Geometric loss functions for shape analysis

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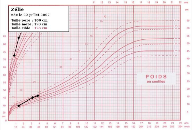
ENS Paris, ENS Paris-Saclay, Imperial College London.

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).

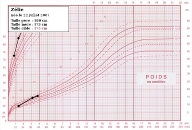
The medical imaging pipeline [Ptr19, EPW+11]



Valuable information

Sensor data

The medical imaging pipeline [Ptr19, EPW+11]



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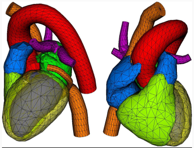

High-level description

Raw image

Sensor data

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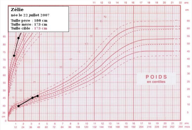

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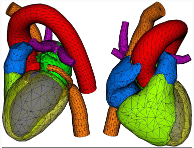

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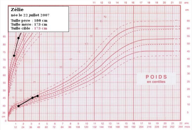

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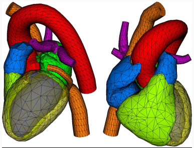

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Computational anatomy

Raw image

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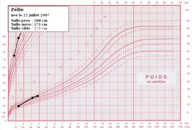

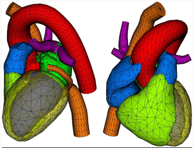

Valuable information

Statistics

High-level description

Computational anatomy

Raw image

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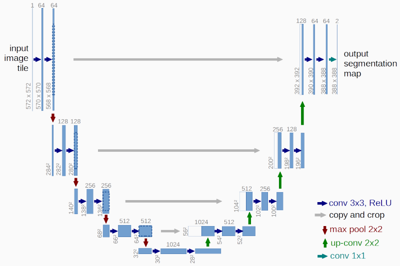
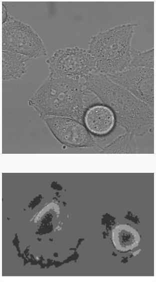
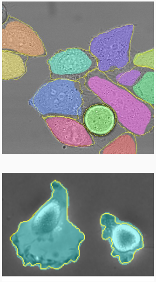
Segmentation with U-nets [RFB15]



Architecture



Input



Output

Geometric problems are becoming increasingly relevant

Geometric questions on segmented shapes:

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- 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 $\rightarrow$ CNNs" revolution in our field,
we need to **revamp our numerical toolbox**.

Outline of the talk

Today, we will talk about:

1. **Fast geometry** with symbolic matrices.
2. Scalable **optimal transport**.
3. Applications and **references**.

Fast geometry with symbolic matrices.

Benjamin Charlier

Joan Glaunès

Deep learning frameworks: unlocking GPUs for research

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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$\implies$ Ideally suited for research.

Efficient algorithms still rely on C++ foundations

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

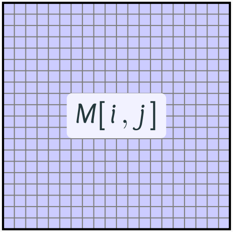
- Linear algebra (cuBLAS).
- Convolutions (cuDNN).
- Fourier (cuFFT) and wavelet transforms (Kymatio).

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.**

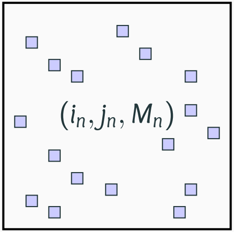
```
RuntimeError: cuda runtime error (2) : out of memory at
/opt/conda/.../THCStorage.cu:66
```

We provide efficient support for distance-like matrices



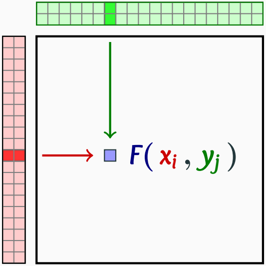
Dense matrix

Coefficients only



Sparse matrix

Coordinates + coeffs



Symbolic matrix

Formula + data

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

KeOps works with PyTorch, NumPy, Matlab and R

```
# Large point cloud in 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
```

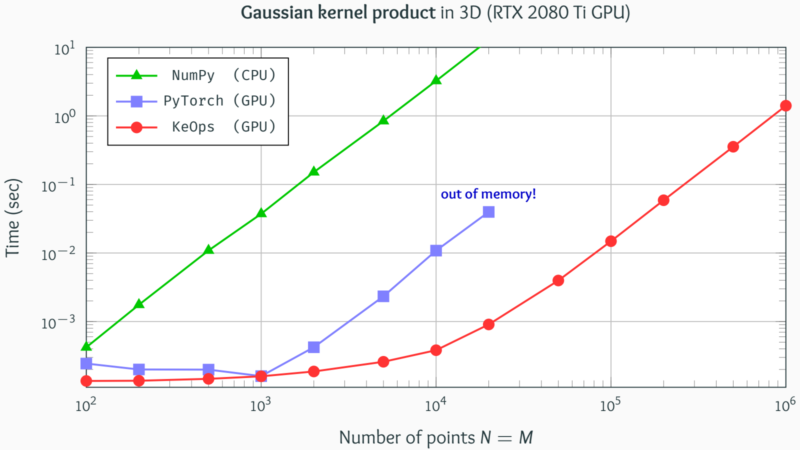
$\Longrightarrow$ $\times$200 acceleration for UMAP on hyperbolic spaces.

KeOps supports:

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

Scaling up to large datasets

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



The KeOps library

+ **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`

→ Kriging, splines, Gaussian processes, **kernel** methods.

→ Geometry processing, **geometric** deep learning.

Computational optimal transport

Thibault Séjourné

F.-X. Vialard

Gabriel Peyré

We need robust loss functions for shape analysis

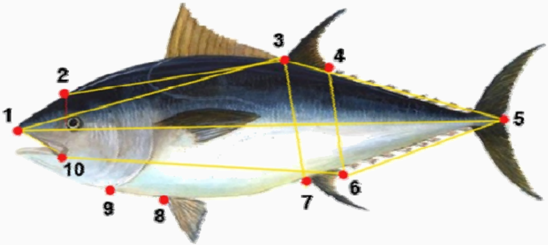
Working with point clouds is now **easier than ever**.
We can protoype new geometric algorithms in minutes.

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

$\Longrightarrow$ 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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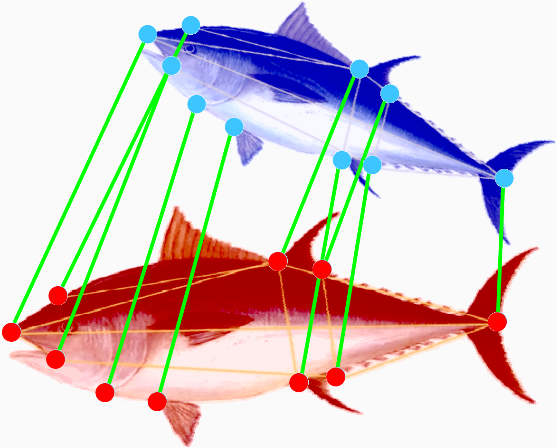

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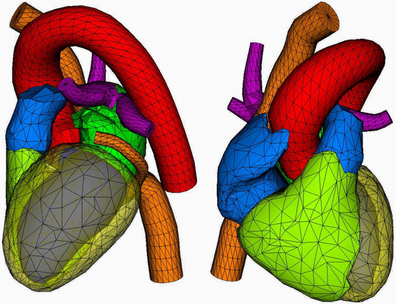
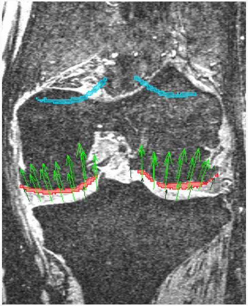
Unfortunately, medical data is often weakly labeled [EPW+11]



Surface meshes

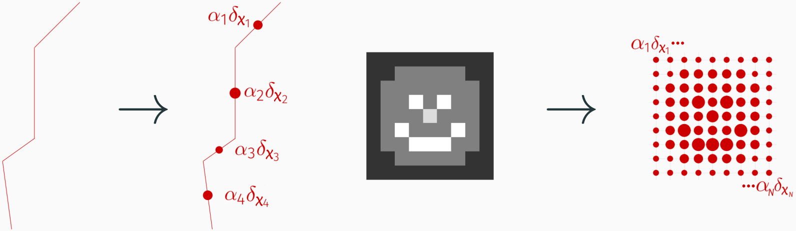


Segmentation masks

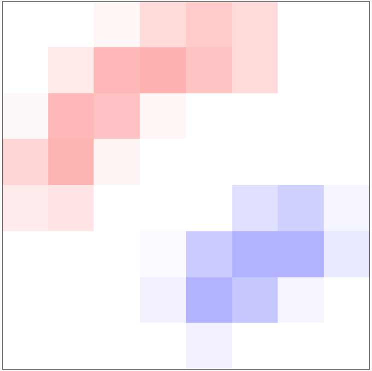
Encoding unlabeled shapes as measures

Let's enforce sampling invariance:

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



A baseline setting: density registration



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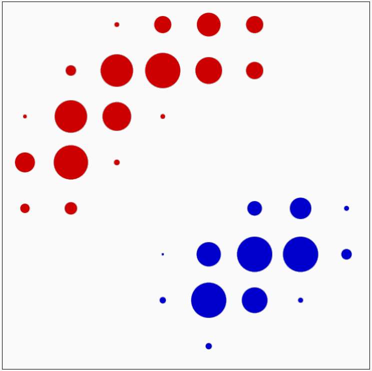

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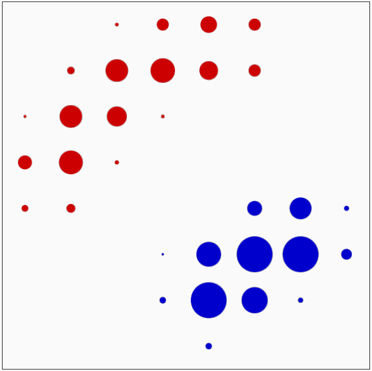

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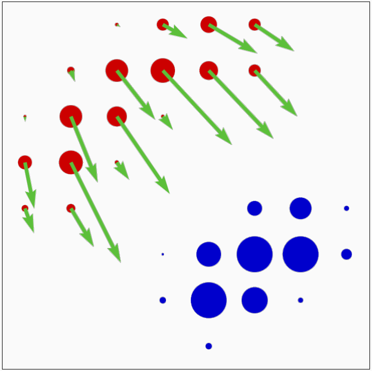

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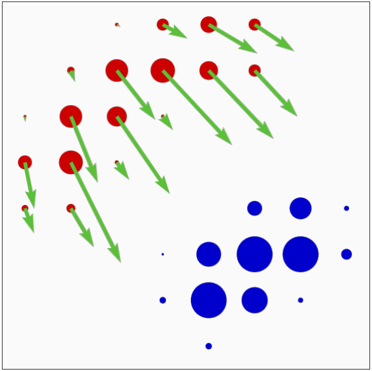
Display $v_i \;=\; -\frac{1}{\alpha_i} \nabla_{x_i} \text{Loss}(\alpha, \beta)$.

A baseline setting: density registration



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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.

The Wasserstein distance

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

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Simple toy example in 1D :

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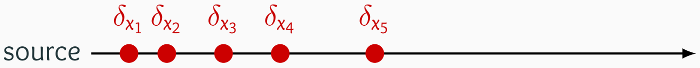

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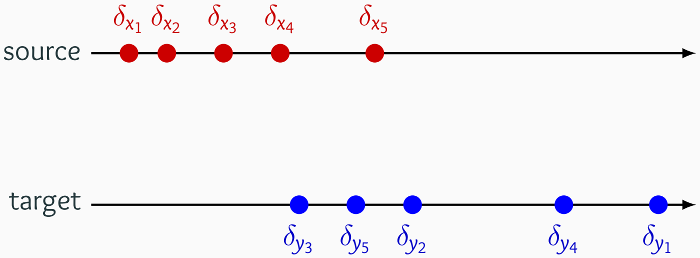

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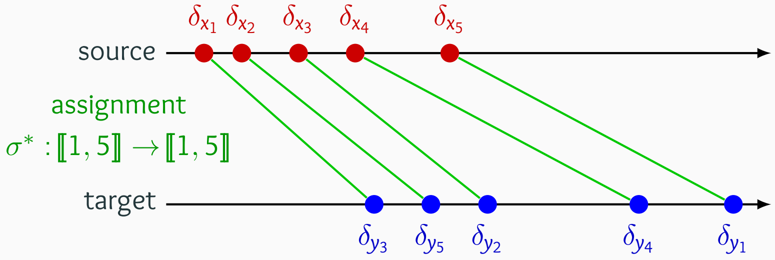

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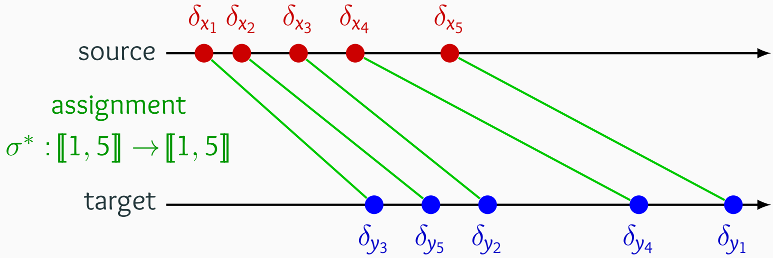

$$\mathrm{OT}(\alpha, \beta) \;=\; \frac{1}{2N} \sum_{i=1}^{N} \left| x_i - y_{\sigma^*(i)} \right|^2$$

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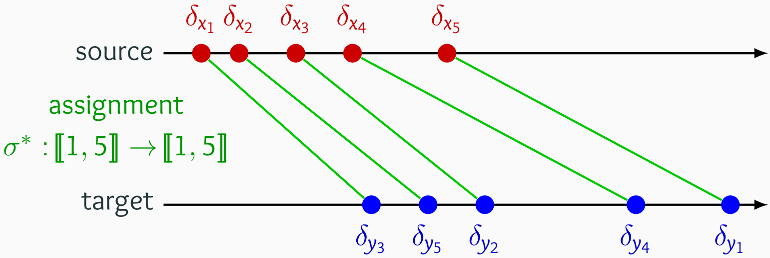
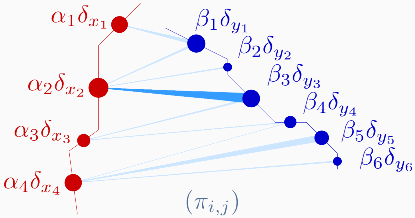
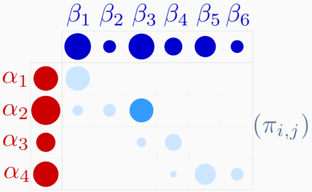


$$\mathrm{OT}(\alpha, \beta) \;=\; \frac{1}{2N} \sum_{i=1}^{N} \left| x_i - y_{\sigma^*(i)} \right|^2 \;=\; \min_{\sigma \in \mathcal{S}_N} \frac{1}{2N} \sum_{i=1}^{N} \left| x_i - y_{\sigma(i)} \right|^2$$

Optimal transport generalizes sorting to D > 1





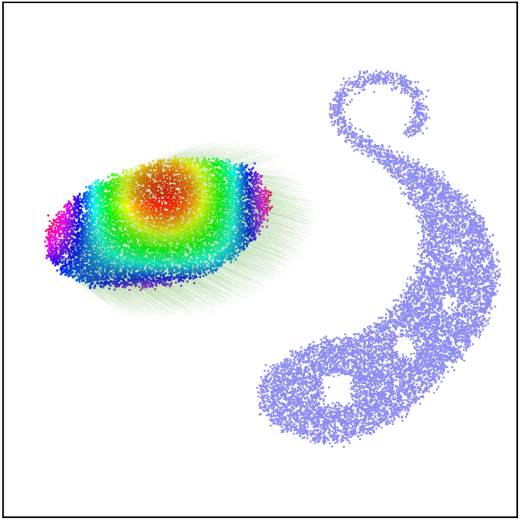
Minimize over N-by-M matrices (transport plans) π :

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

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

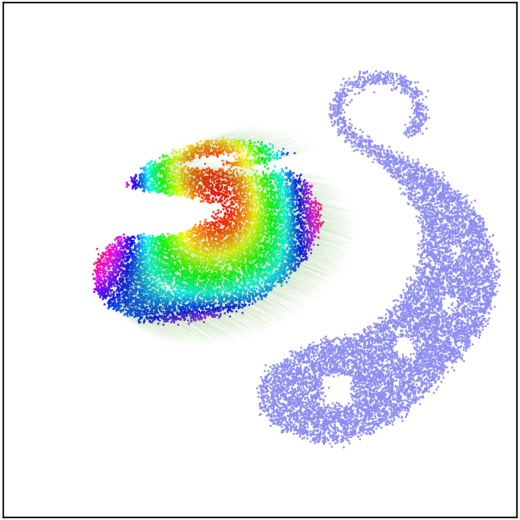
$$\sum_j \pi_{i,j} = \alpha_i, \quad \sum_i \pi_{i,j} = \beta_j.$$

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



$t = .00$

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

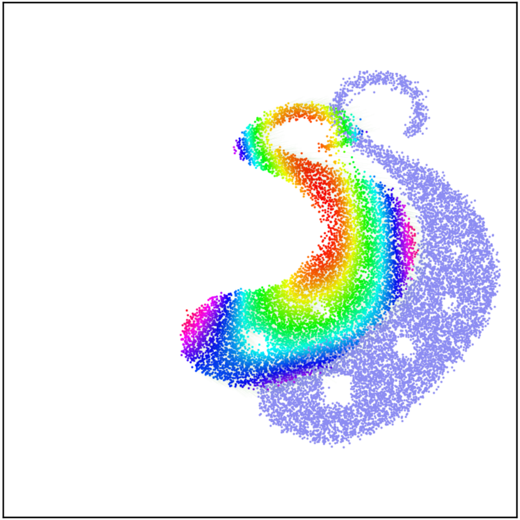


$t = .25$

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

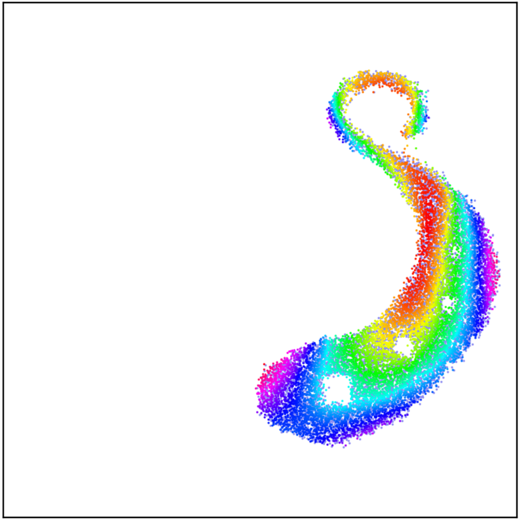
$t = .50$

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



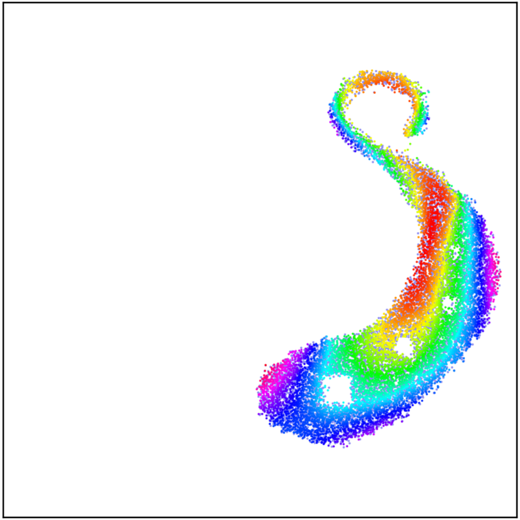
$t = 1.00$

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: $x_i \leftarrow x_i - \delta t \frac{1}{\alpha_i} \nabla_{x_i} \mathrm{OT}(\alpha, \beta)$



$t = 10.00$

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.**

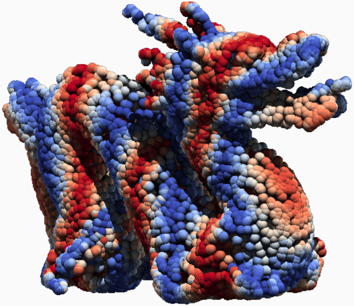
$\Longrightarrow$ Generalized **QuickSort** algorithm.

Scaling up optimal transport to anatomical data

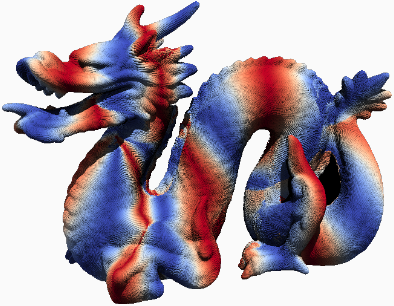
These progresses add up to a $\times 100$ - $\times 1000$ **acceleration:**

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`

$\Longrightarrow$ `pip install geomloss` $\Longleftarrow$

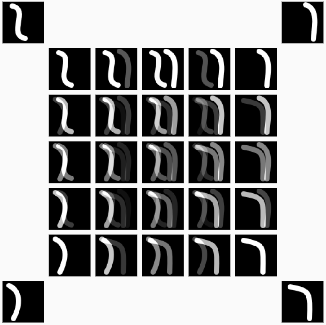
```
# Large point clouds in [0,1]^3
import torch
x = torch.rand(100000, 3, requires_grad=True).cuda()
y = torch.rand(200000, 3).cuda()

# Define a Wasserstein loss between sampled measures
from geomloss import SamplesLoss
loss = SamplesLoss(loss="sinkhorn", p=2)
L = loss(x, y)  # By default, use constant weights
```

Soon: efficient support for **bitmaps**, **meshes** and generic metrics.

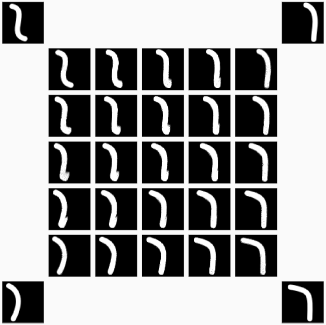
Affordable geometric interpolation [AC11]

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



Linear barycenters

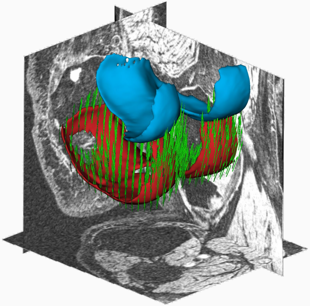
$\text{Loss}(\alpha, \beta) = \|\alpha - \beta\|^2_{L^2}$



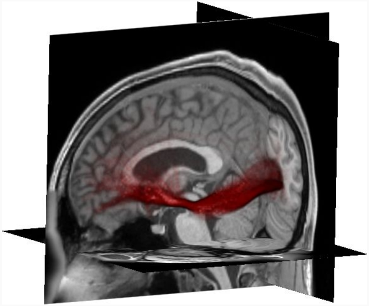
Wasserstein barycenters

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

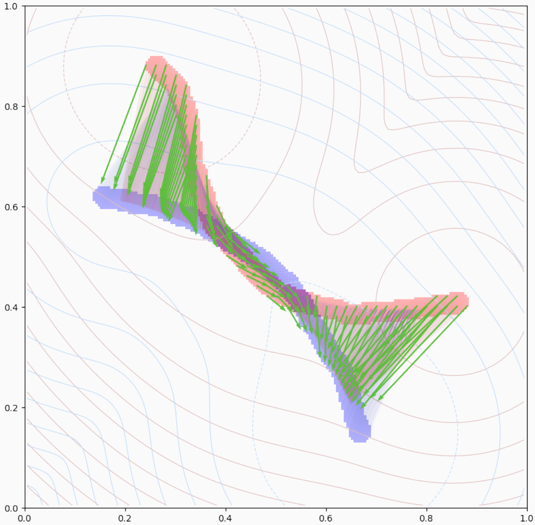
Applications to medical imaging



Knee caps

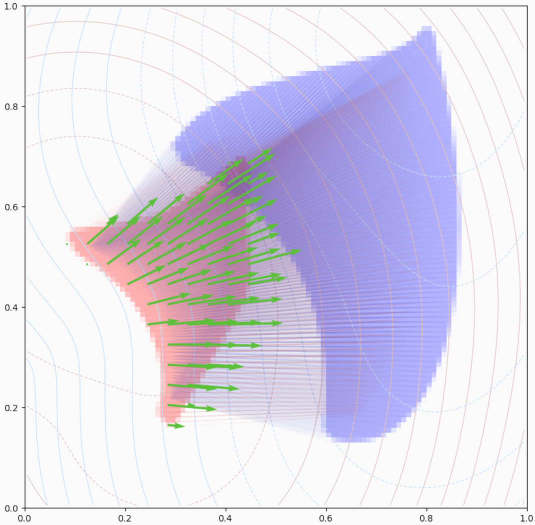


White matter bundles



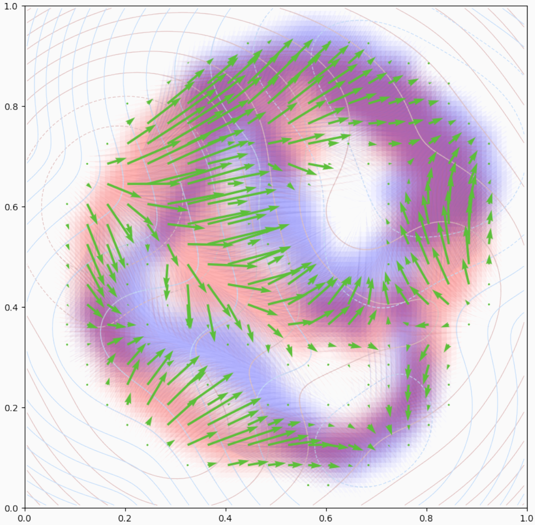
A high-quality gradient...

A global and geometric loss function



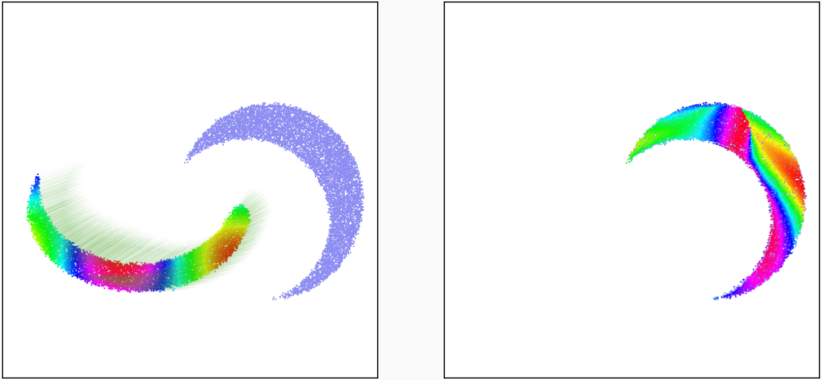
A high-quality gradient…

A global and geometric loss function



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

Optimal transport = cheap'n easy registration? Beware!



Before After

Conclusion

Key points

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

- Optimal Transport = **generalized sorting**:
  $\longrightarrow$ Geometric gradients.
  $\longrightarrow$ Super-fast $O(N \log N)$ solvers.

- Going forward, we must develop **topology-aware**, **data-driven**, efficient yet **robust** shape models.

Reaching out to students and engineers is a priority

Online documentation:

$\Longrightarrow$ `www.kernel-operations.io` $\Longleftarrow$

PhD thesis, written as an introduction to the field:

Geometric data analysis, beyond convolutions

`www.jeanfeydy.com/geometric_data_analysis.pdf`

Thank you for your attention.

Any questions?

M. Agueh and G. Carlier.
Barycenters in the Wasserstein space.
SIAM Journal on Mathematical Analysis, 43(2):904–924, 2011.

Dimitri P Bertsekas.
A distributed algorithm for the assignment problem.
Lab. for Information and Decision Systems Working Paper, M.I.T., Cambridge, MA, 1979.

Y. Brenier.
Polar factorization and monotone rearrangement of vector-valued functions.
Comm. Pure Appl. Math., 44(4):375–417, 1991.

Brian Curless and Marc Levoy.
A volumetric method for building complex models from range images.
In *Proceedings of the 23rd annual conference on Computer graphics and interactive techniques*, pages 303–312. ACM, 1996.

Christophe Chnafa, Simon Mendez, and Franck Nicoud.
Image-based large-eddy simulation in a realistic left heart.
Computers & Fluids, 94:173–187, 2014.

Lénaïc Chizat, Gabriel Peyré, Bernhard Schmitzer, and François-Xavier Vialard.
Unbalanced optimal transport: Dynamic and kantorovich formulations.
Journal of Functional Analysis, 274(11):3090–3123, 2018.

Haili Chui and Anand Rangarajan.
A new algorithm for non-rigid point matching.
In *Computer Vision and Pattern Recognition, 2000. Proceedings. IEEE Conference on*, volume 2, pages 44–51. IEEE, 2000.

Adam Conner-Simons and Rachel Gordon.
Using ai to predict breast cancer and personalize care.
http://news.mit.edu/2019/
using-ai-predict-breast-cancer-and-personalize-c
2019.
MIT CSAIL.

Marco Cuturi.
Sinkhorn distances: Lightspeed computation of optimal transport.
In *Advances in Neural Information Processing Systems*, pages 2292–2300, 2013.

References v

Olivier Ecabert, Jochen Peters, Matthew J Walker, Thomas Ivanc, Cristian Lorenz, Jens von Berg, Jonathan Lessick, Mani Vembar, and Jürgen Weese.
Segmentation of the heart and great vessels in CT images using a model-based adaptation framework.
Medical image analysis, 15(6):863–876, 2011.

Steven Gold, Anand Rangarajan, Chien-Ping Lu, Suguna Pappu, and Eric Mjolsness.
New algorithms for 2d and 3d point matching: Pose estimation and correspondence.
Pattern recognition, 31(8):1019–1031, 1998.

Leonid V Kantorovich.
On the translocation of masses.
In *Dokl. Akad. Nauk. USSR (NS)*, volume 37, pages 199–201, 1942.

Irene Kaltenmark, Benjamin Charlier, and Nicolas Charon.
A general framework for curve and surface comparison and registration with oriented varifolds.
In *Computer Vision and Pattern Recognition (CVPR)*, 2017.

Harold W Kuhn.
The Hungarian method for the assignment problem.
Naval research logistics quarterly, 2(1-2):83–97, 1955.

Jeffrey J Kosowsky and Alan L Yuille.
The invisible hand algorithm: Solving the assignment problem with statistical physics.
Neural networks, 7(3):477–490, 1994.

Bruno Lévy.
A numerical algorithm for l2 semi-discrete optimal transport in 3d.
ESAIM: Mathematical Modelling and Numerical Analysis, 49(6):1693–1715, 2015.

Christian Ledig, Andreas Schuh, Ricardo Guerrero, Rolf A Heckemann, and Daniel Rueckert.
Structural brain imaging in Alzheimer's disease and mild cognitive impairment: biomarker analysis and shared morphometry database.
Scientific reports, 8(1):11258, 2018.

Stéphane Mallat.
Understanding deep convolutional networks.
Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences, 374(2065):20150203, 2016.

Quentin Mérigot.
A multiscale approach to optimal transport.
In *Computer Graphics Forum*, volume 30, pages 1583–1592. Wiley Online Library, 2011.

Yaroslav Nikulin and Roman Novak.
Exploring the neural algorithm of artistic style.
arXiv preprint arXiv:1602.07188, 2016.

Moses Olafenwa.
Object detection with 10 lines of code.
`https://towardsdatascience.com/object-detection-with-10-lines-of-code-d6cb4d86f`
2018.

Towards Data Science.

Maurice Peemen, Bart Mesman, and Henk Corporaal.
Speed sign detection and recognition by convolutional neural networks.
In *Proceedings of the 8th international automotive congress*, pages 162–170. sn, 2011.

Ptrump16.
Irm picture.
`https://commons.wikimedia.org/w/index.php?curid=64157788`, 2019.
CC BY-SA 4.0.

Olaf Ronneberger, Philipp Fischer, and Thomas Brox.
U-net: Convolutional networks for biomedical image segmentation.
In *International Conference on Medical image computing and computer-assisted intervention*, pages 234–241. Springer, 2015.

Bernhard Schmitzer.
Stabilized sparse scaling algorithms for entropy regularized transport problems.
SIAM Journal on Scientific Computing, 41(3):A1443–A1481, 2019.

Donglai Wei, Bolei Zhou, Antonio Torralba, and William T Freeman.
mNeuron: A Matlab plugin to visualize neurons from deep models.
Massachusetts Institute of Technology, 2017.