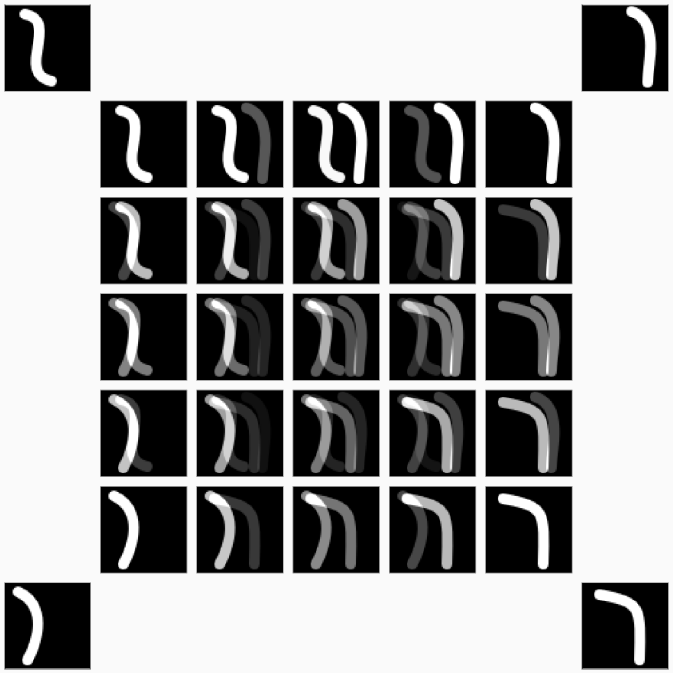

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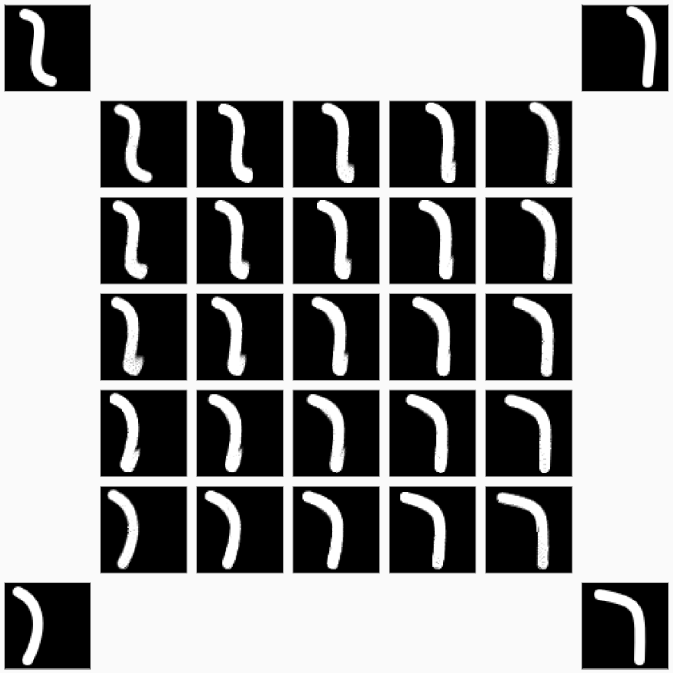
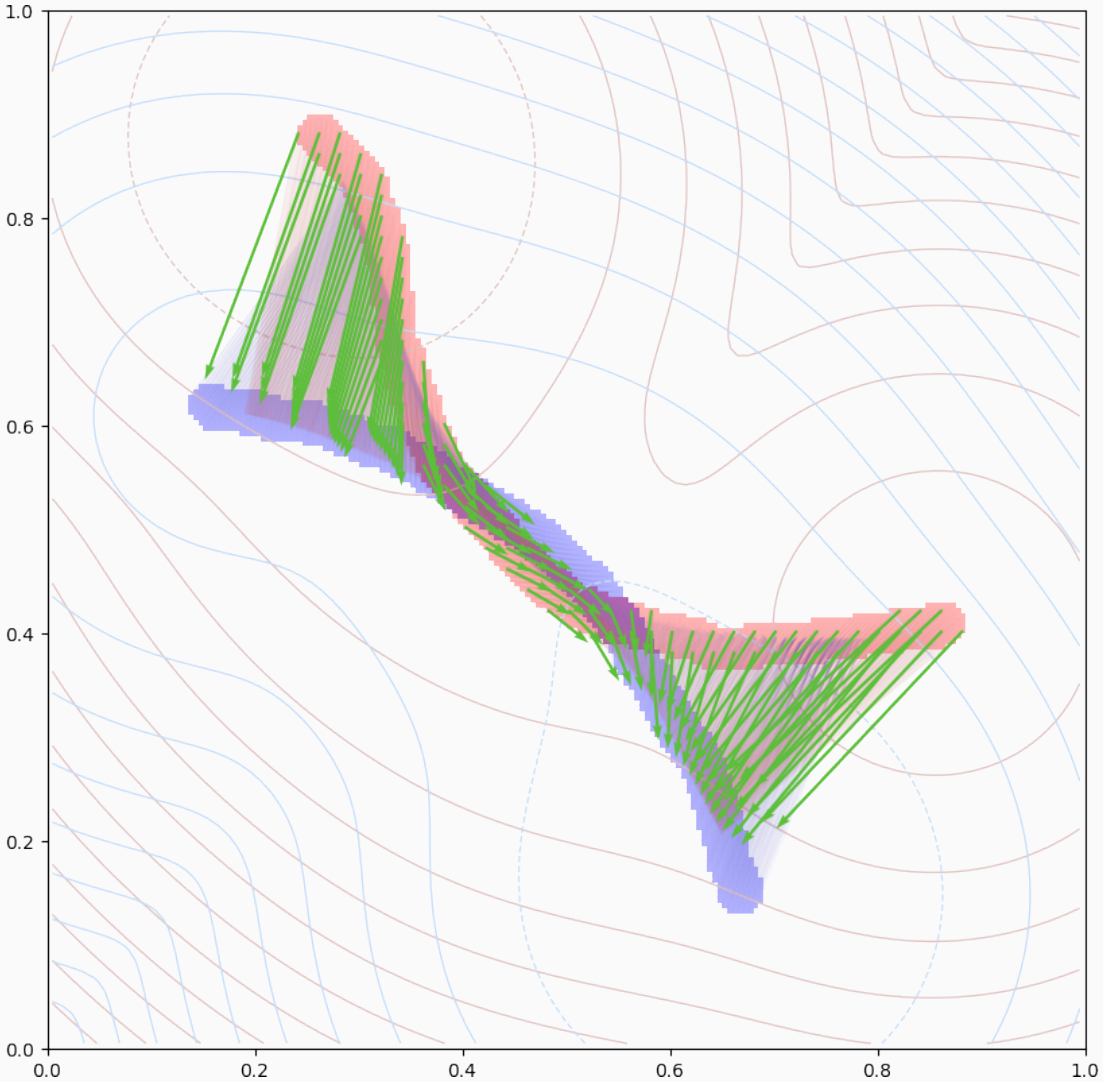


Wasserstein barycenters

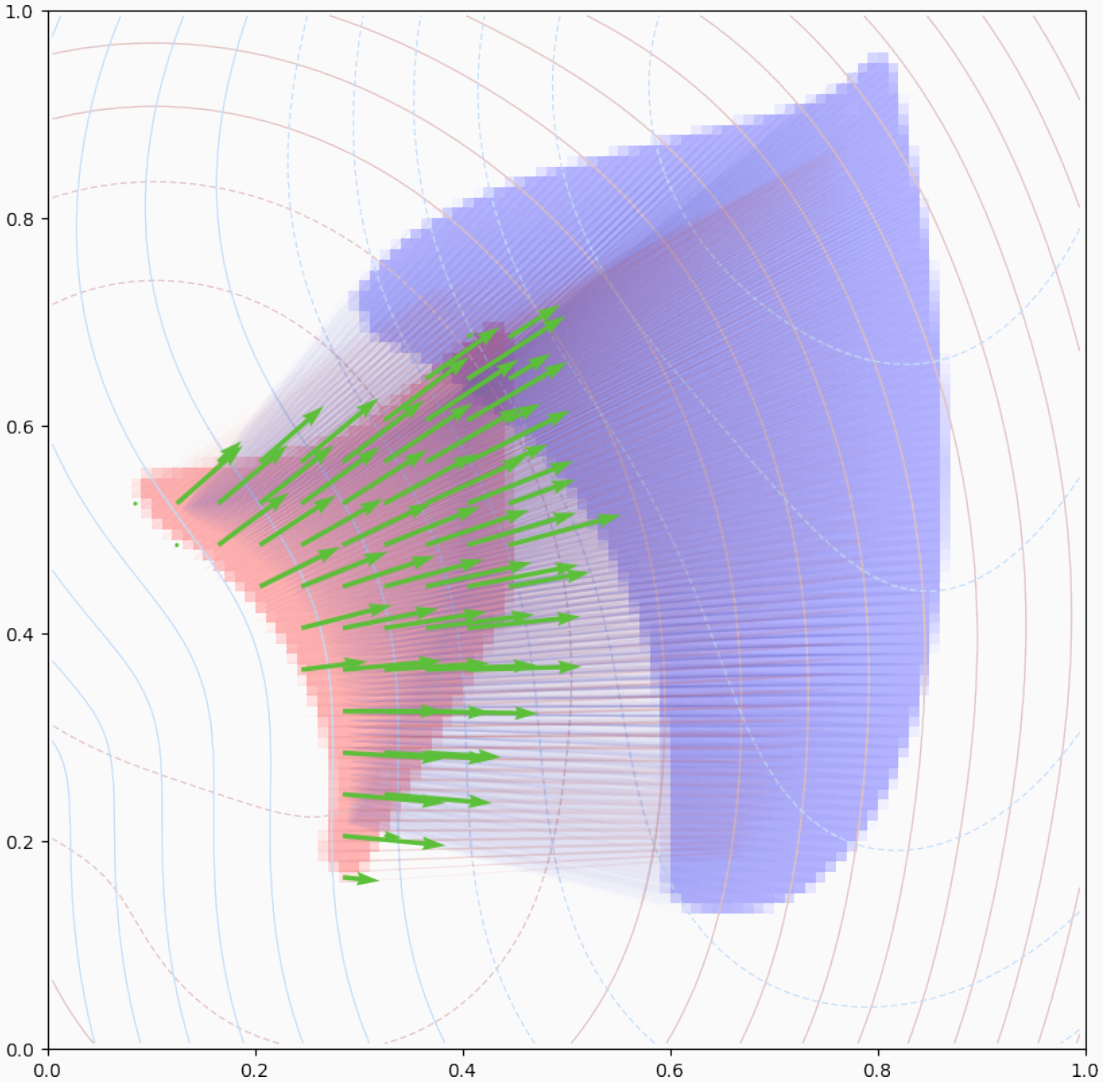
$\text{Loss}(\alpha, \beta) = \text{OT}(\alpha, \beta)$

A robust loss function



A high-quality gradient...

A robust loss function



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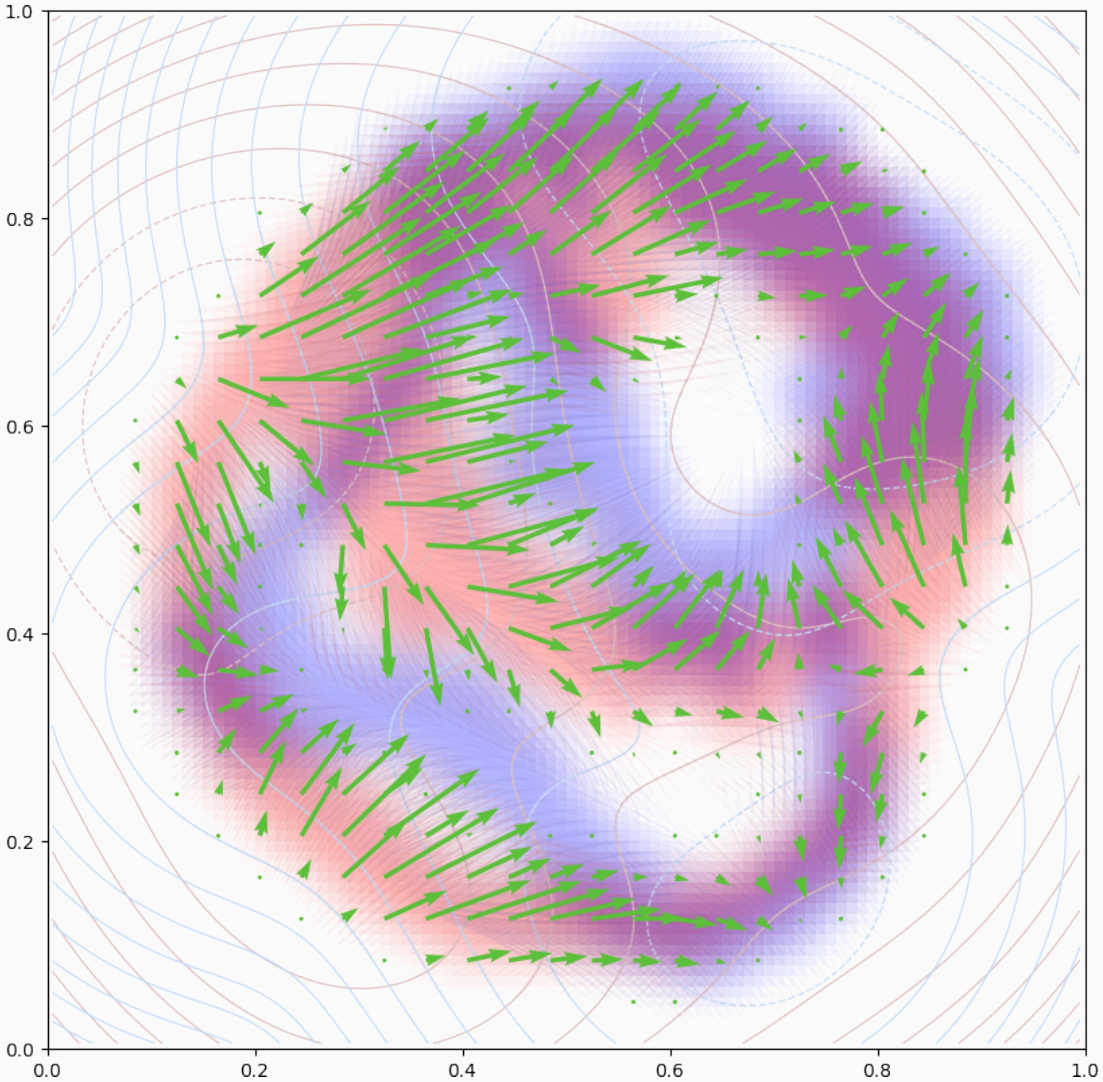
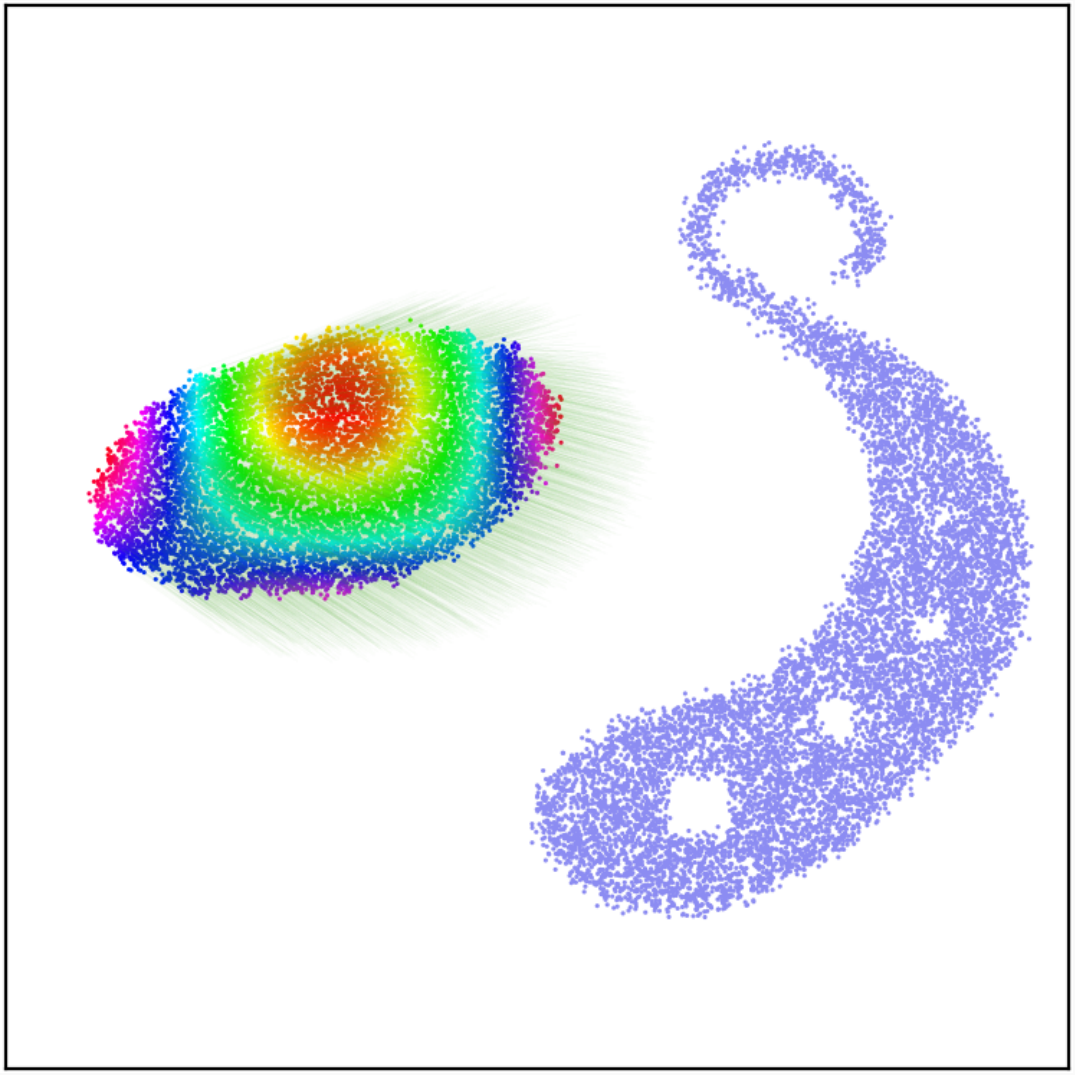


A high-quality gradient... But no preservation of topology!

Gradient descent with OT: cheap'n easy registration?



Iteration 0

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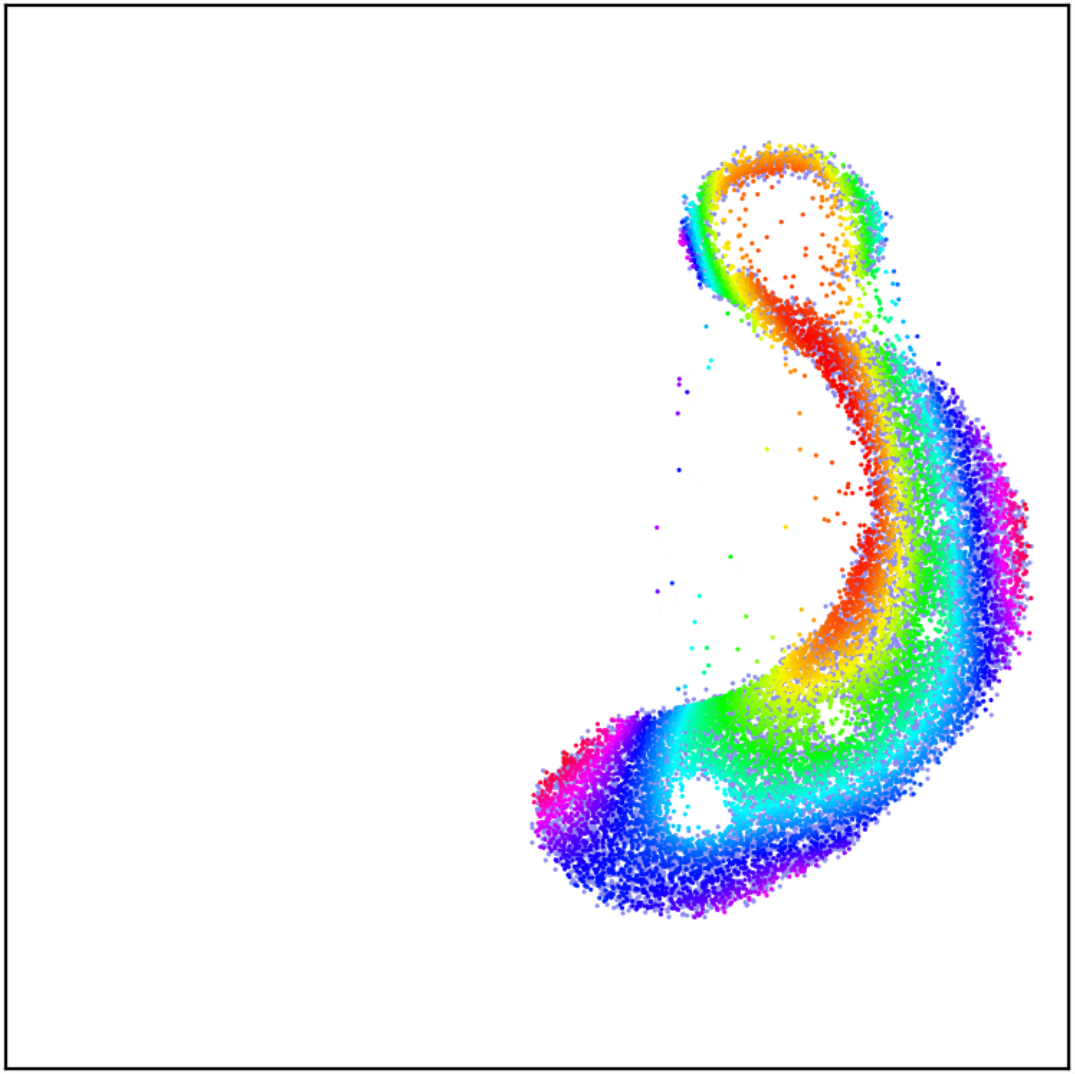

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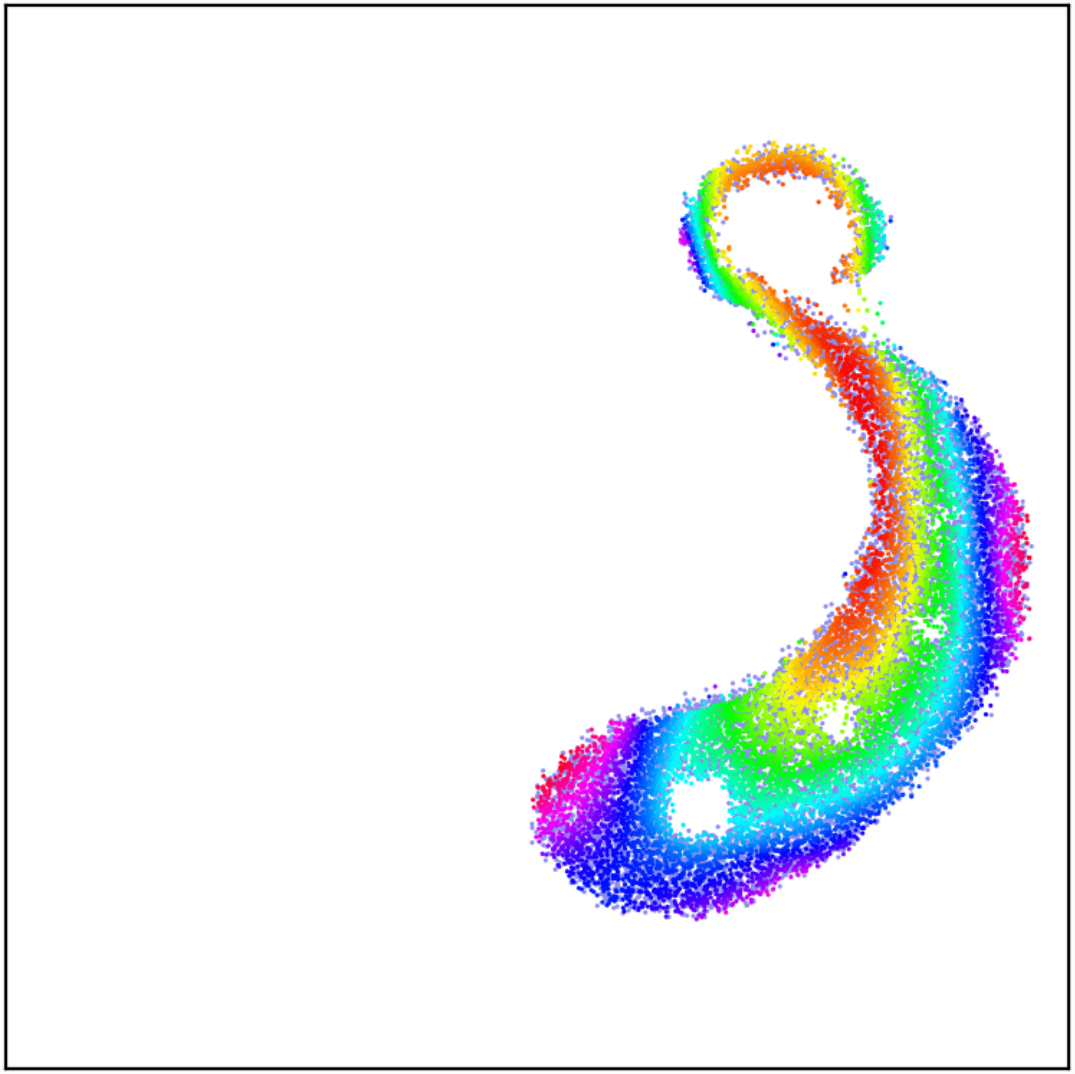

Iteration 2

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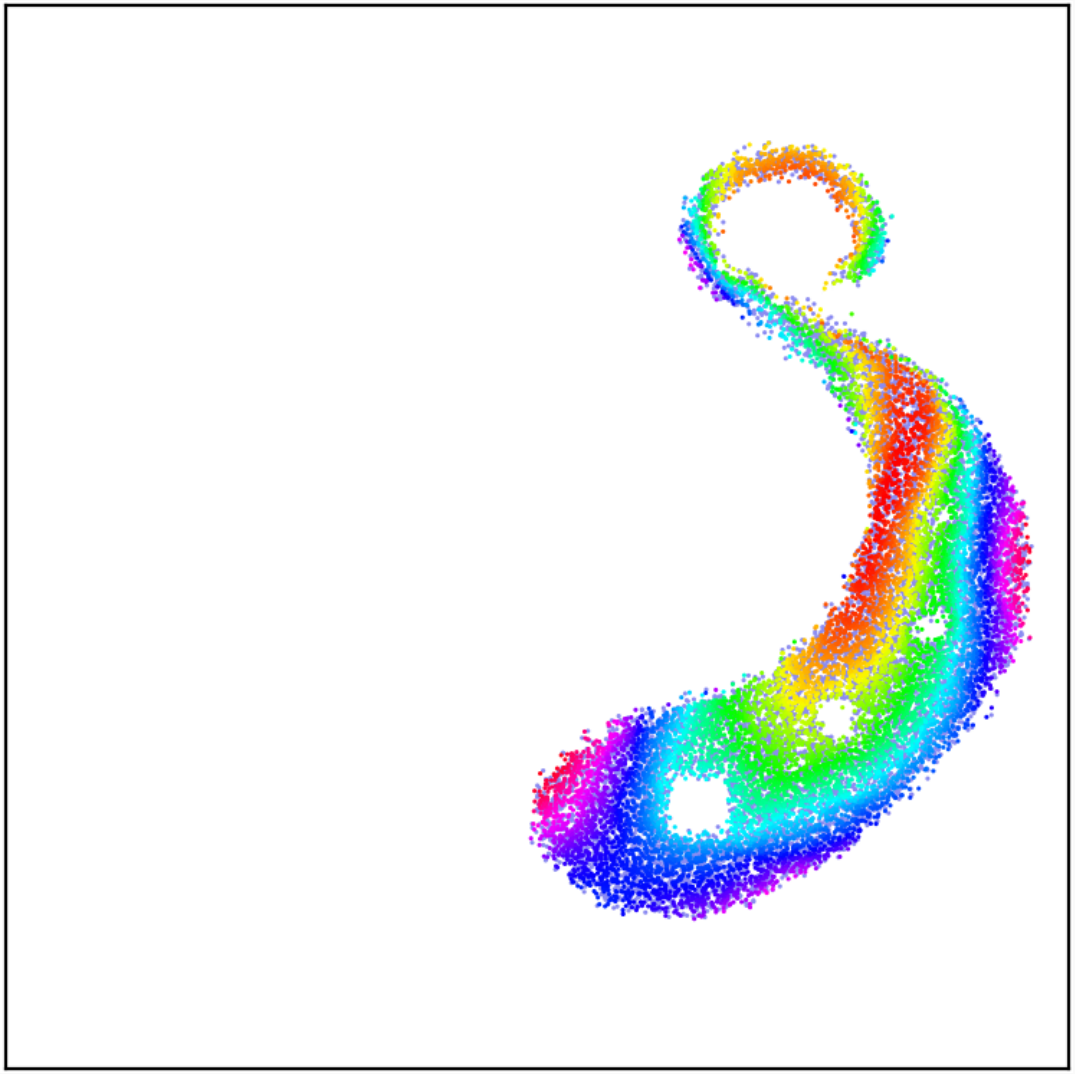

Iteration 10

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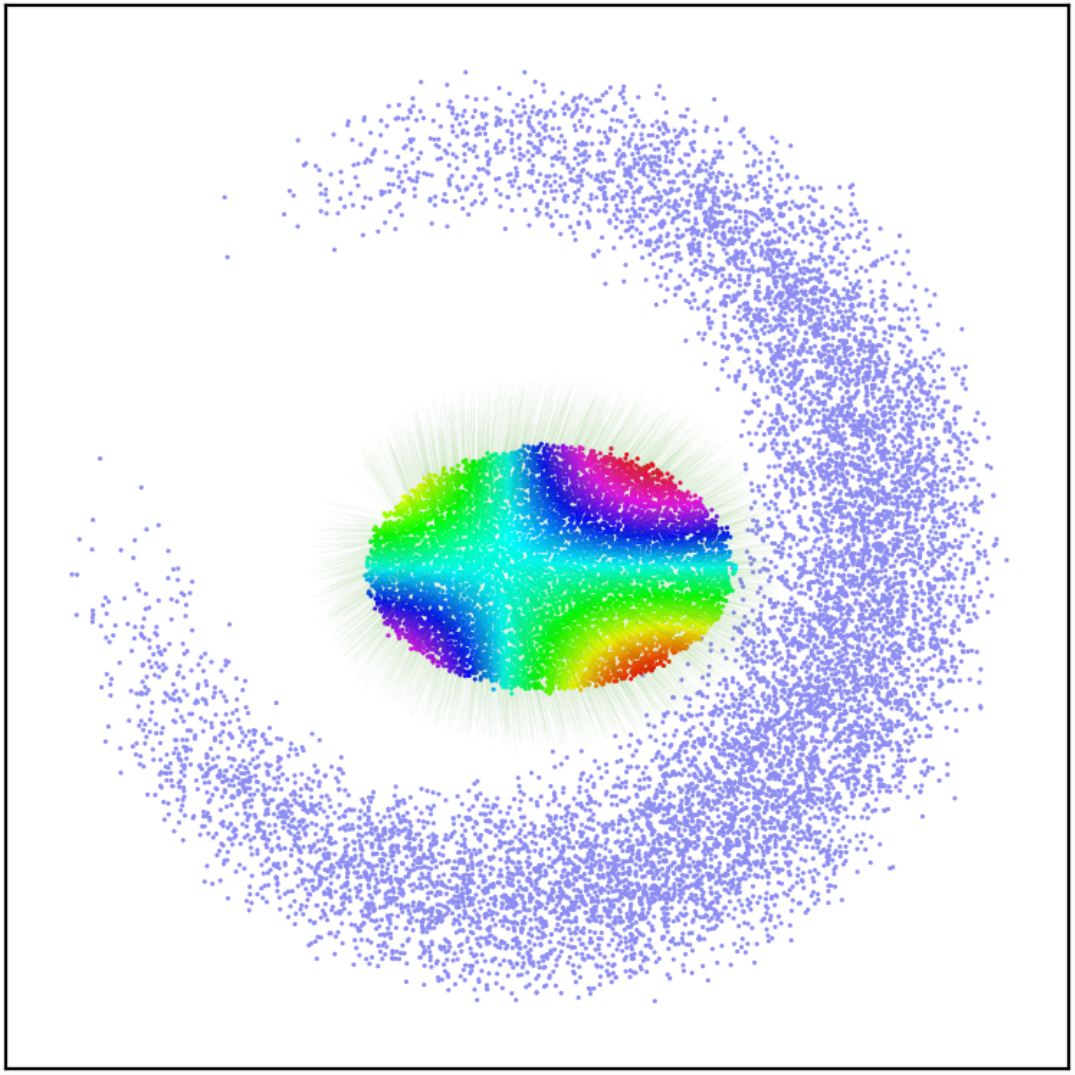

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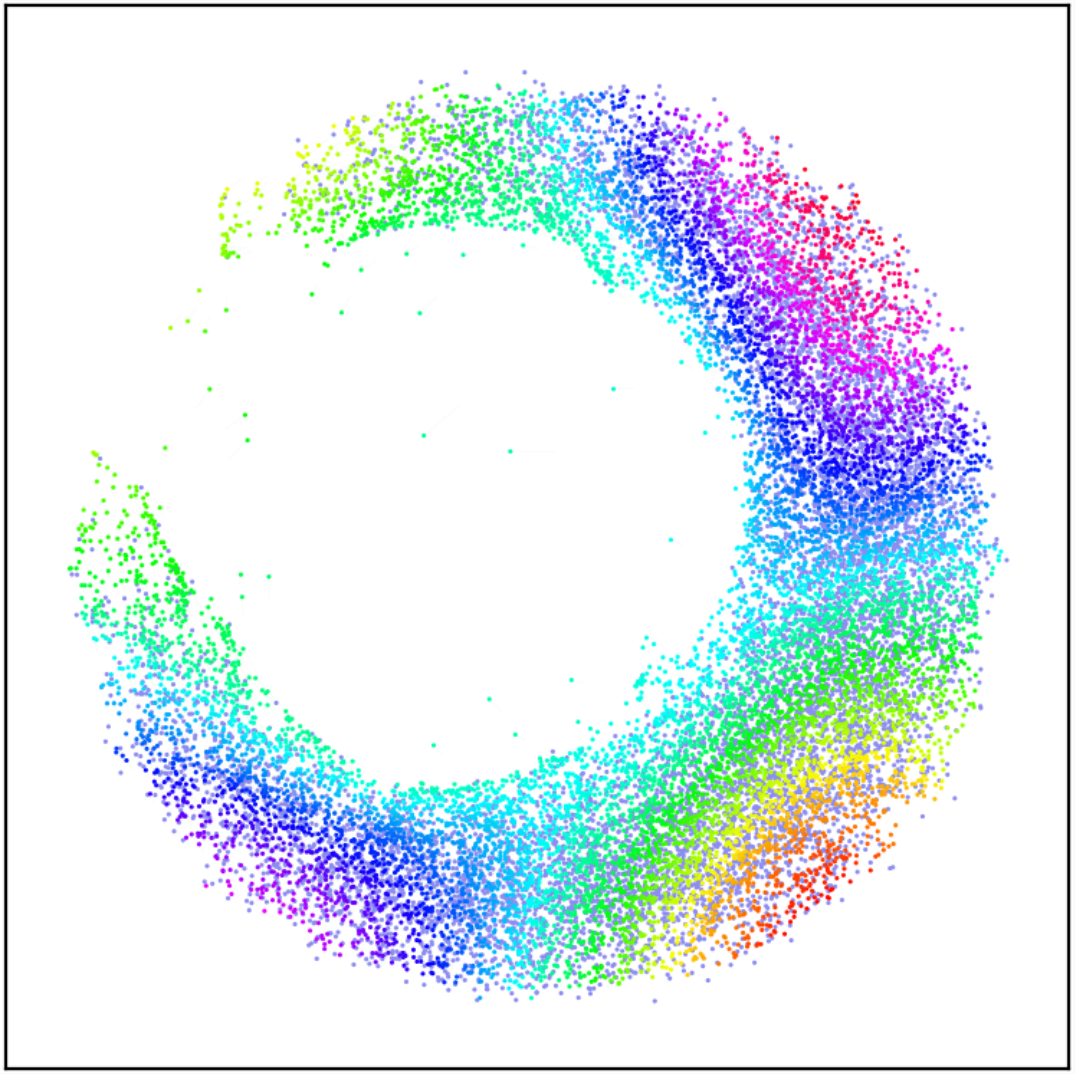

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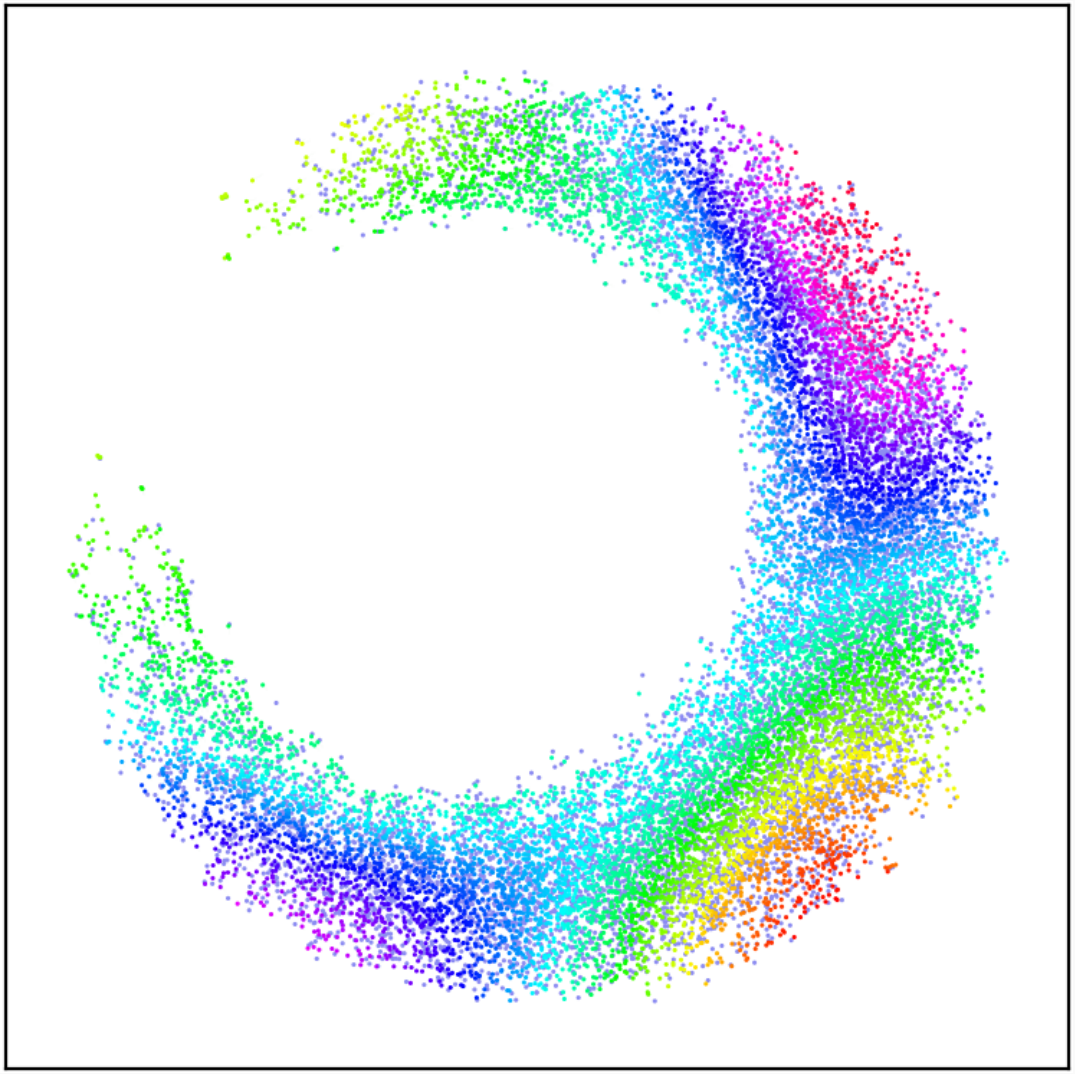

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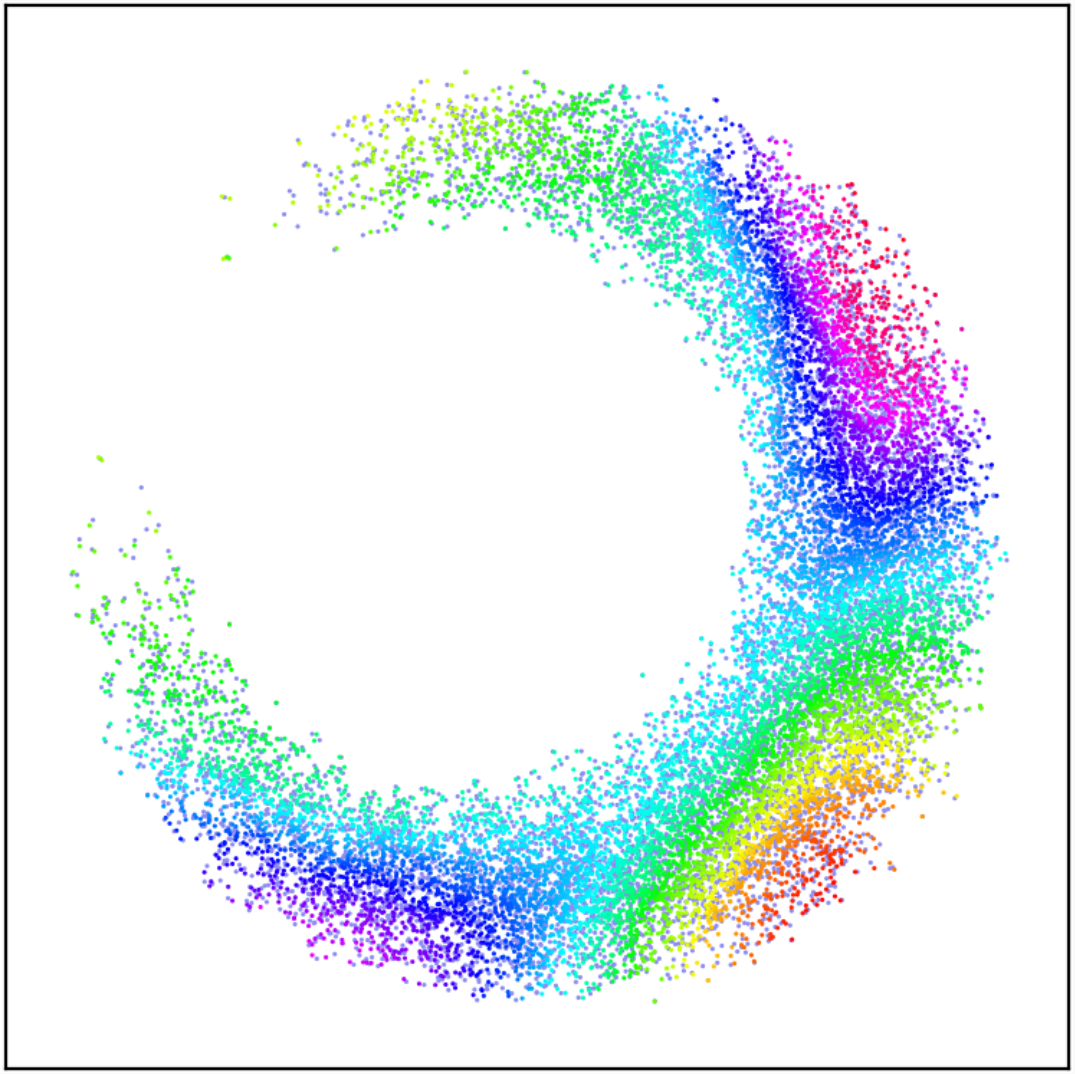

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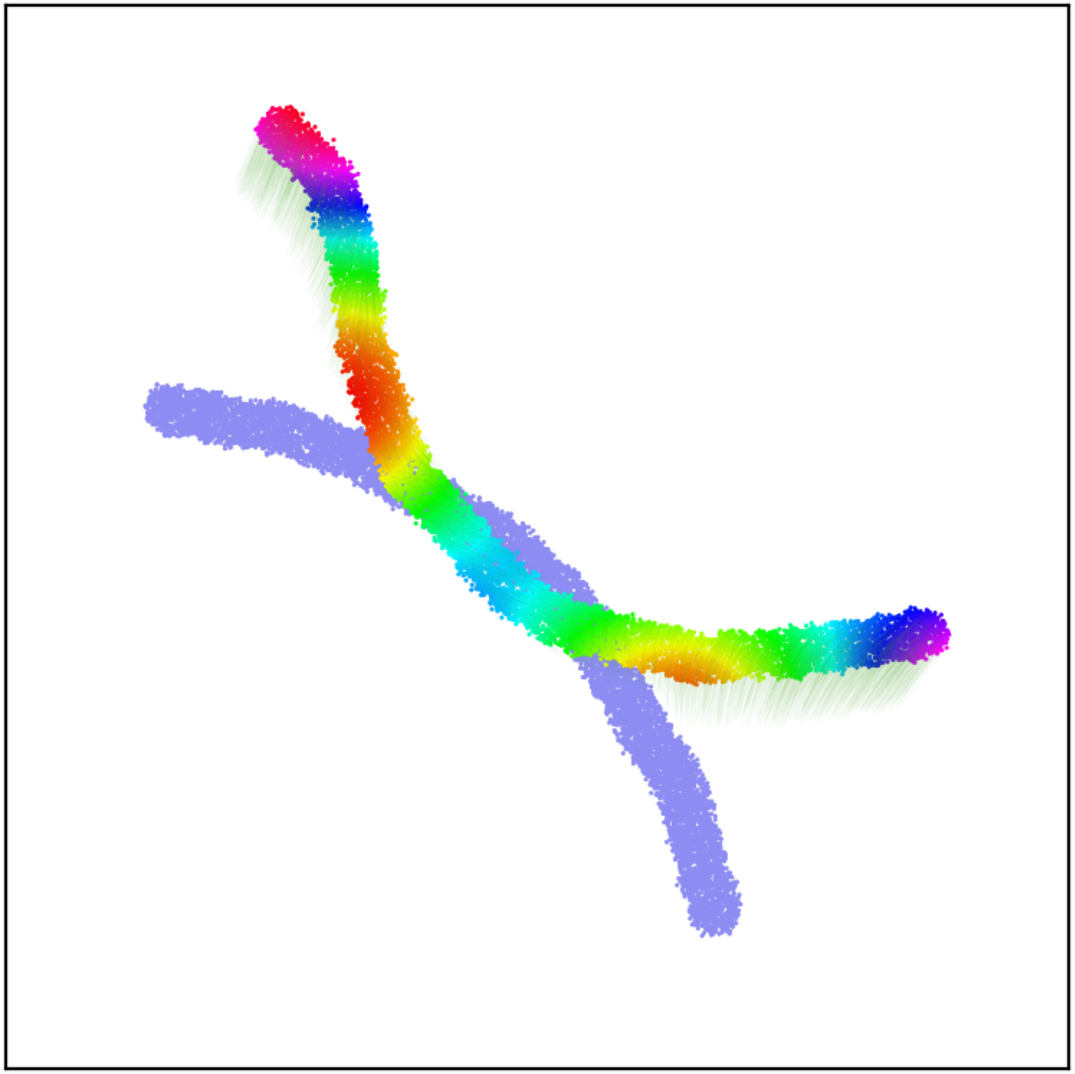

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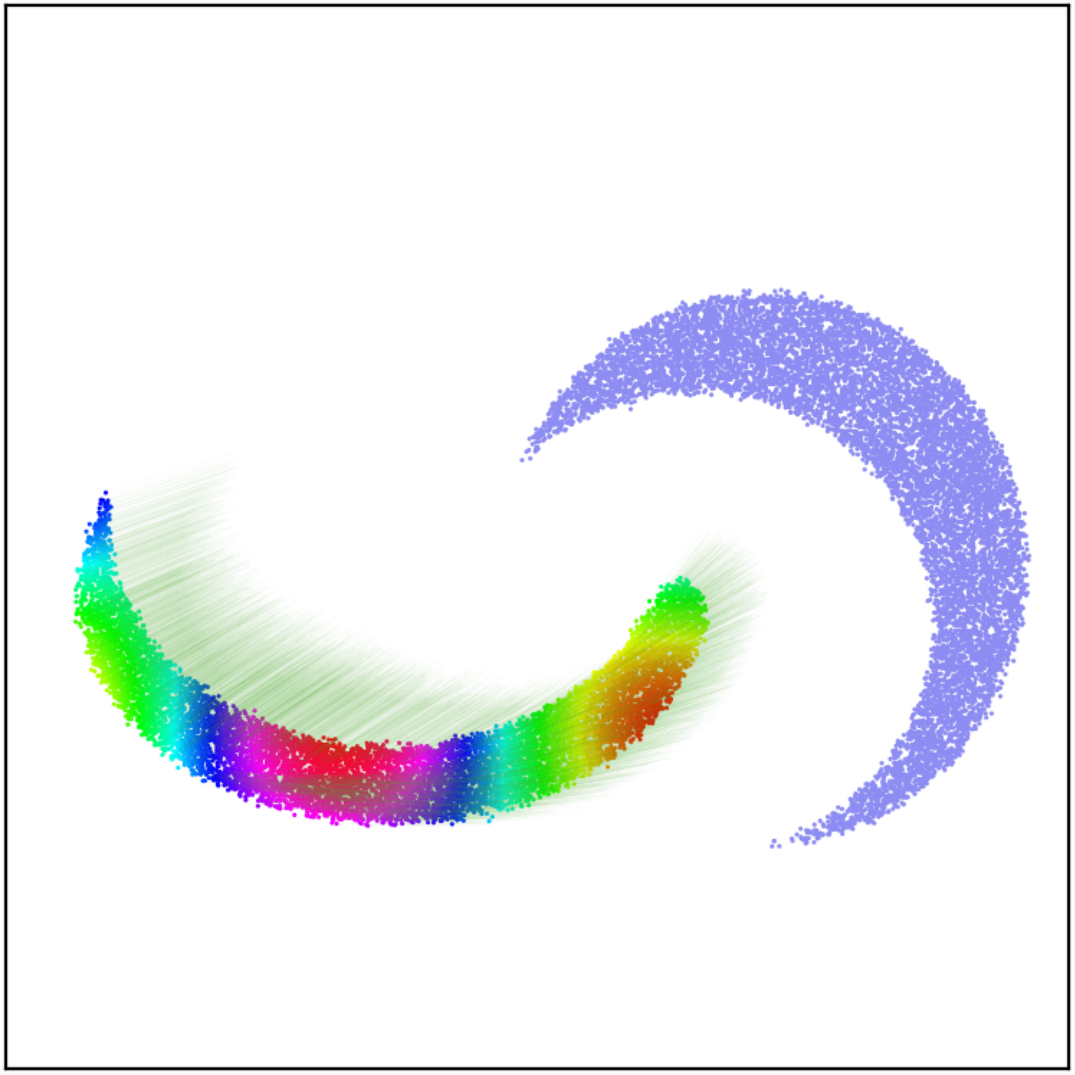

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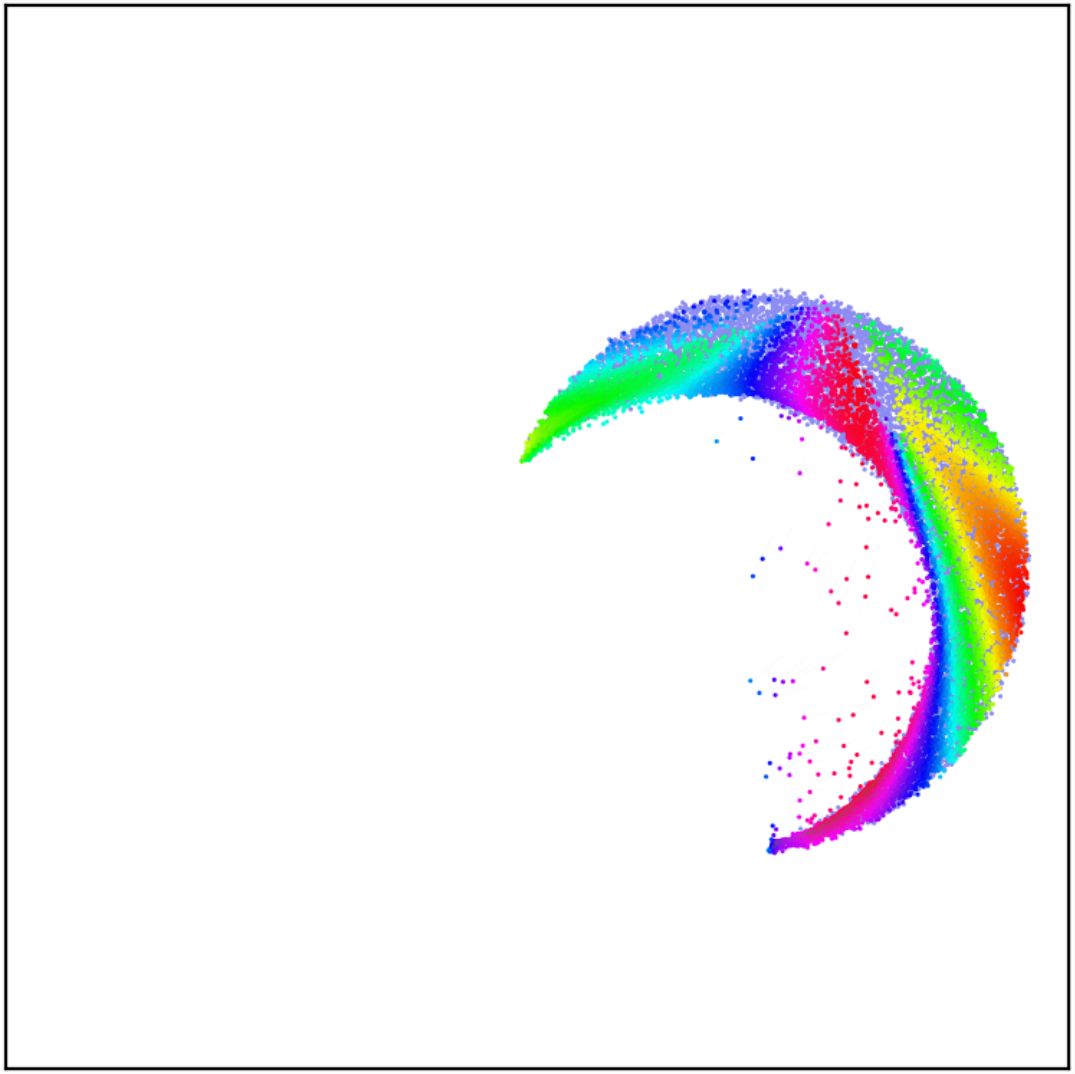

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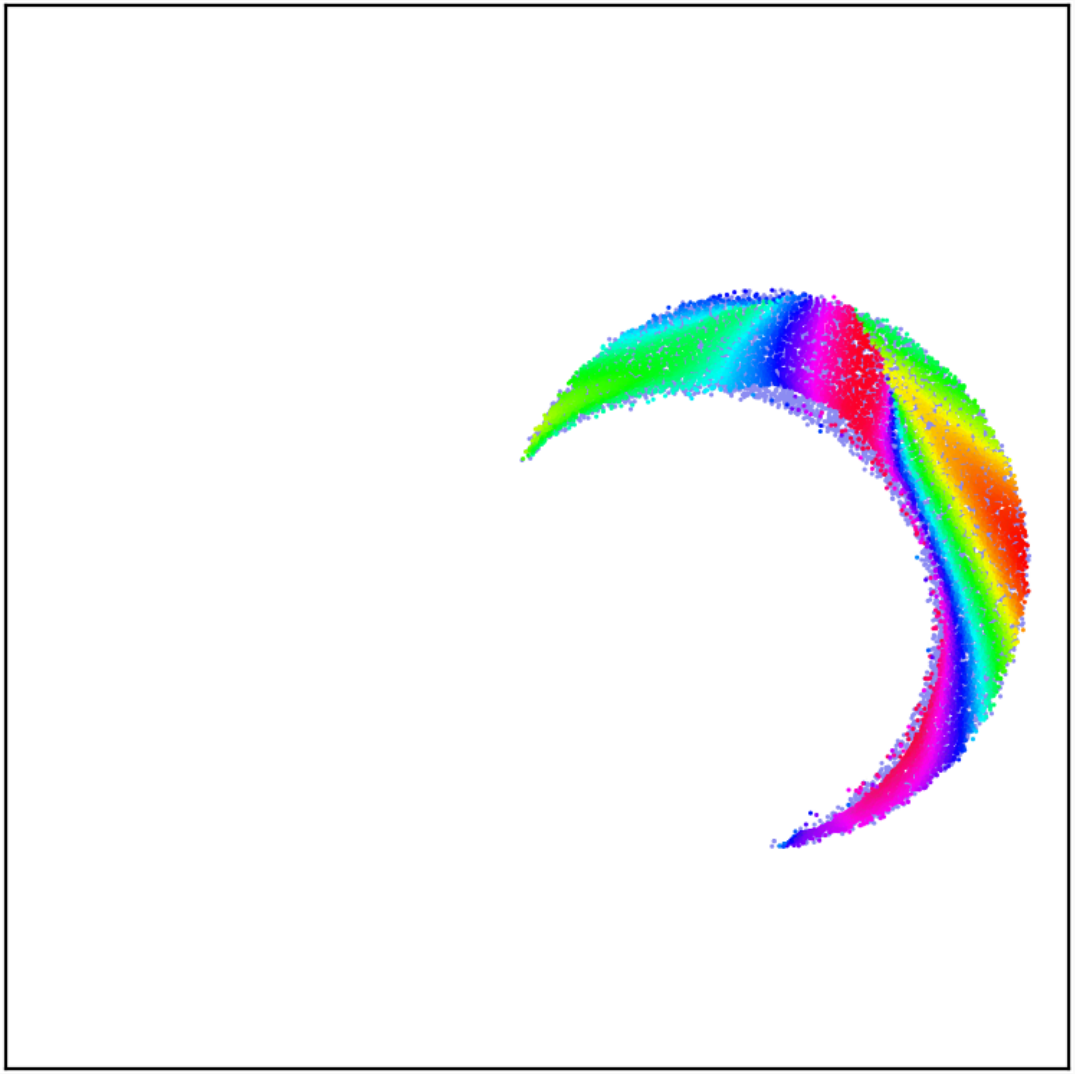

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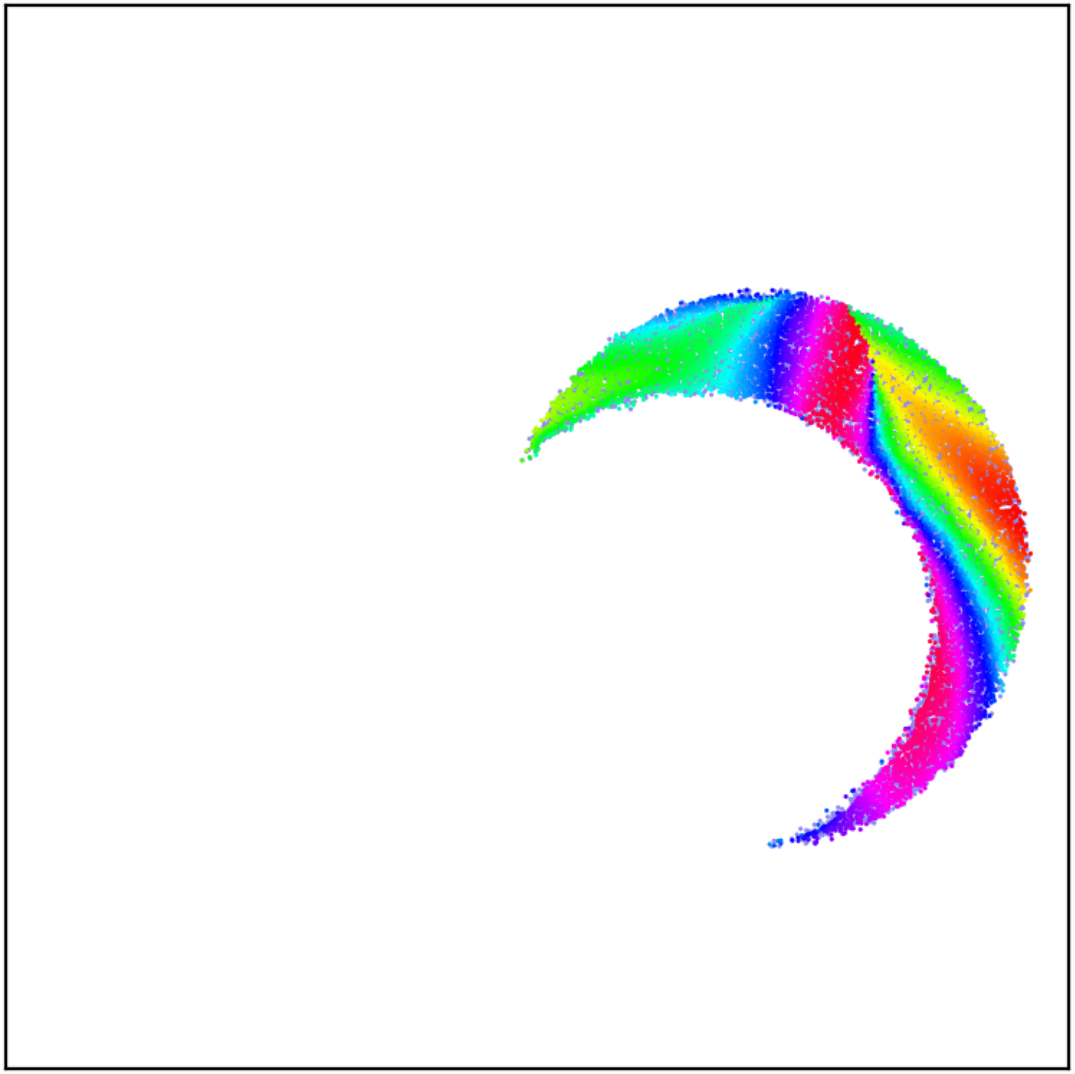

Iteration 10

Conclusion

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**, available in January.

We should go further

Topology-aware registration is a hard, non-convex problem.

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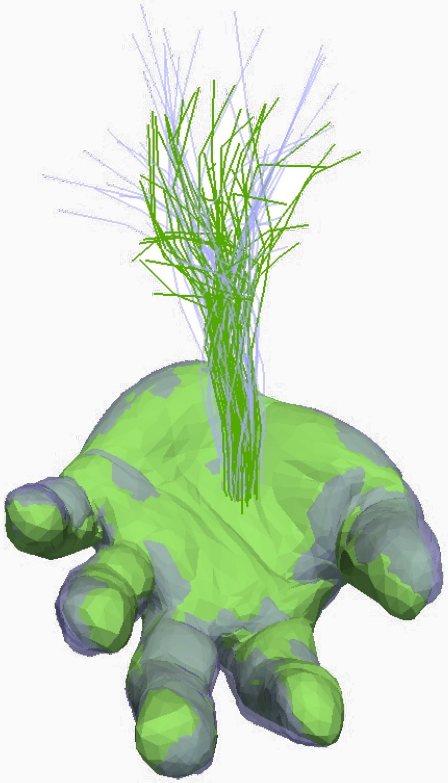
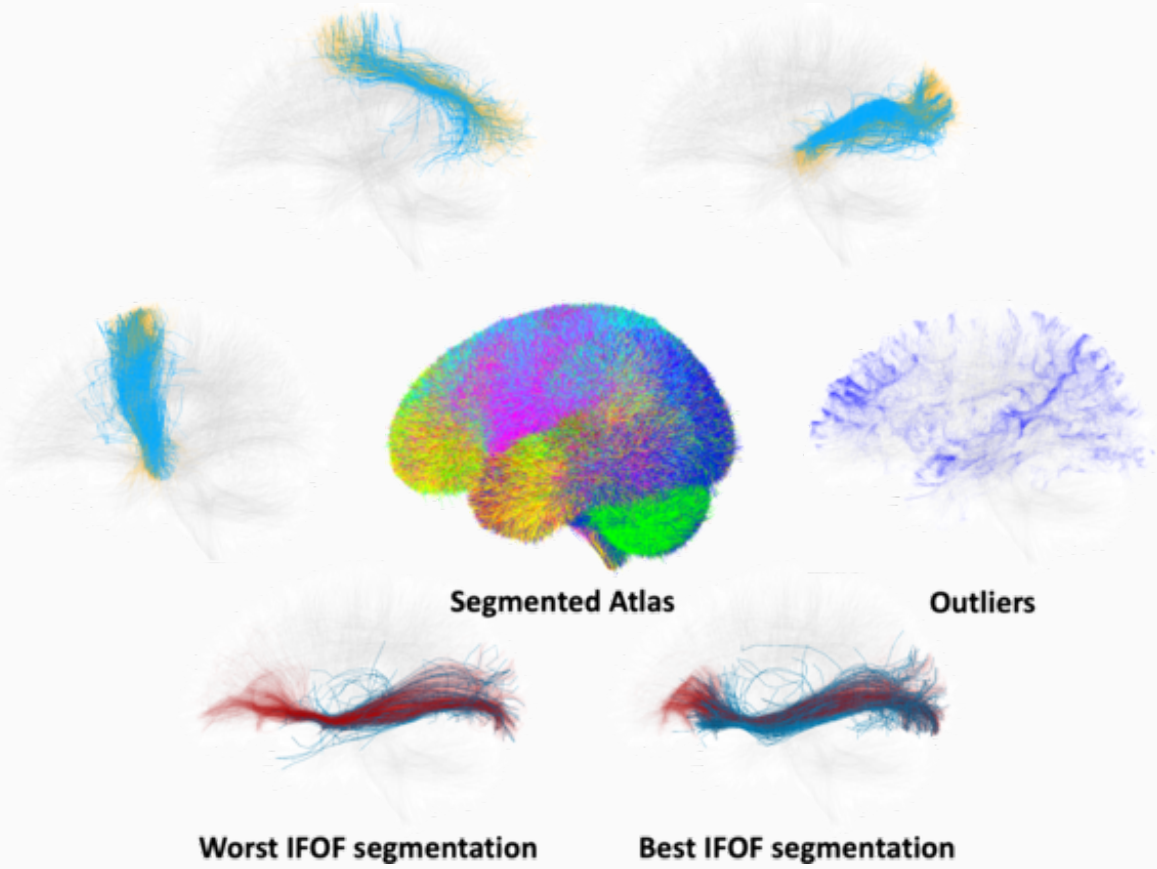
(3^{rd} half)

My work so far: theory, implementation and proofs of concept





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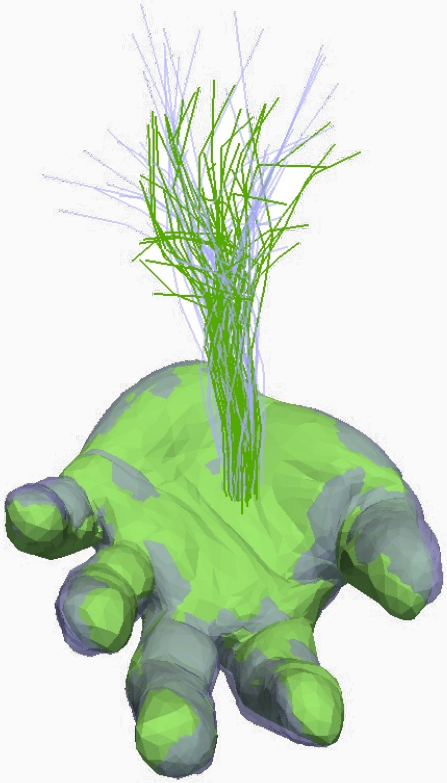
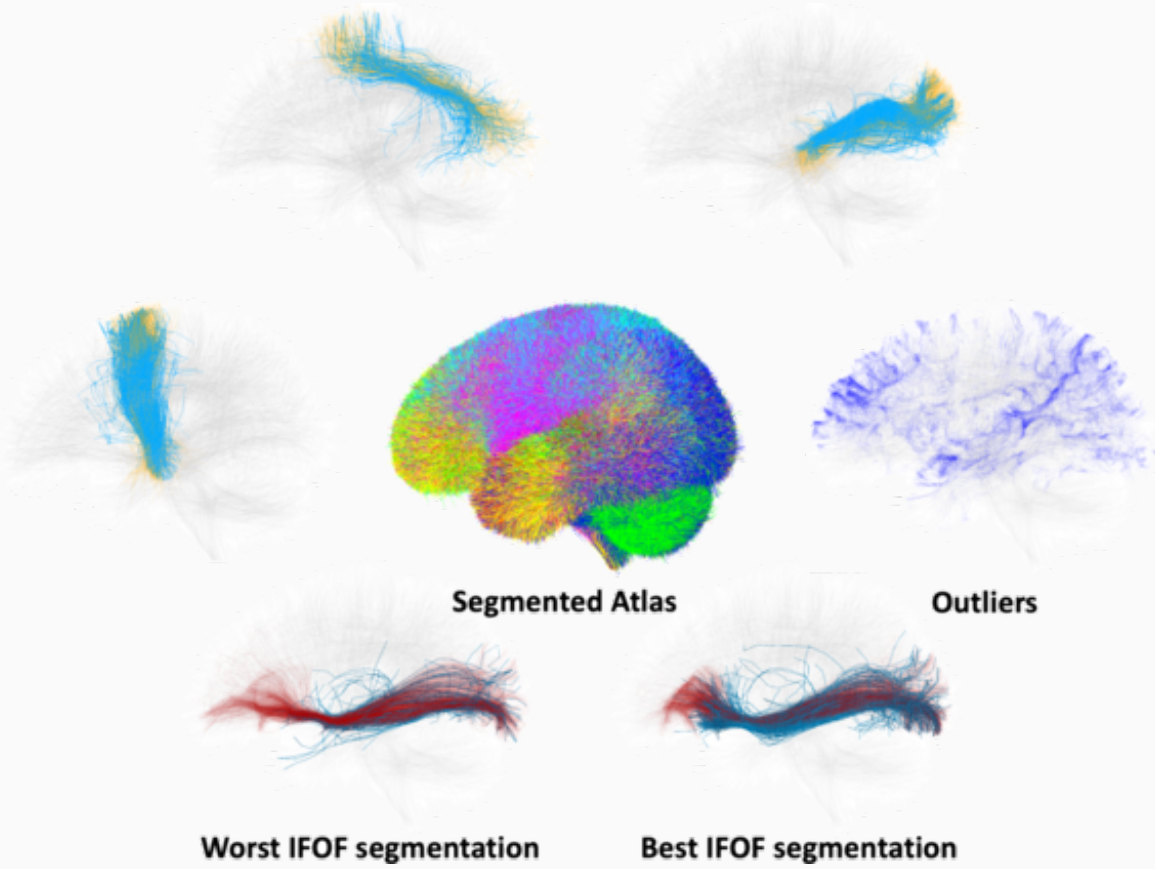


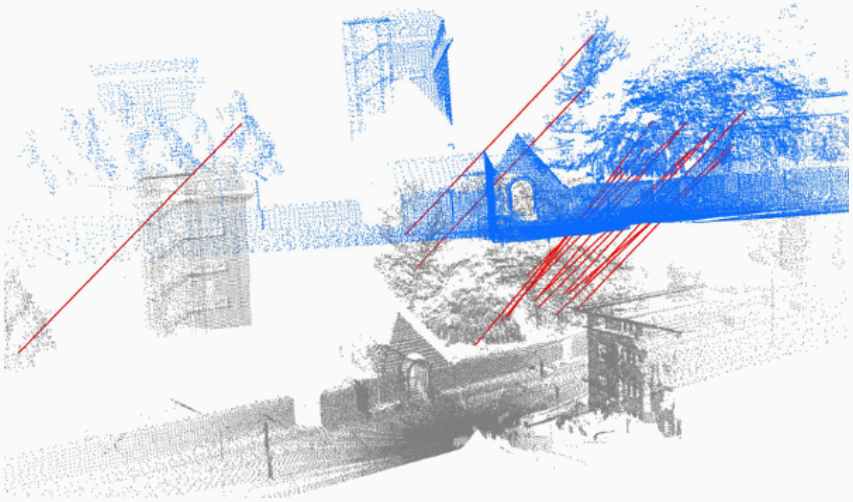


Theorems, libraries, documentation… But no real validation :–(

Thank you for your attention.

Let’s have a chat!

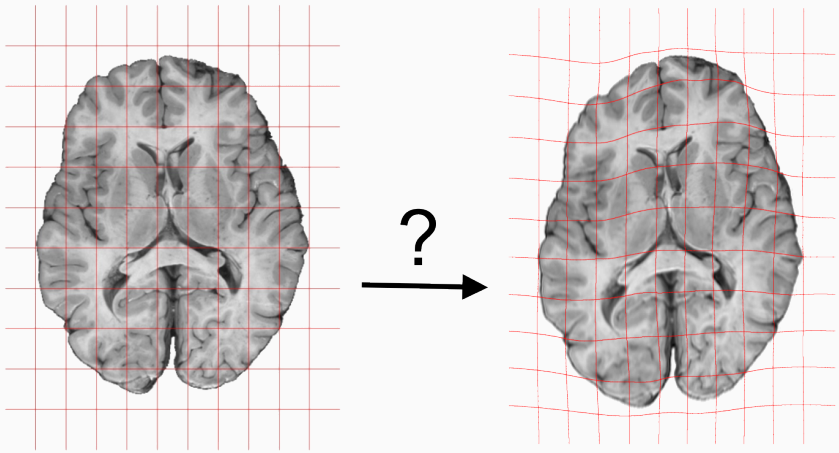
First setting: processing of point clouds



From the documentation of the Point Cloud Library.

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

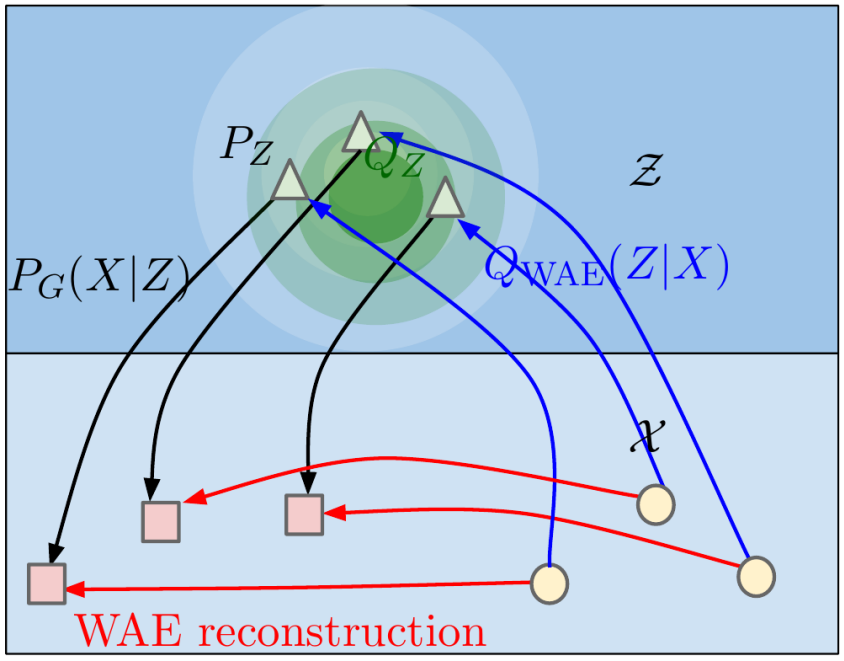
Second setting: medical imaging



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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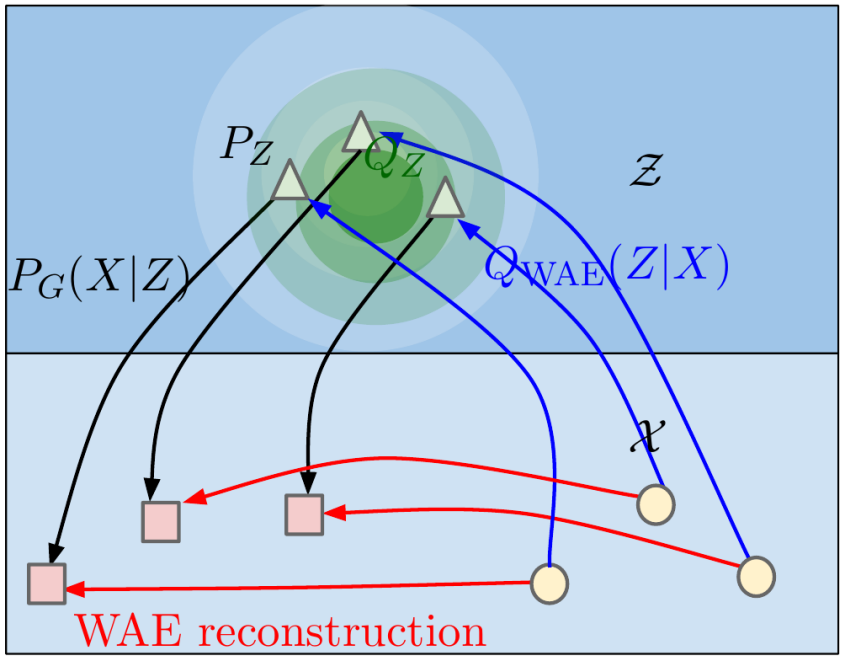

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Which **Loss** function
should we use?

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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  - zero geometry
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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?

References

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- *Optimal Transport for diffeomorphic registration*,
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