Fast geometric libraries for vision and data sciences

.

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Who am I?

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

2012–2016 ENS Paris, mathematics.

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

2016–2019 PhD thesis in **medical imaging** with Alain Trouvé at ENS Cachan.

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

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

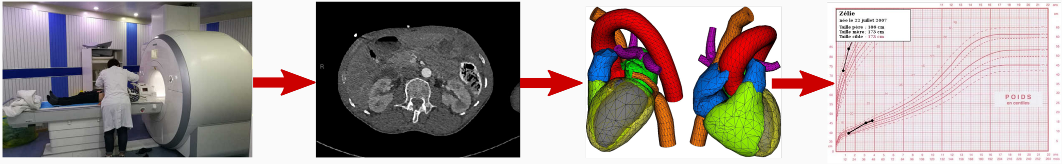
Close ties with **healthcare**:

2015 Image denoising with **Siemens Healthcare** in Princeton.

2019+ MasterClass AI–Imaging, for **radiology interns** in the University of Paris.

2020+ Colloquium on **Medical imaging in the AI era** at the Paris Brain Institute.

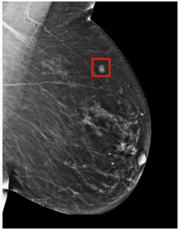
Our motivation: medical data analysis



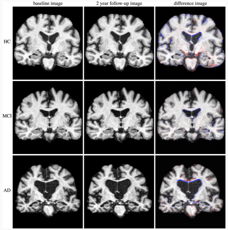
Three main **characteristics**:

- **Heterogeneous data:** patient history, images, etc.
- Small stratified samples: 10 – 1 000 patients per group.
- Dealing with **outliers** and the **heavy tails** of our distributions is a priority.

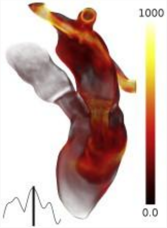
Computational anatomy [CSG19, LSG+18, CMN14]



Detect a pattern.



Analyze a variation.



Register a model.

Some characteristics, in the wider context of computer vision research:

- **Standard acquisitions**, without occlusions.
- **Precision** work (at millimeter scale).
- Need for **guarantees** of robustness and regularity.

A field that is moving fast

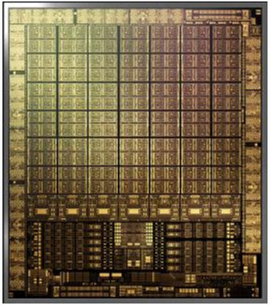
Target. Design models that combine medical **expertise** with modern **datasets.**

Challenge. The advent of **Graphics Processing Units** (GPU):

- Incredible **value for money:**

  $1\,000€ \simeq 1\,000$ cores $\simeq 10^{12}$ operations/s.
- **Bottleneck:** constraints on **register** usage.

"User-friendly" Python ecosystem, consolidated around a **small number of key operations.**



7,000 cores
in a single GPU.

My project: a long-term investiment in the foundations of our field

Solution. **Expand the standard toolbox** in data sciences
to deal with the challenges of the healthcare industry.

Ease the development of **advanced models**,
without compromising on numerical performance.

In-depth work, numerical **foundations** $\longrightarrow$ **high-level** applications:

1. Efficient manipulation of **"symbolic" matrices** (distances, kernel, etc.).
2. **Optimal transport:** generalized sorting methods.
3. Geometric **deep learning** and **biomedical** applications.

Future of these tools and **clinical perspectives**.

1. Symbolic matrices

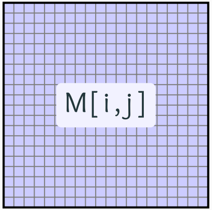
Computing libraries represent most objects as tensors

Context. Constrained **memory accesses** on the GPU:

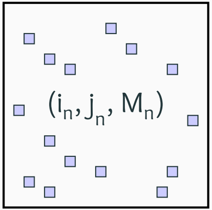
- **Long access times** to the registers penalize the use of large **dense** arrays.
- Hard-wired **contiguous** memory accesses penalize the use of **sparse** matrices.

Challenge. In order to reach optimal run times:

- **Restrict** ourselves to operations that are supported by the constructor: convolutions, FFT, etc.
- Develop new routines from scratch in C++/CUDA (FAISS, KPConv...): **several months of work.**



Dense array



Sparse matrix

The KeOps library: efficient support for symbolic matrices

Solution. KeOps – `www.kernel-operations.io`:

- For PyTorch, NumPy, Matlab and R, on **CPU and GPU.**
- **Automatic differentiation.**
- Just-in-time **compilation** of **optimized** C++ schemes, triggered for every new **reduction:** sum, min, etc.

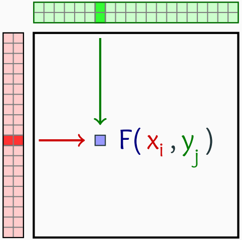
If the formula "F" is simple ($\leqslant$ 100 arithmetic operations):

"100k $\times$ 100k" computation $\rightarrow$ 10ms – 100ms,

"1M $\times$ 1M" computation $\rightarrow$ 1s – 10s.

Hardware ceiling of 10^{12} operations/s.

$\times$**10 to** $\times$**100 speed-up** vs standard GPU implementations for a wide range of problems.



Symbolic matric

Formula + data

- Distances $d(x_i,y_j)$.
- Kernel $k(x_i,y_j)$.
- Numerous transforms.

A first example: efficient nearest neighbor search in dimension 50

Create large point clouds using **standard PyTorch syntax:**

```
import torch
N, M, D = 10**6, 10**6, 50
x = torch.rand(N, 1, D).cuda()  # (1M,  1, 50) array
y = torch.rand(1, M, D).cuda()  # ( 1, 1M, 50) array
```

Turn **dense** arrays into **symbolic** matrices:

```
from pykeops.torch import LazyTensor
x_i, y_j = LazyTensor(x), LazyTensor(y)
```

Create a large **symbolic matrix** of squared distances:

```
D_ij = ((x_i - y_j) ** 2).sum(dim=2)  # (1M, 1M) symbolic
```

Use an `.argmin()` **reduction**to perform a nearest neighbor query:

```
indices_i = D_ij.argmin(dim=1)  # -> standard torch tensor
```

The KeOps library combines performance with flexibility

Script of the previous slide = efficient nearest neighbor query,
on par with the bruteforce CUDA scheme of the **FAISS** library...
And can be used with **any metric**!

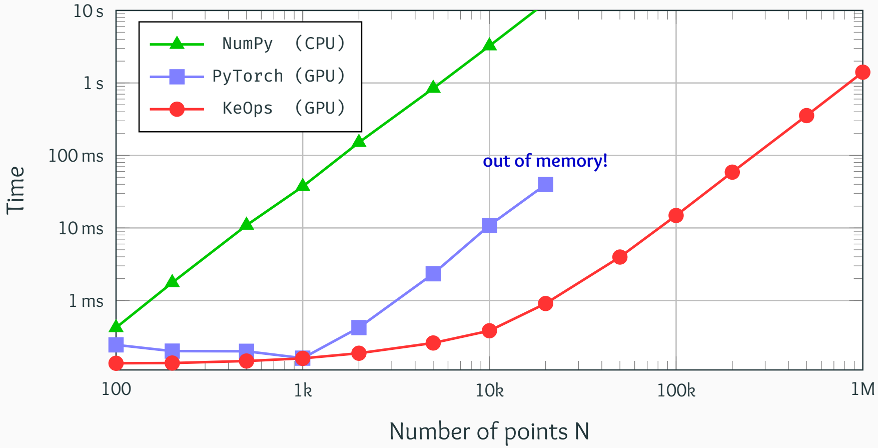
```
D_ij = ((x_i - x_j) ** 2).sum(dim=2)     # Euclidean
M_ij =  (x_i - x_j).abs().sum(dim=2)     # Manhattan
C_ij = 1 - (x_i | x_j)                   # Cosine
H_ij = D_ij / (x_i[...,0] * x_j[...,0])  # Hyperbolic
```

KeOps supports arbitrary **formulas** and **variables** with:

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

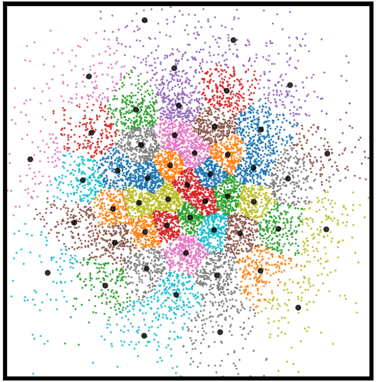
KeOps lets users work with millions of points at a time

Benchmark of a Gaussian **convolution**
between **clouds of N 3D points** on a RTX 2080 Ti GPU.

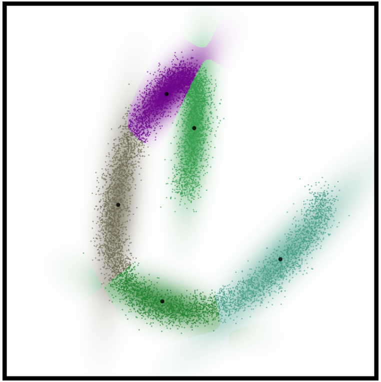


Applications

KeOps is a good fit for machine learning research



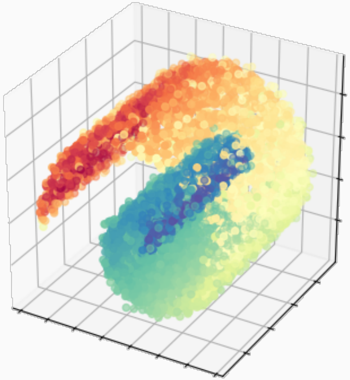
K-Means.



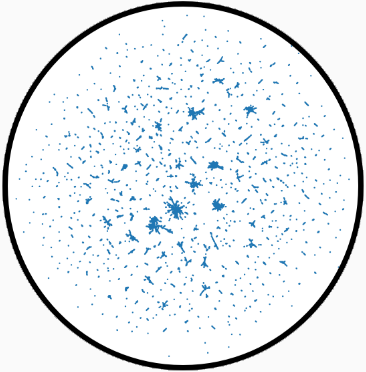
Gaussian Mixture Model.

Use **any** kernel, metric or formula **you** like!

KeOps is a good fit for machine learning research



Spectral analysis.

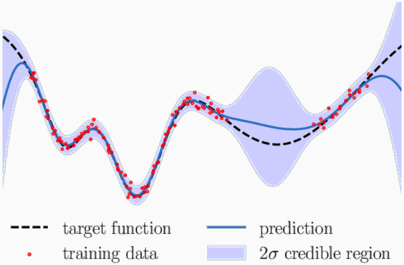


UMAP in hyperbolic space.

Use **any** kernel, metric or formula **you** like!

Applications to Kriging, spline, Gaussian process, kernel regression

A standard tool for regression [Lec18]:



Under the hood, solve a **kernel linear system:**

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

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

Applications to Kriging, spline, Gaussian process, kernel regression

KeOps symbolic tensors $(K_{xx})_{i,j} = k(x_i, x_j)$ **:**

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

  7h avec 8 GPUs $\longrightarrow$ 15mn avec 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).

2. Optimal transport

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

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

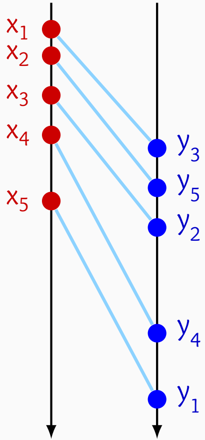
$$\text{OT}(A, B) = \min_{\sigma \in \mathcal{S}_N} \frac{1}{2N} \sum_{i=1}^{N} \| x_i - y_{\sigma(i)} \|^2$$

Generalizes **sorting** to metric spaces.

Linear problem on the permutation matrix P:

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

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



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

Key properties of this distance “up to permutations”

The Wasserstein distance $\sqrt{\text{OT}}(\text{A}, \text{B})$ is:

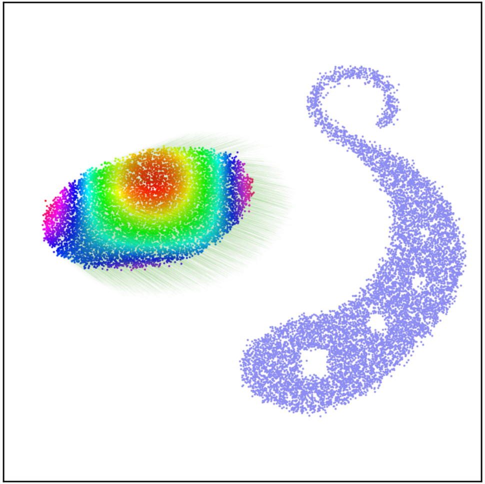
- **Symmetric:** $\text{OT}(\text{A}, \text{B}) = \text{OT}(\text{B}, \text{A})\,.$
- **Positive:** $\text{OT}(\text{A}, \text{B}) \geqslant 0\,.$
- **Definite:** $\text{OT}(\text{A}, \text{B}) = 0 \iff \text{A} = \text{B}\,.$
- **Translation-aware:** $\text{OT}(\text{A}, \ \text{Translate}_{\vec{v}}(\text{A})\,)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

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

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

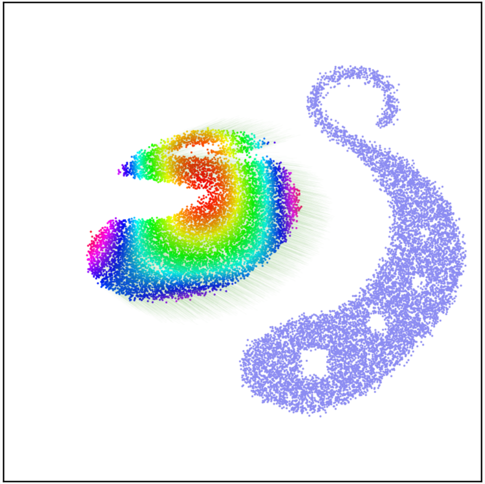
$\Longrightarrow$ Appealing generalization of an **increasing mapping.**

A simple example in 2D



t = .00

A simple example in 2D



$t = .25$

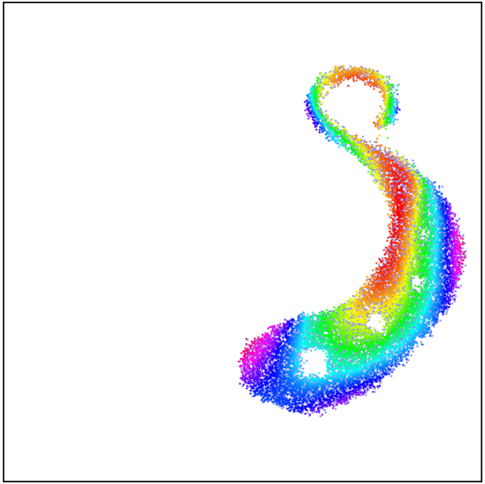
A simple example in 2D

t = .50

A simple example in 2D

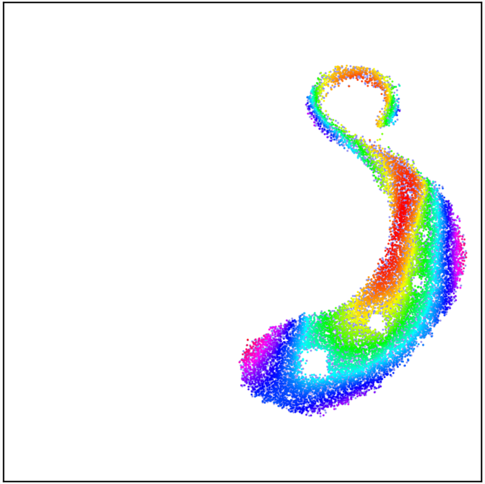
$t = 1.00$

A simple example in 2D



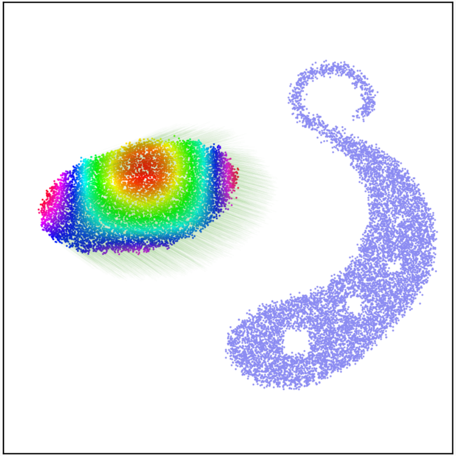
$t = 5.00$

A simple example in 2D

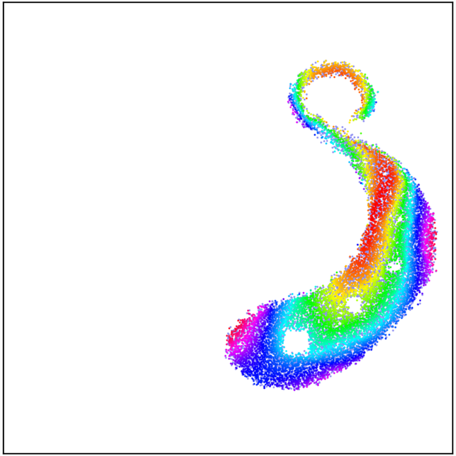


$t = 10.00$

An efficient model... but beware of tears!

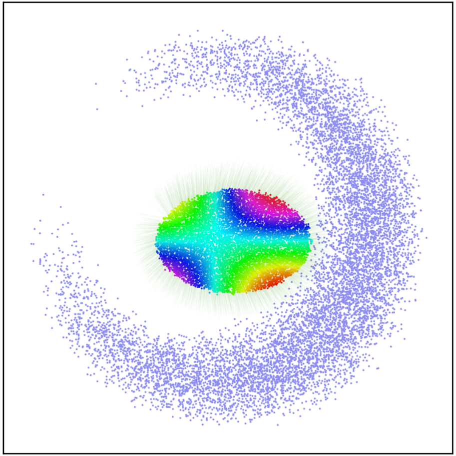


Before

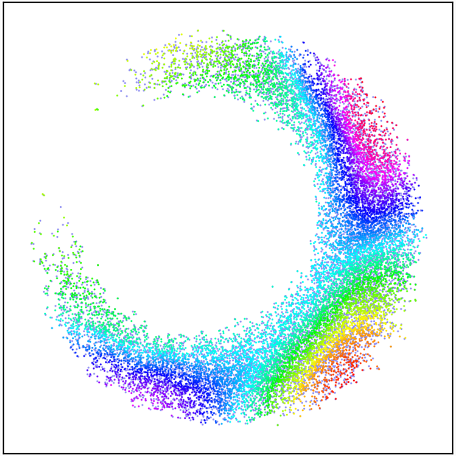


After

An efficient model... but beware of tears!

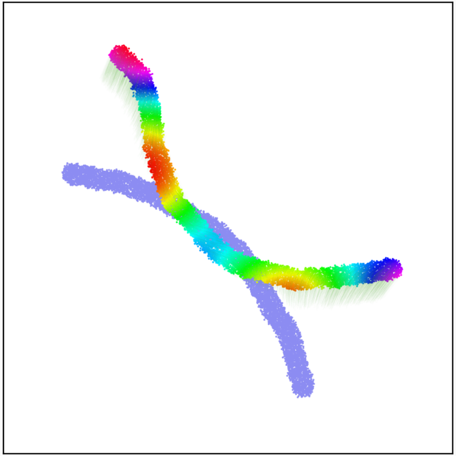


Before



After

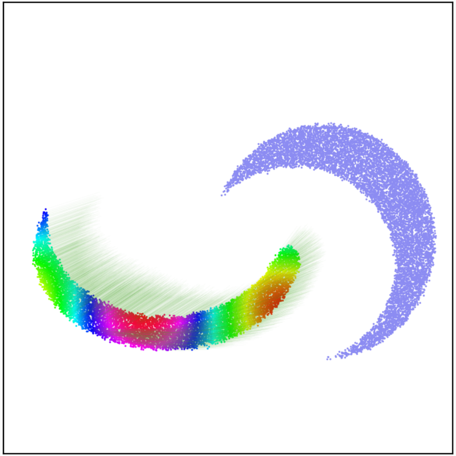
An efficient model... but beware of tears!



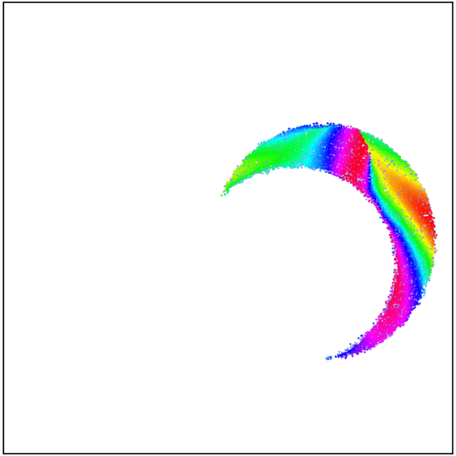
Before

After

An efficient model… but beware of tears!



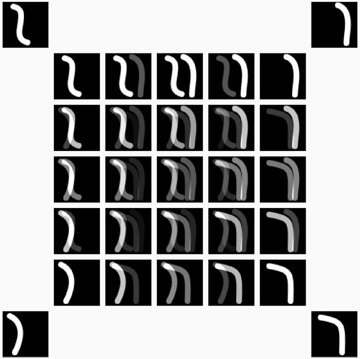
Before



After

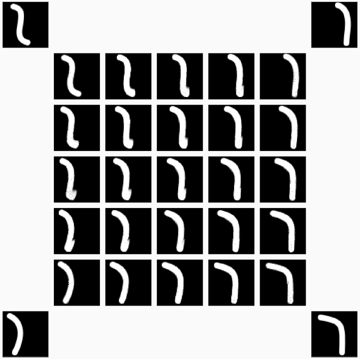
Geometric solutions to least square problems [AC11]

$$\text{Barycenter } \color{red}{A^*} = \arg\min_{\color{red}{A}} \sum_{i=1}^{4} \lambda_i \, \text{Loss}(\color{red}{A}, \color{blue}{B_i}) \, .$$



Euclidean barycenters.

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



Wasserstein barycenters.

$$\text{Loss}(\color{red}{A}, \color{blue}{B}) = \text{OT}(\color{red}{A}, \color{blue}{B})$$

Regularization and entropic bias

Challenge. Linear assignment: hard to solve in the general case.

Structure of the distance matrix $\| x_i - y_j \|$

$\Longrightarrow$ **Speed-up** computations.

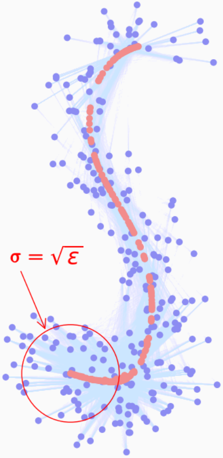
Fundamental tool: **regularized transport**

$\text{OT}_\varepsilon(A, B) \simeq \text{OT}(A, B) +$ **entropic penalty** with strength $\varepsilon > 0$.

Smooth and strictly **convex** approximation: easier to study, most popular **Sinkhorn** (or "*SoftAssign*") algorithm.

On the other hand, does **not** define a **distance:**

$\text{OT}_\varepsilon(B, B) > 0.$



$\arg\min_A \text{OT}_\varepsilon(A, B).$

Theoretical solution: guarantees of robustness to entropic bias

Solution. **Sinkhorn divergences** are defined with:

$$\mathrm{S}_\varepsilon(\mathrm{A},\mathrm{B}) = \mathrm{OT}_\varepsilon(\mathrm{A},\mathrm{B}) - \tfrac{1}{2}\mathrm{OT}_\varepsilon(\mathrm{A},\mathrm{A}) - \tfrac{1}{2}\mathrm{OT}_\varepsilon(\mathrm{B},\mathrm{B})$$

in order to get a null value when $\mathrm{A} = \mathrm{B}$.

Theorem (S_ε is well suited for optimization)

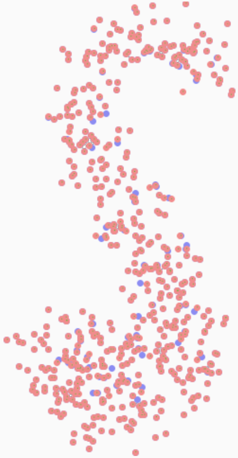
For all samples A and B :

$$S_\varepsilon(A,B) \geqslant 0 \quad \text{with equality iff. } A = B,$$

$$A \mapsto S_\varepsilon(A,B) \quad \text{is convex, differentiable}$$

and metrizes the convergence in law.

*We generalize this result to positive Radon **measures**, arbitrary **metrics** $\|x_i - y_j\|$ and to the "**unbalanced**" setting.*



$\arg\min_{\mathrm{A}} \mathrm{S}_\varepsilon(\mathrm{A},\mathrm{B})$.

How should we solve the OT problem?

Key dates for discrete optimal transport with N points:

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

- **Solution,** today: **Multiscale Sinkhorn algorithm, on the GPU.**

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

Scaling up optimal transport to anatomical data

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

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

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

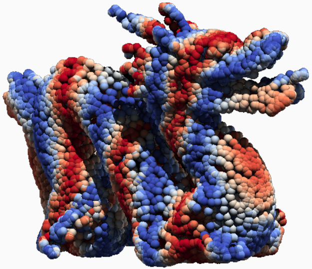
`pip install geomloss`

+

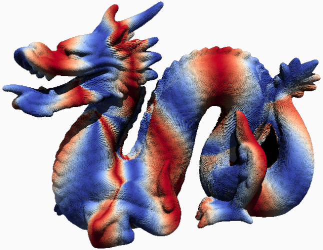
modern GPU

(1 000 €)

$\Longrightarrow$



10k points in 30-50ms



100k points in 100-200ms

3. Geometric deep learning

Design task-specific trainable models

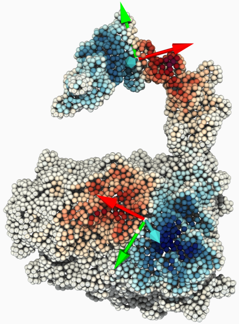
Context. Trainable models on **non-Euclidean domains** (point clouds, surfaces, graphs, etc.), beyond 2D/3D images.

Challenge. In spite of growing interest in the industry, these models still **lack support** on the numerical side. C++/CUDA is (often) required to reach top performance.

Solution. Using KeOps, with a few lines of Python:

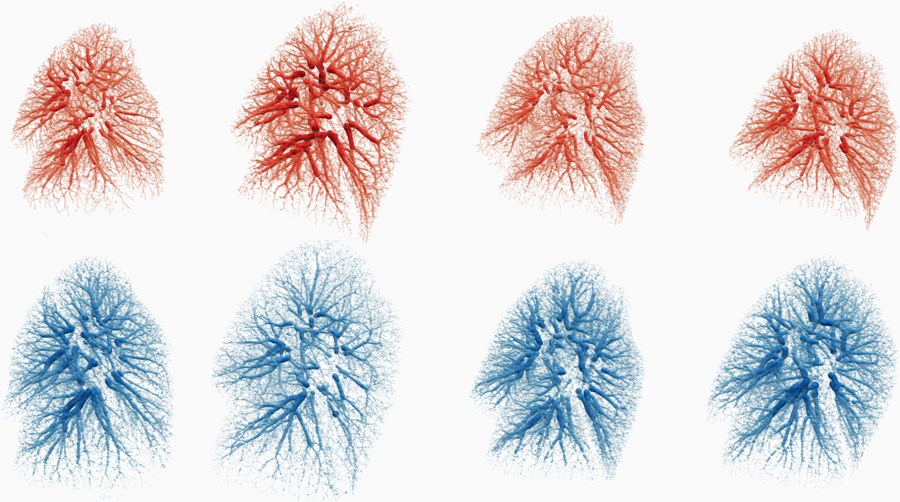
- **Local** interactions: K-nearest neighbors.
- **Global** interactions: generalized convolutions.

Modelling **freedom**
$\Longrightarrow$ **Domain-specific** priors.



Quasi-geodesic convolution on a protein surface.

Lung registration “Exhale – Inhale”



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

Three-steps registration

We combine:

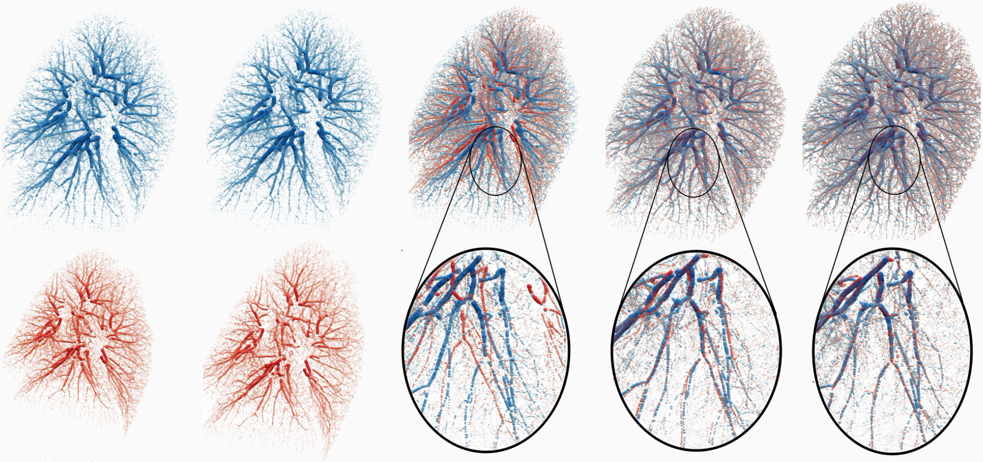
1. Global **pre-alignment:** OT + affine deformation.
2. **Deep prediction** "at centimeter scale": multi-scale neural network + diffeomorphism.
3. **Fine-tuning** "at millimeter scale": OT + spline regularization.

This **pragmatic** method:

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

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

Three-steps registration



0. Input data
1. Pre-alignment
Zoom !
2. Deep registration
3. Fine-tuning

Conclusion

Key points

- **Symbolic** matrices are to **geometric** ML what
  sparse matrices are to **graph** processing:

  $\longrightarrow$ KeOps: **x30 speed-up** vs. PyTorch, TF et JAX.

  $\longrightarrow$ Useful in a wide range of settings.

- Optimal Transport = **generalized sorting** :

  $\longrightarrow$ Geometric gradients.

  $\longrightarrow$ Super-fast $O(\mathrm{N} \log \mathrm{N})$ solvers.

- These tools open **new paths** for geometers and statisticians:

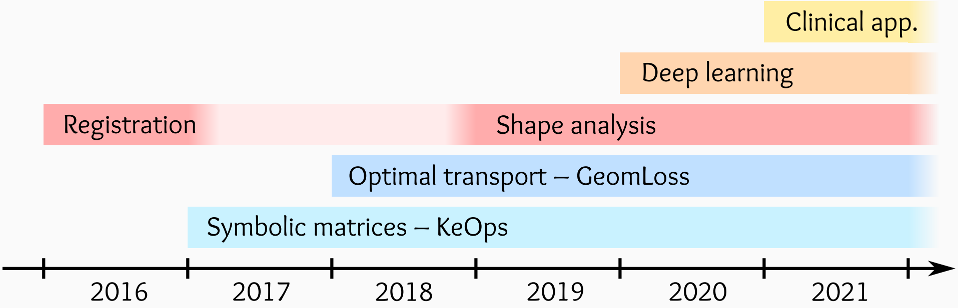
  $\longrightarrow$ GPUs are more **versatile** than you think.

  $\longrightarrow$ Ongoing work to provide **fast GPU backends** to researchers, going beyond what Google and Facebook are ready to pay for.

Summary: a long-term investment that is starting to bear fruits

Two major evolutions:

- "Big" geometric problem: $N > \mathbf{10k} \longrightarrow N > \mathbf{1M}$.
- Optimal transport: linear **problem** + generalized **quicksort**.



Genuine team work

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+ Marc Niethammer, Bruno Correia, Michael Bronstein...

Our contribution to the community

KeOps and GeomLoss are:

- **Fast** : 10 to 1,000 speedup vs. standard GPU implementations.
- **Memory-efficient:** $O(\mathrm{N})$, not $O(\mathrm{N}^2)$.
- **Versatile**, with a **transparent** interface: freedom!
- **Powerful and well-documented:** research-friendly.

- **Slow** with **large vectors** of dimension $\mathrm{D} > 100$.

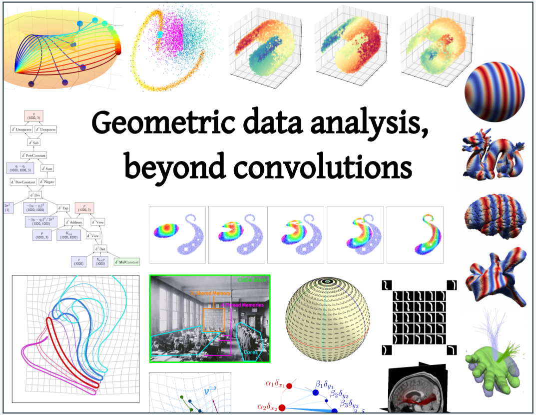
Coming soon:

→ **Approximation strategies** (Nyström, etc.) in KeOps.

→ Wasserstein **barycenters** and **grid images** in GeomLoss.

Documentation and tutorials are available online

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



www.jeanfeydy.com/geometric_data_analysis.pdf

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