

Geometric data analysis, beyond convolutions

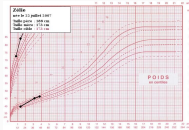
Jean Feydy,
under the supervision of Alain Trounev.

Online PhD defense — July 2, 2020.

ENS Paris, ENS Paris-Saclay, Imperial College London.

Joint work with B. Charlier, J. Glaunès (numerical foundations),
T. Séjourné, F.-X. Vialard, G. Peyré (optimal transport theory),
P. Roussillon, P. Gori (applications to neuroanatomy).

The medical imaging pipeline [Ptr19, EPW⁺11]

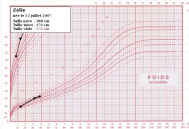


Valuable information

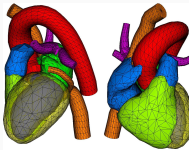


Sensor data

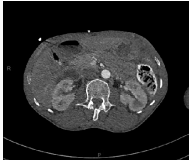
The medical imaging pipeline [Ptr19, EPW⁺11]



Valuable information



High-level description

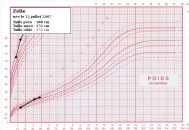


Raw image

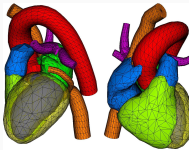


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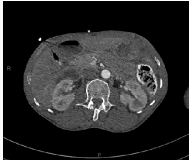
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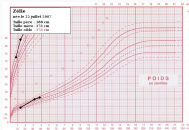
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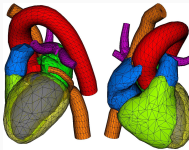
Sensor data

Signal processing

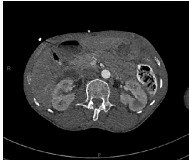
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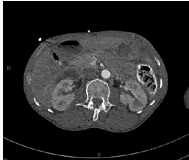
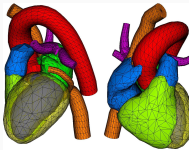
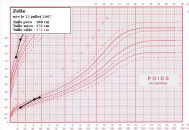


Sensor data

Computational anatomy

Signal processing

The medical imaging pipeline [Ptr19, EPW⁺11]



Valuable information

Statistics

High-level description

Computational anatomy

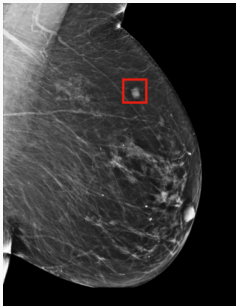
Raw image

Signal processing

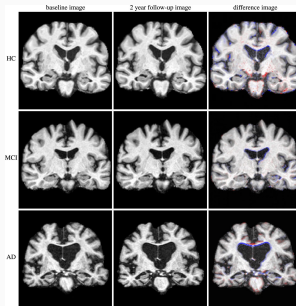
Sensor data

Computational anatomy [CSG19, LSG⁺18, CMN14]

Three main problems:



Spot patterns



Analyze variations



Fit models

The key operation for imaging: filtering, aka. “convolution product”

Convolution = weighted average of the neighboring pixels :

Cheap generalization of the **product** “ $a \cdot x$ ”,
parameterized by the coefficients of a **small filter** φ .



The diagram illustrates the convolution operation. On the left, a small gray square filter with a white center pixel is shown, labeled φ below it. This is followed by a star symbol \star . In the middle, a grayscale image of a heart is shown, labeled x below it. To the right of the heart image is an equals sign $=$. On the far right, the resulting blurred heart image is shown, labeled $\varphi \star x$ below it.

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The diagram illustrates the convolution operation. On the left, a small 5x5 grayscale filter, labeled φ , is shown. This filter is convolved with a larger grayscale image of a heart, labeled x . The result is a blurred version of the heart image, labeled $\varphi \star x$. The convolution operation is represented by a star symbol \star between the filter and the image, and an equals sign $=$ between the result and the blurred image.

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Convolution = weighted average of the neighboring pixels :

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The diagram illustrates the convolution operation. On the left, a small 2x2 filter φ is shown, consisting of a black square and a white square. This filter is convolved with an input image x , which is a grayscale image of a heart. The result is a filtered image $\varphi \star x$, which shows the heart image with the filter applied, resulting in a blurred or smoothed appearance.

$$\varphi \star x = \varphi \star x$$

The key operation for imaging: filtering, aka. “convolution product”

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The diagram illustrates the convolution operation. On the left, a small filter φ is shown as a 2x2 grid with black and white squares. This is followed by a star symbol \star representing convolution. In the middle is the input image x , a grayscale image of a heart. To the right of the input image is an equals sign $=$. On the far right is the output image $\varphi \star x$, which is a grayscale image of a heart with enhanced edges, representing the result of the convolution operation.

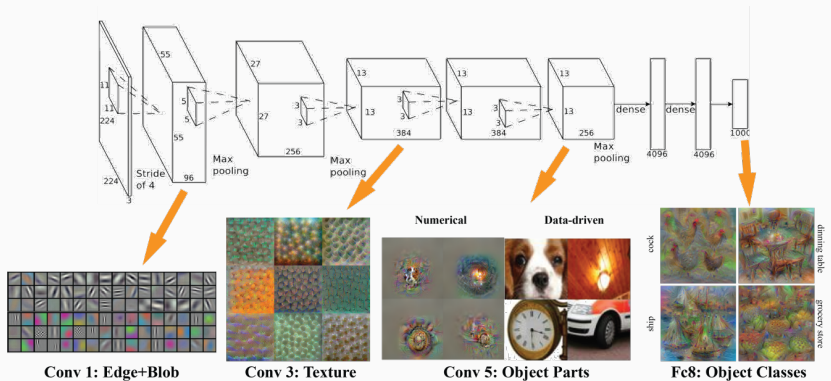
φ x $\varphi \star x$

Combine convolutions + pointwise operations + zooms/unzooms.

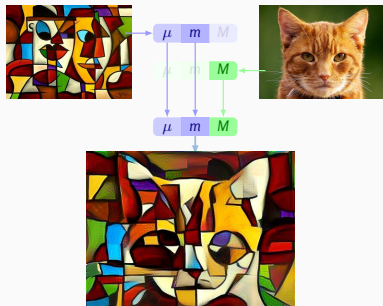
How do we pick the convolution weights?

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

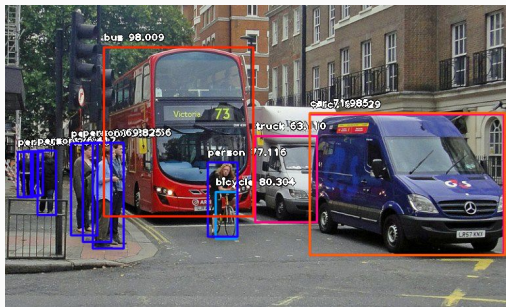
Explicit wavelets \longrightarrow **Data-driven** Convolutional Neural Networks



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

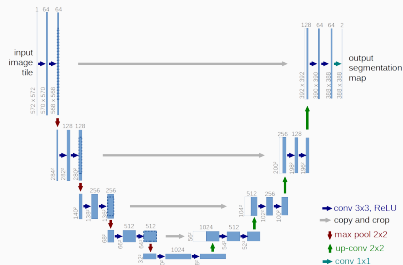


Texture processing

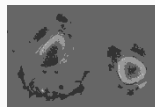
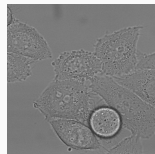


Object detection

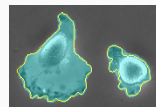
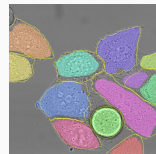
Segmentation with U-nets [RFB15]



Architecture



Input



Output

Shape analysis is still a very open problem

Geometric questions on segmented shapes:

Shape analysis is still a very open problem

Geometric questions on segmented shapes:

- Is this **heart** beating all right?
- How should we reconstruct this **mandible**?
- Has this **brain** grown or shrunk since last year?
- Can we link these anatomical changes to **other signals**?

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Over the last 30 years, **robust methods** have been designed to answer these questions.

Today, we want to improve them with **data-driven** insights.

This is challenging.

To replicate the “wavelets → CNNs” revolution in our field, we need to **revamp our numerical toolbox**.

Geometric data analysis, beyond convolutions:

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- Focus on **geometric data**:
segmentation maps, point clouds, surface meshes, etc.
- Focus on **geometric methods**:
K-nearest neighbors, kernel methods, optimal transport, etc.
- Provide new **computational routines**:
expand the toolbox for data sciences.

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We work with 10^3 - 10^6 points in dimension 2 to 10.

We focus on geometry and speed.

Today, we will talk about:

1. **Fast geometry** with symbolic matrices.
2. Scalable **optimal transport**.
3. New directions for **computational anatomy**.

Fast geometry with symbolic matrices.

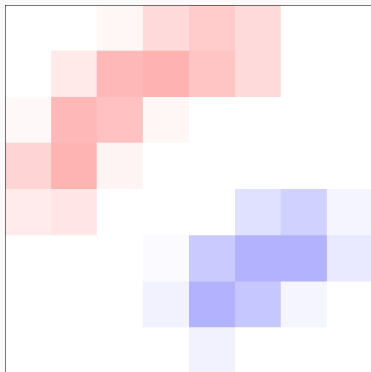


Benjamin Charlier



Joan Glaunès

Working with images – implicit coordinates

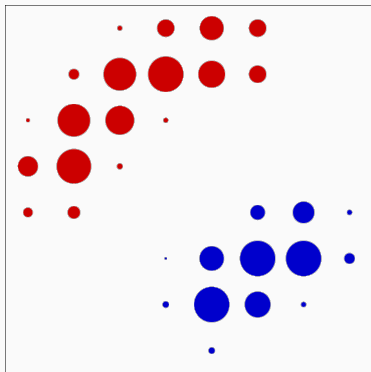


$N_x = 8, N_y = 8, N_z = 1$
 $C = 3$ (RGB channels)

Bitmap images and volumes:

- (N_x, N_y, N_z, C) pixels.
 - .bmp, .png, .jpg
 - Eulerian.
-
- + **Standard** for radiology.
 - + Easy to find neighbors.
 - + Fast **convolutions**.
 - + Fast Fourier transforms.
-
- Precision vs. Memory.
 - Cumbersome **deformations**.

Working with point clouds – explicit coordinates



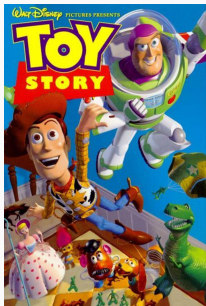
$N = 31, D = 2,$
 $C = 3$ (RGB channels)

Point clouds, sampled data:

- (N, D) coordinates.
 - (N, C) signals.
 - .svg
 - Lagrangian.
- + Compact representation.
- + High precision for geometry.
- + **Easy to deform.**
- Cumbersome convolutions and Fourier transforms.

We can now get the best of both worlds

Video games: millions of **textured triangles**, processed in real-time.



1995



Today

In research, 1,000,000 is the new 10,000 [CL96]



11k triangles



871k triangles

Thank God for the gamers!



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

Incredible performance: $\sim 10^{12}$ operations (+, \times , ...) per second.

One catch: complex **memory management**, with 6 types of buffers.

GPU programming is a full-time job.

TensorFlow and PyTorch combine:

- + Array-centric **Python interface**.
- + CPU *and* **GPU** backends.
- + **Automatic differentiation** engine.
- + Excellent support for imaging (convolutions) and linear algebra.

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⇒ Ideally suited for research.

Efficient algorithms still rely on C++ foundations

Explicit C++/CUDA implementations with a Python interface for:

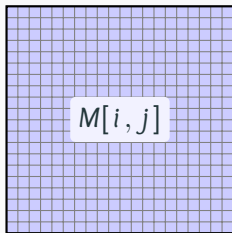
- Linear algebra (cuBLAS).
- Convolutions (cuDNN).
- Fourier (cuFFT) and wavelet transforms (Kymatio).

Geometric algorithms do not benefit from the same level of integration. Researchers can either:

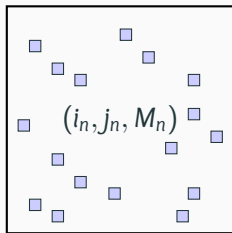
- Work directly in C++/CUDA – cumbersome for data sciences.
- Rely on **explicit distance matrices**.

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

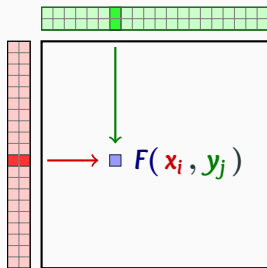
We provide efficient support for distance-like matrices



Dense matrix
Coefficients only



Sparse matrix
Coordinates + coeffs



Symbolic matrix
Formula + data



`pip install pykeops`



KeOps works with PyTorch, NumPy, Matlab and R

```
# Large point cloud in  $\mathbb{R}^{50}$ :  
import torch  
N, D = 10**6, 50  
x = torch.rand(N, D).cuda() # (1M, 50) array  
  
# Compute the nearest neighbor of every point:  
from pykeops.torch import LazyTensor  
x_i = LazyTensor(x.view(N, 1, D)) # x_i is a "column"  
x_j = LazyTensor(x.view(1, N, D)) # x_j is a "line"  
D_ij = ((x_i - x_j)**2).sum(dim=2) # (N, M) symbolic  
indices_i = D_ij.argmin(dim=1)    # -> (N,) dense
```

On par with reference C++/CUDA libraries (FAISS-GPU).

Combining performance and flexibility

We can work with arbitrary formulas:

```
D_ij = ((x_i - x_j) ** 2).sum(dim=2)      # Euclidean
M_ij = (x_i - x_j).abs().sum(dim=2)      # Manhattan
C_ij = 1 - (x_i | x_j)                   # Cosine
H_ij = D_ij / (x_i[...,0] * x_j[...,0]) # Hyperbolic
```

⇒ ×200 acceleration for UMAP on hyperbolic spaces.

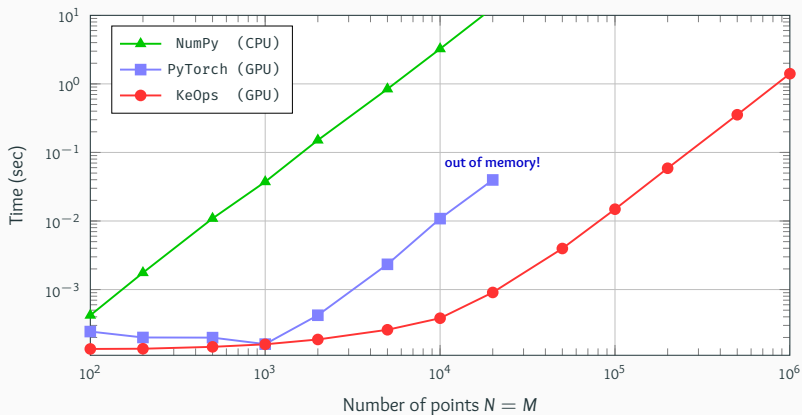
KeOps supports:

- **Reductions:** sum, log-sum-exp, K-min, matrix-vector product, etc.
- **Operations:** +, ×, sqrt, exp, neural networks, etc.
- **Advanced schemes:** block-wise sparsity, numerical stability, etc.
- **Automatic differentiation:** seamless integration with PyTorch.

Scaling up to large datasets

$$a_i \leftarrow \sum_{j=1}^M \underbrace{\exp(-\|x_i - y_j\|^2 / 2\sigma^2)}_{k(x_i, y_j)} b_j, \quad \forall i \in \llbracket 1, N \rrbracket$$

Gaussian kernel product in 3D (RTX 2080 Ti GPU)



- + **Cross-platform:** C++, R, Matlab, NumPy *and* PyTorch.
- + **Versatile:** many operations, variables, reductions.
- + **Efficient:** $O(N)$ memory, competitive runtimes.
- + **Powerful:** automatic differentiation, block-sparsity, etc.
- + **Transparent:** interface with **SciPy**, GPytorch, etc.
- + **Fully documented:**
`www.kernel-operations.io`
- Requires a C++/CUDA environment (nvcc).
- Slow-down when $D > 100$.

Solve a **kernel linear system**:

$$(\lambda \text{Id} + K_{xx}) a = b \quad \text{i.e.} \quad a \leftarrow (\lambda \text{Id} + K_{xx})^{-1} b$$

where $\lambda \geq 0$ and $(K_{xx})_{i,j} = k(x_i, x_j)$ is a positive definite matrix.

KeOps symbolic tensors:

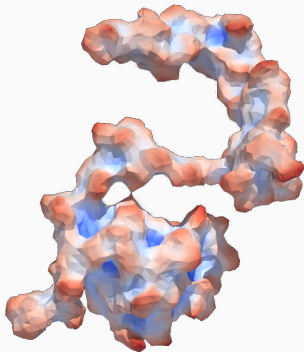
- Can be fed to **standard solvers**: SciPy, GPytorch, etc.
- On the 3DRoad dataset ($N = 278k$, $D = 3$):

7h with 8 GPUs \rightarrow 15mn with 1 GPU.

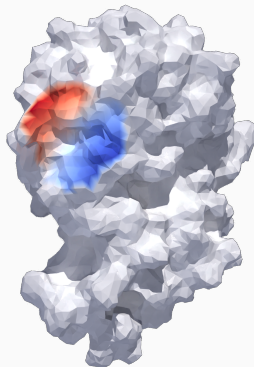
- Provide a **fast backend for research codes**: see e.g.
*Kernel methods through the roof: handling **billions of points** efficiently*, by G. Meanti, L. Carratino, L. Rosasco, A. Rudi (2020).

Applications to geometric deep learning

Fast prototyping of geometry processing algorithms:



Mean curvature



Mesh convolution

The KeOps library provides:

- **Good performance** on geometric problems, with all the **convenient features** of a deep learning library.
- A first **stable release** last year; 23k downloads so far.
- The computational **foundations** of this thesis.

Computational optimal transport



Thibault Séjourné



F.-X. Vialard



Gabriel Peyré

We need robust loss functions for shape analysis

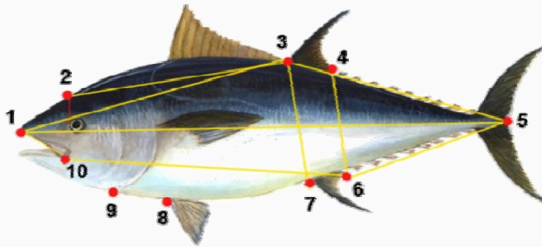
Working with point clouds is now **easier than ever**.
We can prototype new geometric algorithms in minutes.

But how should we **measure success** and **errors**?

⇒ We must develop **geometric loss functions**
to compute distances between shapes.

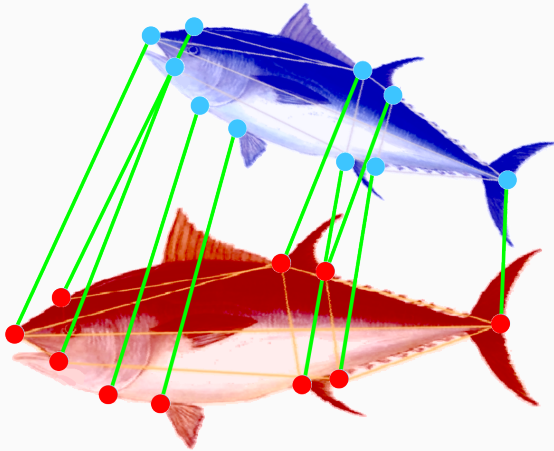
High-quality gradients will improve the **robustness**
of registration or training algorithms
and allow us to **focus on our models**.

Life is easy when you have landmarks...



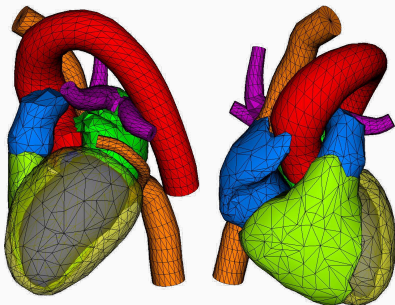
Anatomical landmarks from *A morphometric approach for the analysis of body shape in bluefin tuna*, Addis et al., 2009.

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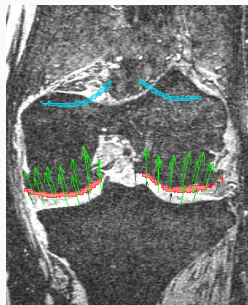


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Unfortunately, medical data is often weakly labeled [EPW⁺11]



Surface meshes

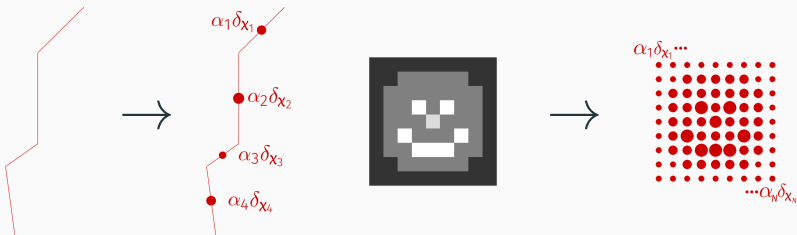


Segmentation masks

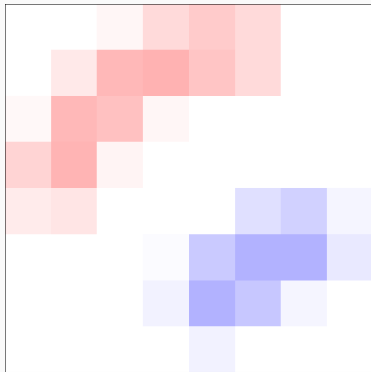
Encoding unlabeled shapes as measures

Let's enforce sampling invariance:

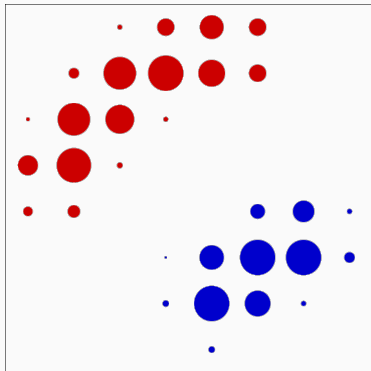
$$A \longrightarrow \alpha = \sum_{i=1}^N \alpha_i \delta_{x_i}, \quad B \longrightarrow \beta = \sum_{j=1}^M \beta_j \delta_{y_j}.$$



A baseline setting: density registration

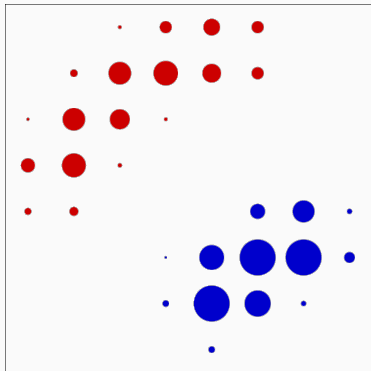


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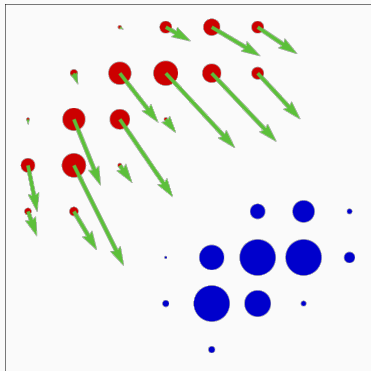
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$$\sum_{i=1}^N \alpha_i = 1 = \sum_{j=1}^M \beta_j$$

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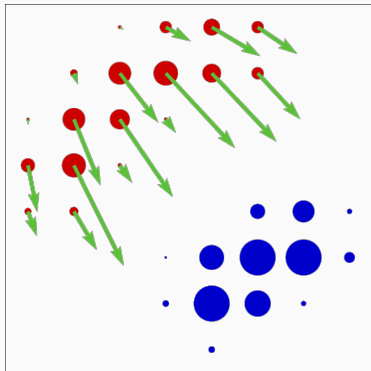


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Display $v_i = -\frac{1}{\alpha_i} \nabla_{x_i} \text{Loss}(\alpha, \beta).$

A baseline setting: density registration



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

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

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

Seamless extensions to:

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

The Wasserstein distance

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

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Simple toy example in 1D:

The Wasserstein distance

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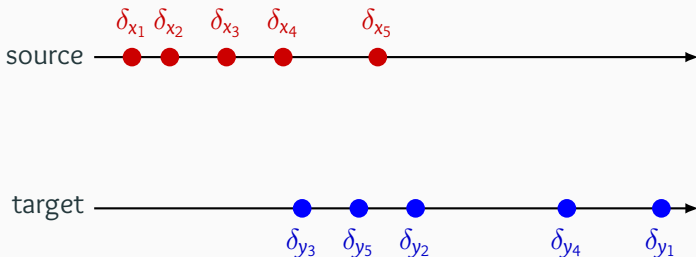
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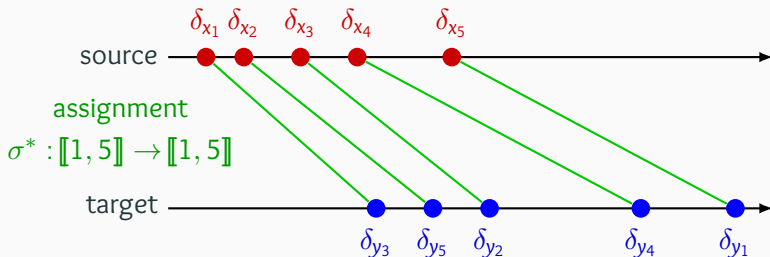
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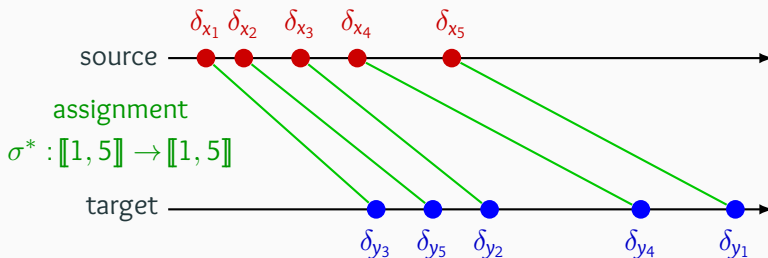
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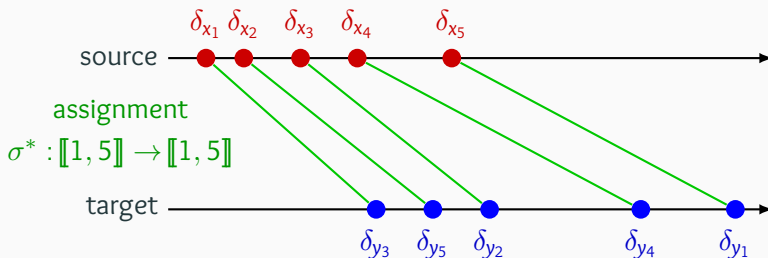


$$\text{OT}(\alpha, \beta) = \frac{1}{2N} \sum_{i=1}^N |x_i - y_{\sigma^*(i)}|^2$$

The Wasserstein distance

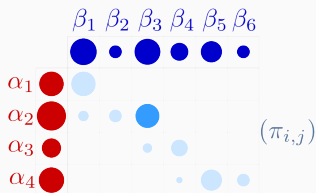
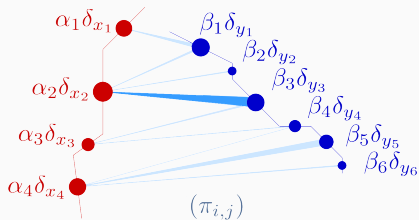
We need **clean gradients**, without artifacts.

Simple toy example in 1D:



$$\text{OT}(\alpha, \beta) = \frac{1}{2N} \sum_{i=1}^N |\mathbf{x}_i - \mathbf{y}_{\sigma^*(i)}|^2 = \min_{\sigma \in \mathcal{S}_N} \frac{1}{2N} \sum_{i=1}^N |\mathbf{x}_i - \mathbf{y}_{\sigma(i)}|^2$$

Optimal transport generalizes sorting to $D > 1$



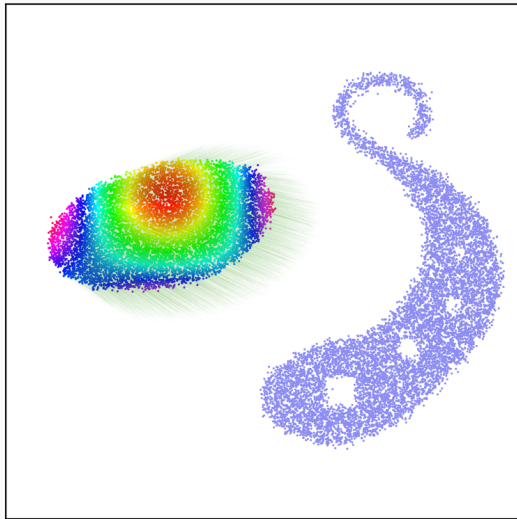
Minimize over N -by- M matrices
(transport plans) π :

$$\text{OT}(\alpha, \beta) = \min_{\pi} \underbrace{\sum_{i,j} \pi_{i,j} \cdot \frac{1}{2} |\mathbf{x}_i - \mathbf{y}_j|^2}_{\text{transport cost}}$$

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

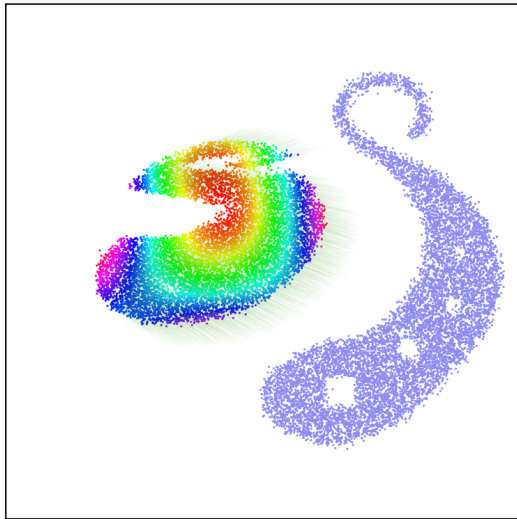
$$\sum_j \pi_{i,j} = \alpha_i, \quad \sum_i \pi_{i,j} = \beta_j.$$

Gradient flow as a toy registration: $x_i \leftarrow x_i - \delta t \frac{1}{\alpha_i} \nabla_{x_i} \text{OT}(\alpha, \beta)$



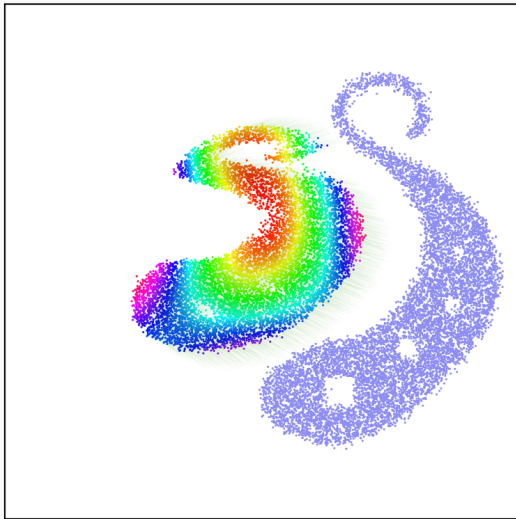
$t = .00$

Gradient flow as a toy registration: $x_i \leftarrow x_i - \delta t \frac{1}{\alpha_i} \nabla_{x_i} \text{OT}(\alpha, \beta)$



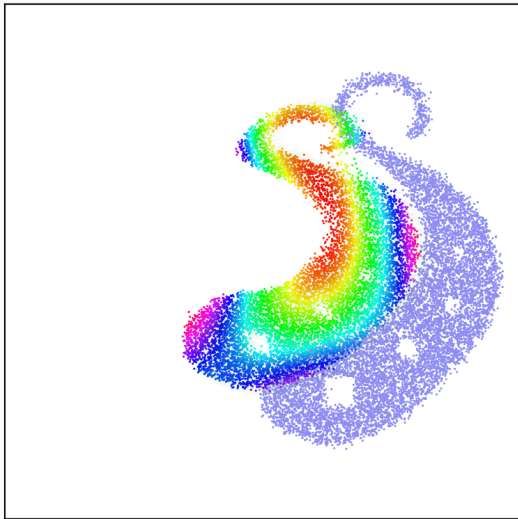
$t = .25$

Gradient flow as a toy registration: $x_i \leftarrow x_i - \delta t \frac{1}{\alpha_i} \nabla_{x_i} \text{OT}(\alpha, \beta)$



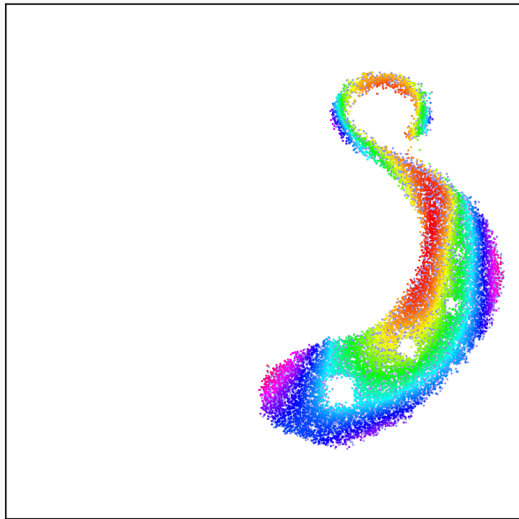
$t = .50$

Gradient flow as a toy registration: $x_i \leftarrow x_i - \delta t \frac{1}{\alpha_i} \nabla_{x_i} \text{OT}(\alpha, \beta)$



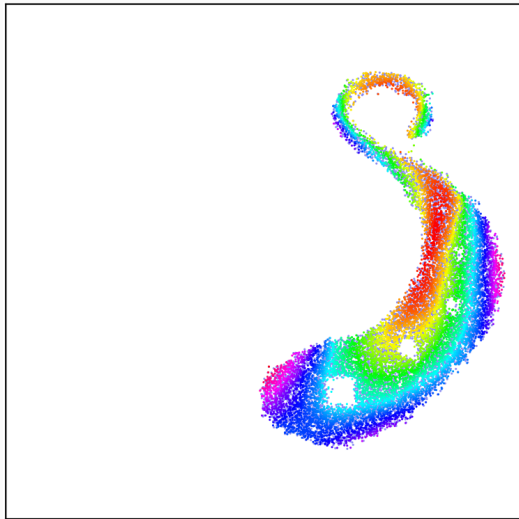
$t = 1.00$

Gradient flow as a toy registration: $x_i \leftarrow x_i - \delta t \frac{1}{\alpha_i} \nabla_{x_i} \text{OT}(\alpha, \beta)$



$t = 5.00$

Gradient flow as a toy registration: $x_i \leftarrow x_i - \delta t \frac{1}{\alpha_i} \nabla_{x_i} \text{OT}(\alpha, \beta)$



$t = 10.00$

Key properties [Bre91]

The Wasserstein loss $\text{OT}(\alpha, \beta)$ is:

- **Symmetric:** $\text{OT}(\alpha, \beta) = \text{OT}(\beta, \alpha).$
- **Positive:** $\text{OT}(\alpha, \beta) \geq 0.$
- **Definite:** $\text{OT}(\alpha, \beta) = 0 \iff \alpha = \beta.$
- **Translation-aware:** $\text{OT}(\alpha, \text{Translate}_{\vec{v}}(\alpha)) = \frac{1}{2} \|\vec{v}\|^2.$
- More generally, OT retrieves the unique **gradient of a convex function** $T = \nabla \varphi$ that maps α onto β :

$$\text{In dimension 1, } (x_i - x_j) \cdot (y_{\sigma(i)} - y_{\sigma(j)}) \geq 0$$

$$\text{In dimension D, } \langle x_i - x_j, T(x_i) - T(x_j) \rangle_{\mathbb{R}^D} \geq 0.$$

\implies Appealing generalization of an **increasing mapping**.

How should we solve the OT problem?

Key dates for discrete optimal transport with N points:

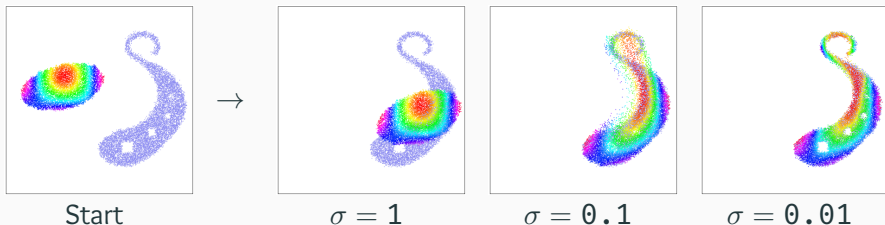
- [Kan42]: **Dual** problem.
- [Kuh55]: **Hungarian** method in $O(N^3)$.
- [Ber79]: **Auction** algorithm in $O(N^2)$.
- [KY94]: **SoftAssign** = Sinkhorn + annealing, in $O(N^2)$.
- [GRL⁺98, CR00]: **Robust Point Matching** = Sinkhorn as a loss.
- [Cut13]: Start of the **GPU era**.
- [Mér11, Lév15,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

⇒ Generalized **QuickSort** algorithm.

Key ingredient: the entropic blur

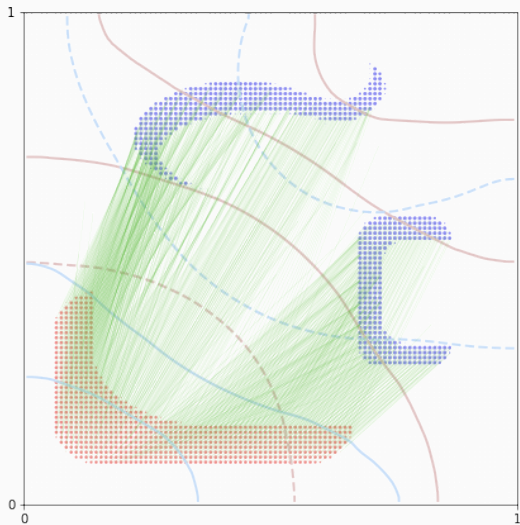
Sinkhorn divergence: with k_σ a Gaussian kernel of deviation σ ,

$$S_\sigma(\alpha, \beta) \simeq \text{OT}(k_\sigma \star \alpha, k_\sigma \star \beta).$$



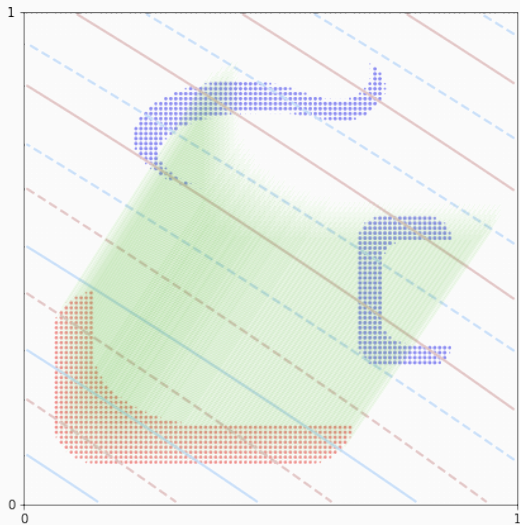
Theorem: If α and β have bounded support, then S_σ is suitable for gradient descent. It is symmetric, **positive**, definite, **convex** and metrizes the convergence in law.

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



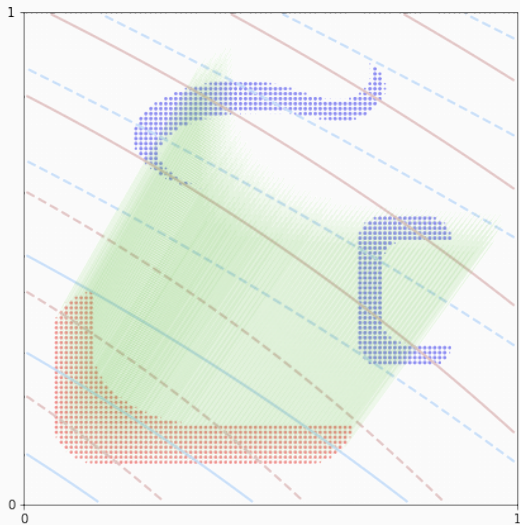
OT plan in 2D.

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



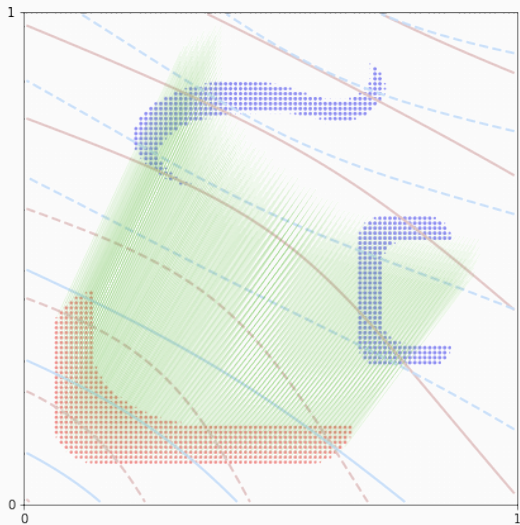
Iteration 0, blur $\sigma = 2^0$

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



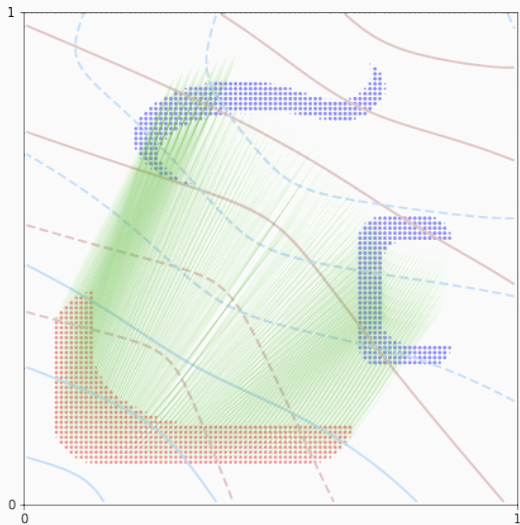
Iteration 1, blur $\sigma = 2^{-1}$

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



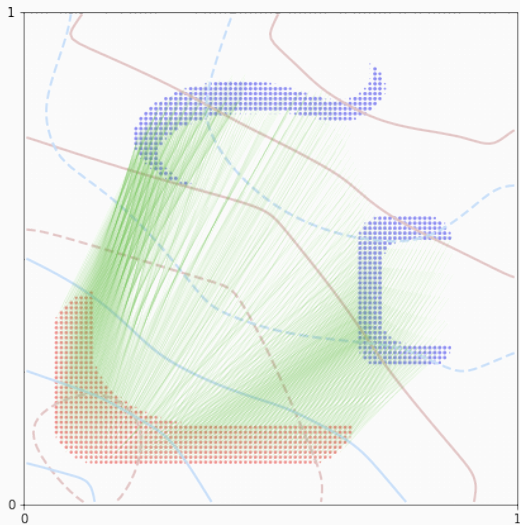
Iteration 2, blur $\sigma = 2^{-2}$

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



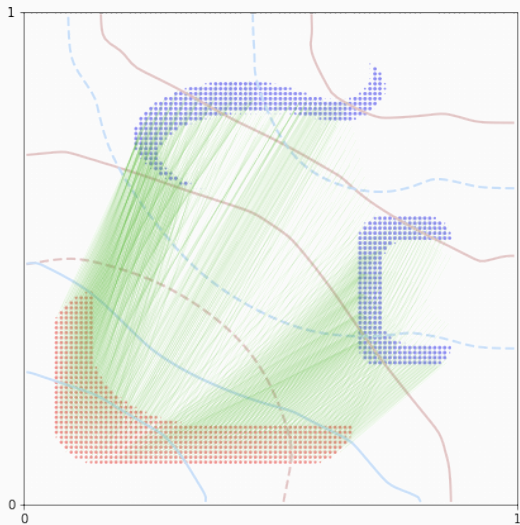
Iteration 3, blur $\sigma = 2^{-3}$

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



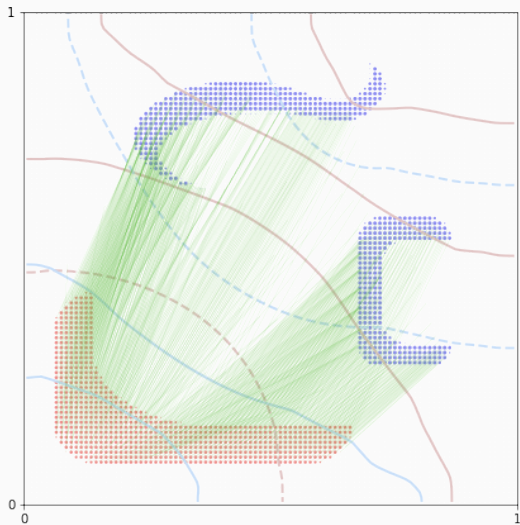
Iteration 4, blur $\sigma = 2^{-4}$

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



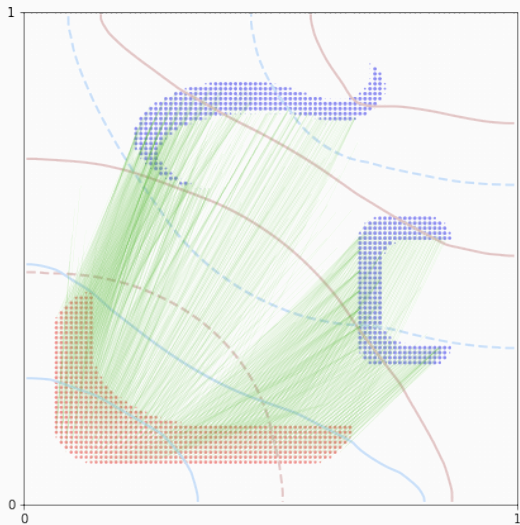
Iteration 5, blur $\sigma = 2^{-5}$

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



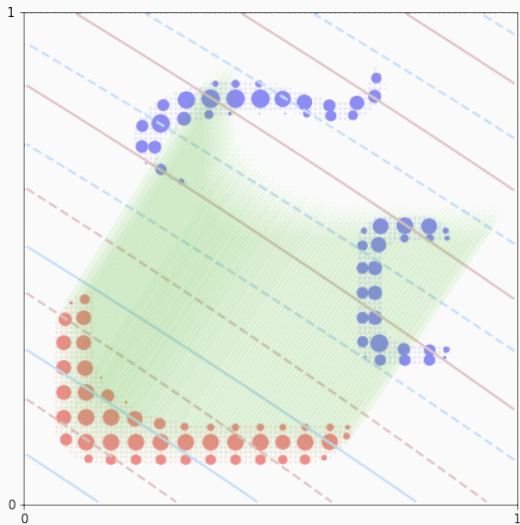
Iteration 6, blur $\sigma = 2^{-6}$

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



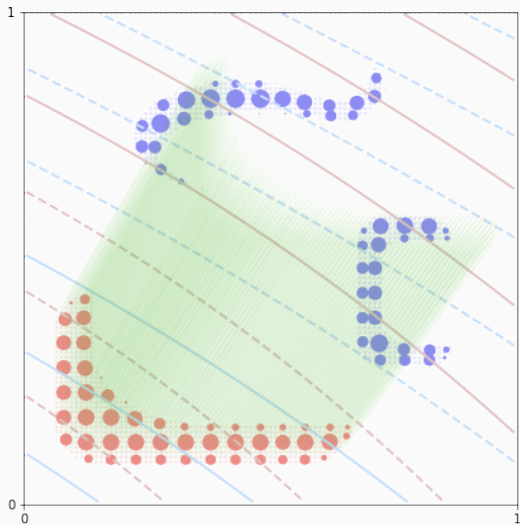
Iteration 7, blur $\sigma = .01$

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



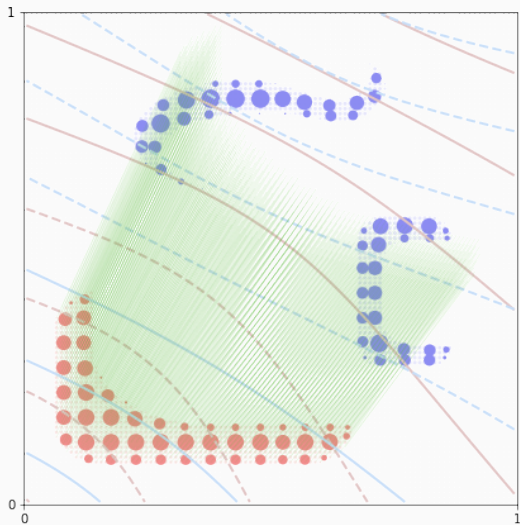
Iteration 0, blur $\sigma = 2^0$

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



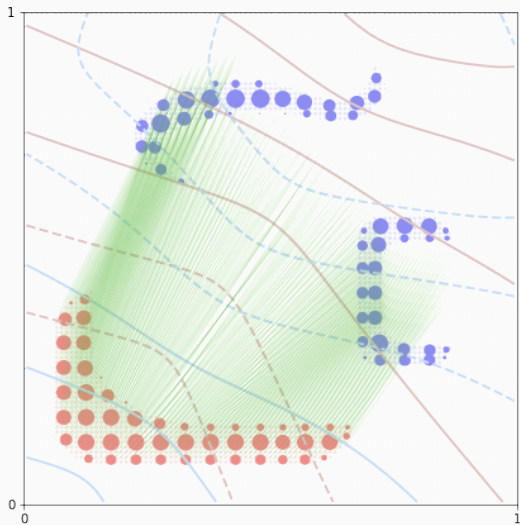
Iteration 1, blur $\sigma = 2^{-1}$

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



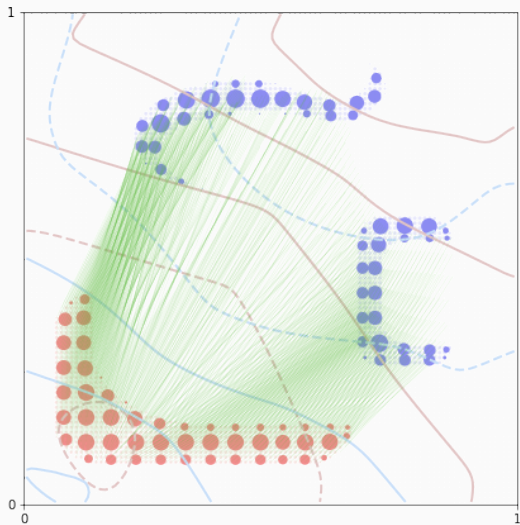
Iteration 2, blur $\sigma = 2^{-2}$

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



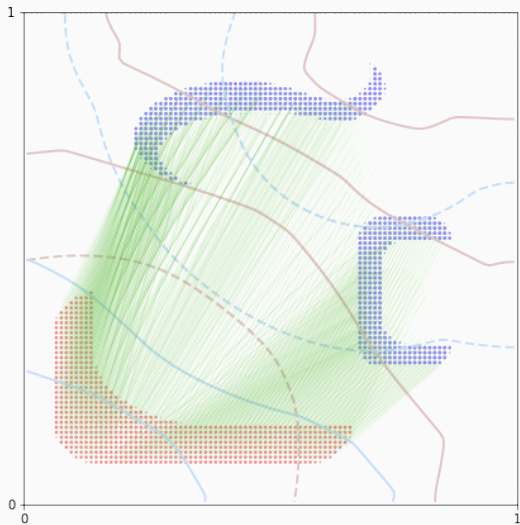
Iteration 3, blur $\sigma = 2^{-3}$

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



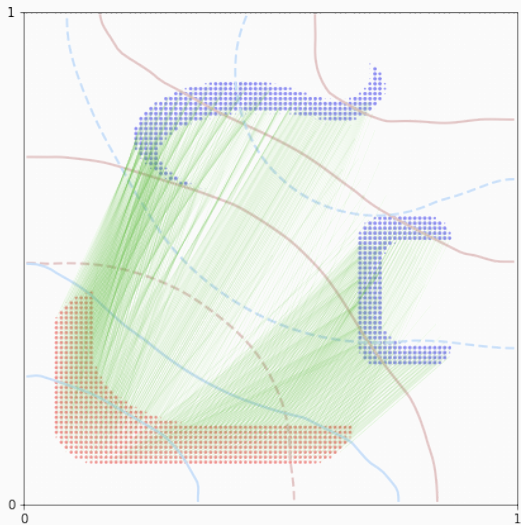
Iteration 4, blur $\sigma = 2^{-4}$

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



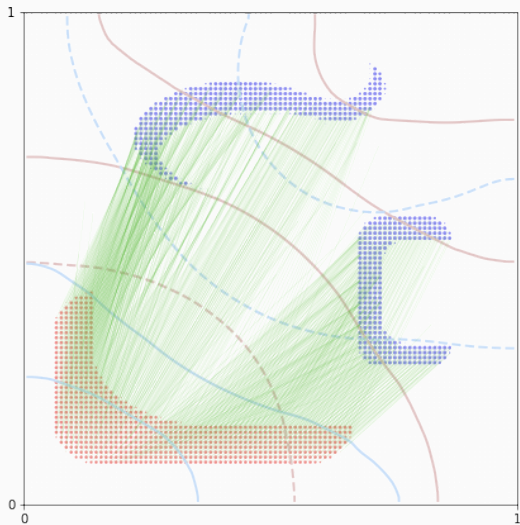
Iteration 5, blur $\sigma = 2^{-5}$

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



Iteration 6, blur $\sigma = 2^{-6}$

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



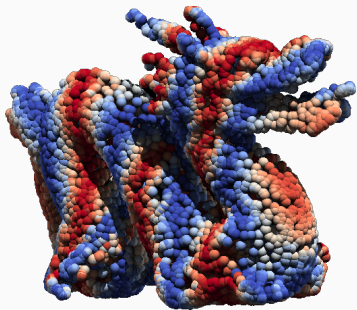
Iteration 7, blur $\sigma = .01$

Scaling up optimal transport to anatomical data

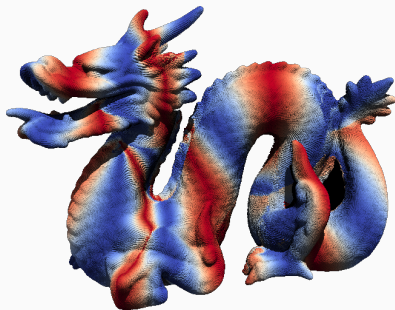
These progresses add up to a $\times 100 - \times 1000$ acceleration:

Sinkhorn GPU $\xrightarrow{\times 10}$ + KeOps $\xrightarrow{\times 10}$ + Annealing $\xrightarrow{\times 10}$ + Multiscale

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



10k points in 30-50ms



100k points in 100-200ms

Geometric Loss functions for PyTorch

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

⇒ pip install geomloss ⇐

```
# Large point clouds in  $[0,1]^3$ 
import torch
x = torch.rand(100000, 3, requires_grad=True).cuda()
y = torch.rand(200000, 3).cuda()

# Define a Wasserstein loss between sampled measures
from geomloss import SamplesLoss
loss = SamplesLoss(loss="sinkhorn", p=2, blur=.05)

L = loss(x, y) # By default, use constant weights
# GeomLoss supports autograd, batch processing, etc.
g_x, = torch.autograd.grad(L, [x])
```

Geometry processing:

- + KeOps provides support for **distance-like matrices**.
- + It **relieves us** from C++/CUDA programming.

Overview of the last two sections

Geometry processing:

- + KeOps provides support for **distance-like matrices**.
- + It **relieves us** from C++/CUDA programming.

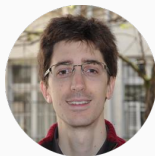
Computational optimal transport:

- + Significant **progress** over the last decade.
- + Efficient solvers are being **packaged** for the global community:
GeomLoss, SD-OT, Geogram, etc.
- Some **challenging settings** remain wide open:
high-dimensional spaces, graphs, etc.
- + The problem is essentially **solved** in three “simple” settings:
imaging, **3D geometry**, fluid mechanics.

New paths for computational anatomy



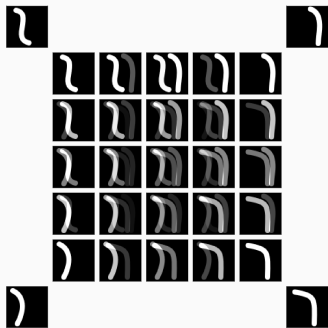
Pierre Roussillon



Pietro Gori

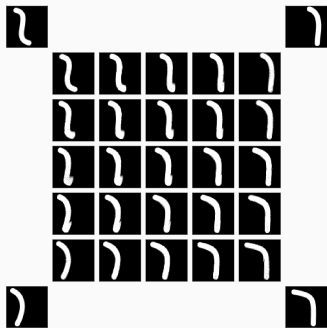
Affordable geometric interpolation [AC11]

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



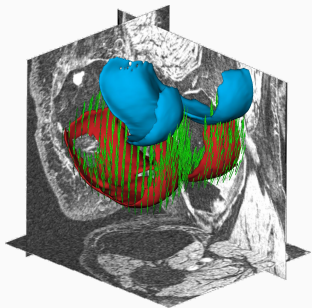
Linear barycenters

$$\text{Loss}(\alpha, \beta) = \|\alpha - \beta\|_{l_2}^2$$

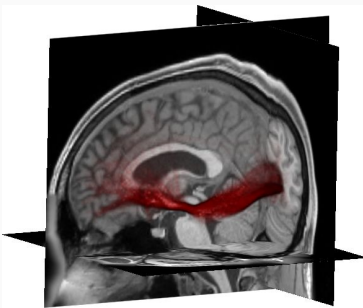


Wasserstein barycenters

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

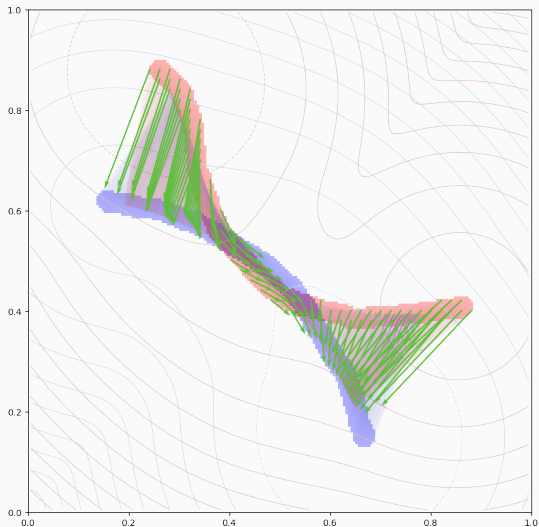


Knee caps



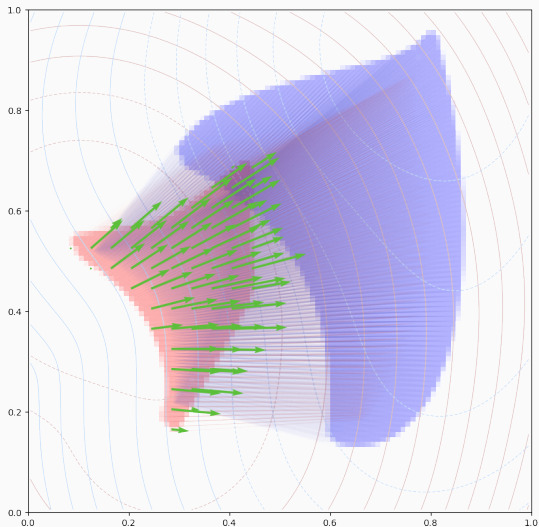
White matter bundles

A global and geometric loss function



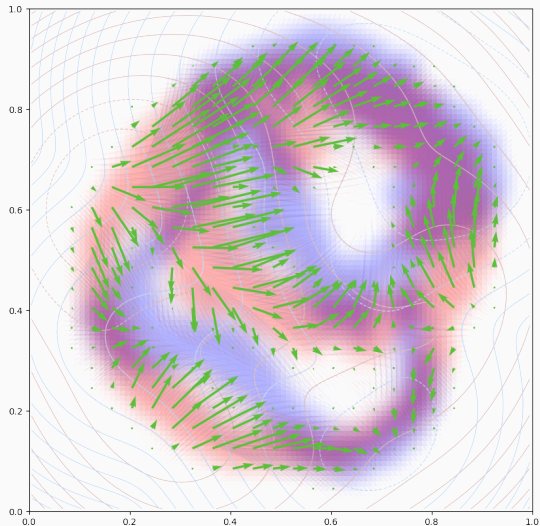
A high-quality gradient...

A global and geometric loss function



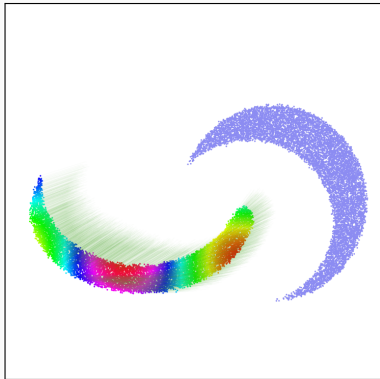
A high-quality gradient...

A global and geometric loss function

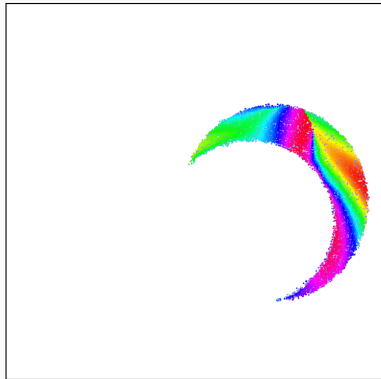


A high-quality gradient... But no preservation of topology!

Optimal transport = cheap'n easy registration? Beware!



Before



After

Topology-aware shape models

Optimal Transport = **independent** particles + mass preservation.

We need stronger metrics.

Topology-aware models are often related to physics:
elastic materials, **fluid** mechanics, etc.

We now have access to **large datasets**, **reliable segmentations**
and efficient **feature detectors**.

Can we plug them into our models?

We are reaching the **limits** of what can be done
with existing **Matlab/C++** codebases.

Since 2017, a new development paradigm

Toolboxes for computational anatomy are becoming increasingly:

- + **Efficient**, with GPU backends.
- + **Differentiable**, to fit in neural pipelines.
- + **Modular** and un-opinionated: freedom!
- + **Easy-to-use** by newcomers.

Since 2017, a new development paradigm

Toolboxes for computational anatomy are becoming increasingly:

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- + **Modular** and un-opinionated: freedom!
- + **Easy-to-use** by newcomers.

KeOps and **GeomLoss** fit within this ecosystem
and support e.g. the **Deformetrica** software.

We look forward to finally **using** them!
(See Chapter 5 for examples of shape models.)

Conclusion

- **Symbolic matrices** are key to performance:
 - KeOps, x30 speed-up vs. PyTorch and TF.
- Optimal Transport = **generalized sorting**:
 - Geometric gradients.
 - Super-fast $O(N \log N)$ solvers.
- Going forward, we must develop **data-driven, efficient yet robust shape models.**

Genuine team work



Alain Trouvé



Thibault Séjourné



F.-X. Vialard



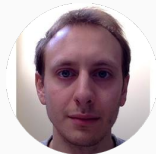
Gabriel Peyré



Benjamin Charlier



Joan Glaunès

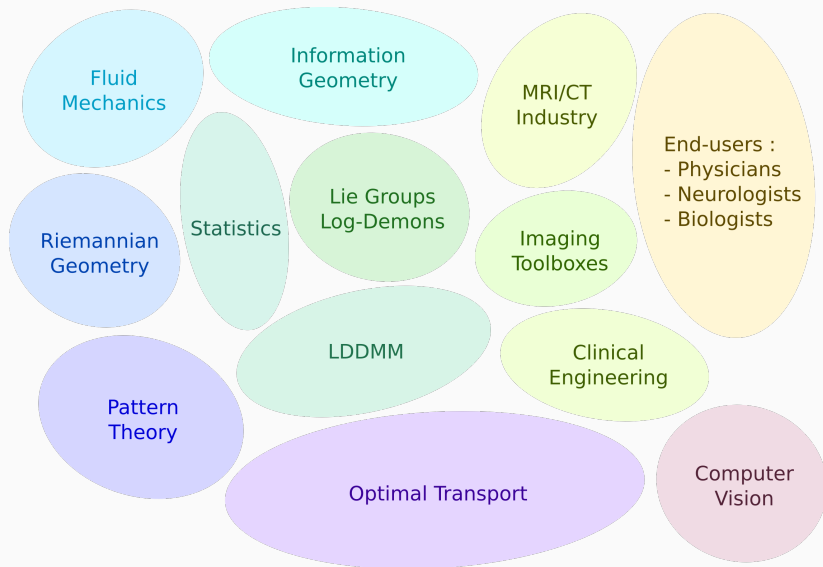


Pierre Roussillon

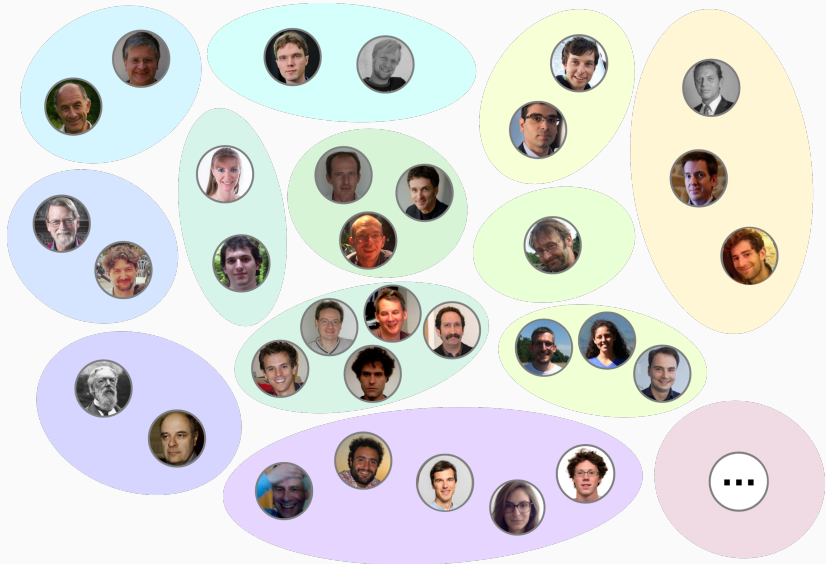


Pietro Gori

Promoting cross-field interactions



Promoting cross-field interactions



Reaching out to students and engineers is a priority

Online documentation:

\Rightarrow `www.kernel-operations.io` \Leftarrow

PhD thesis, written as an introduction to the field:

`www.jeanfeydy.com/geometric_data_analysis.pdf`

Thank you for your attention.

Any questions?

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