Fast libraries for geometric data analysis

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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+ Medical imaging.

2016+ Computational anatomy.

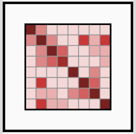
2021+ Public health.

A focus on the geometric side of data sciences

Domain-specific observations on a population of N patients

- MRI/CT images
- Cognitive scores
- Physiological measurements
- Drug consumption history

N-by-N matrix of similarities



General machine learning methods

- Clustering (K-Means...)
- Classification (hierarchical...)
- Regression (kernels...)
- Visualization (UMAP...)

My research is about understanding **similarity structures**.

What are the implicit **priors** that they reflect?

How can we manipulate them **efficiently**?

A field that is moving fast

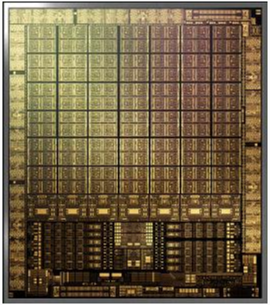
Target. Allow scientists to work with **tailor-made** models as **efficiently** as possible.

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

- Incredible **value for money**:

  $1\,000€ \simeq 1\,000$ cores $\simeq 10^{12}$ operations/s.
- **Bottleneck**: low-level **memory** 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.

Today's talk:

1. Efficient manipulation of **"symbolic" matrices** (distances, kernel, etc.).
2. **Optimal transport**: generalized sorting methods.
3. The long road to **standardization** and **clinical** impact.

1. Symbolic matrices

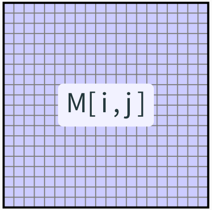
Computing libraries represent most objects as tensors

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

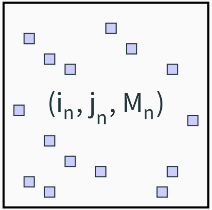
- **Long access times** to the registers penalize the use of large **dense** arrays.
- Hard-wired **contiguous** memory accesses penalize the use of **sparse** matrices.

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.

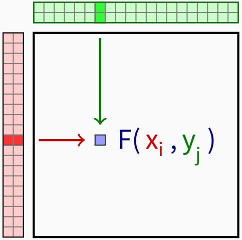
If the formula "F" is simple ($\leqslant$ 100 arithmetic operations):

"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 matrix

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**!

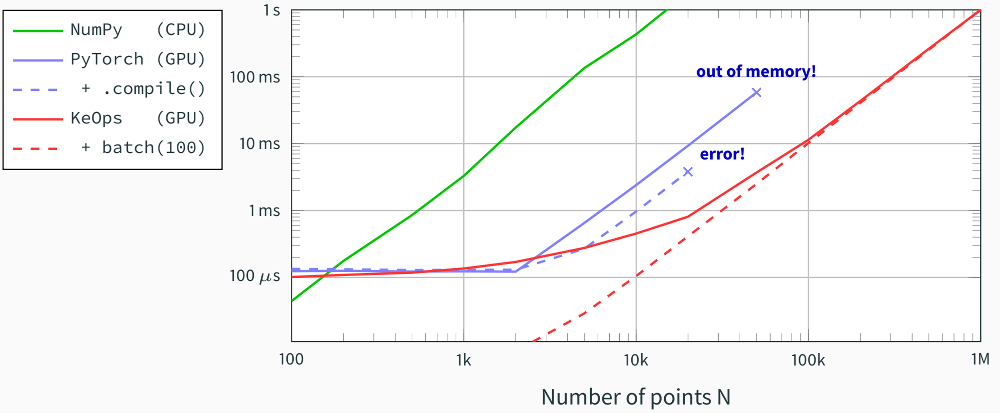
```
D_ij = ((x_i - x_j) ** 2).sum(dim=2)      # Euclidean
M_ij =  (x_i - x_j).abs().sum(dim=2)      # Manhattan
C_ij = 1 - (x_i | x_j)                    # Cosine
H_ij = D_ij / (x_i[...,0] * x_j[...,0])  # Hyperbolic
```

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** $a_i \leftarrow \sum_{j=1}^{N} \exp(-\|x_i - y_j\|^2_{\mathbb{R}^3})\, b_j$
between **clouds of N 3D points** on a A100 GPU.



Yet another ML compiler?

Many impressive tools out there (Numba, Triton, Halide…):

- Focus on **generality** (software + hardware).
- Increasingly easy to use via e.g. PyTorch 2.0.

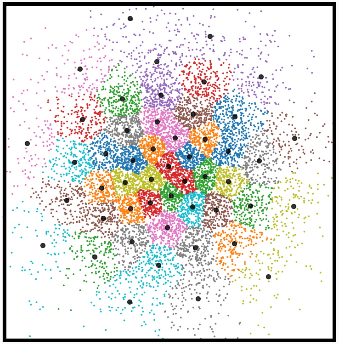
KeOps fills a different niche (a bit like cuFFT, FFTW…):

- Focus on a **single major bottleneck**: geometric interactions.
- **Agnostic** with respect to Euclidean / non-Euclidean formulas.
- Fully compatible with PyTorch, NumPy, R.
- Can actually be **used by mathematicians**.

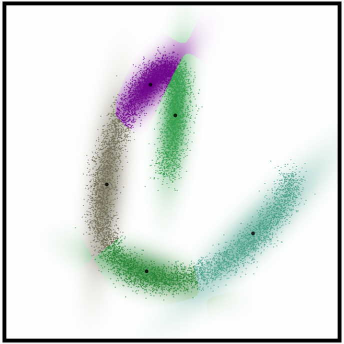
KeOps is a **bridge** between geometers (with a maths background)
and compiler experts (with a CS background).

Applications

KeOps is a good fit for machine learning research



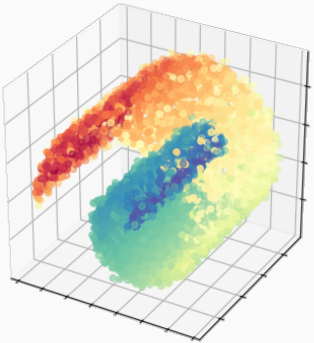
K-Means.



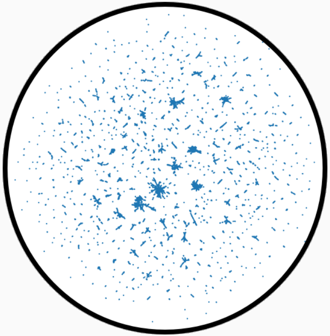
Gaussian Mixture Model.

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

KeOps is a good fit for machine learning research



Spectral analysis.

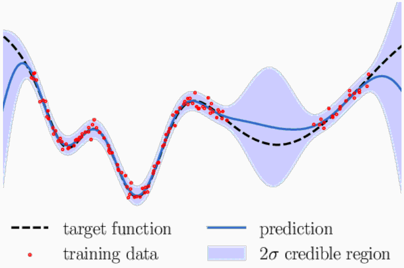


UMAP in hyperbolic space.

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 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).

Geometric deep learning

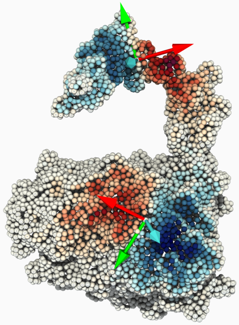
Context. Trainable models on **non-Euclidean domains** (point clouds, surfaces, graphs, etc.), beyond 2D/3D images.

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:

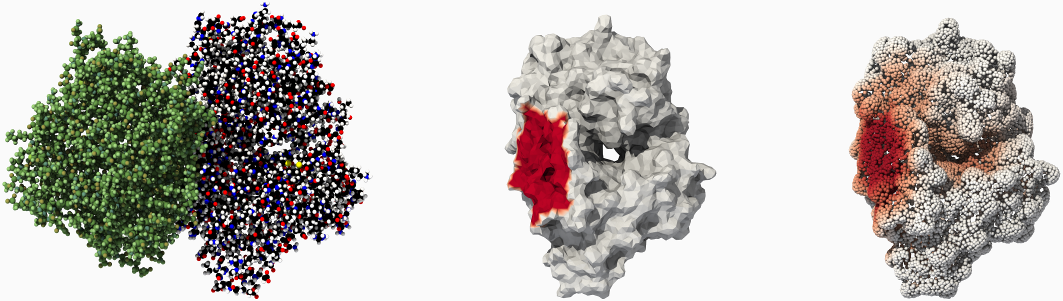
- **Local** interactions: K-nearest neighbors.
- **Global** interactions: generalized convolutions.

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



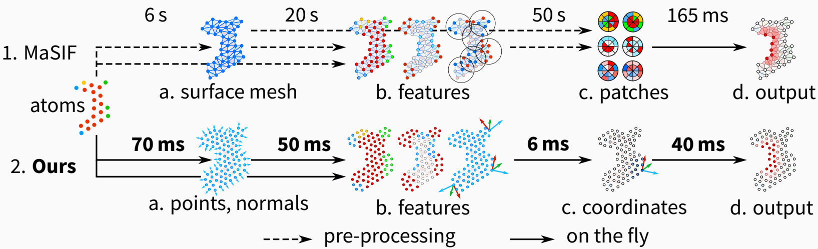
Quasi-geodesic convolution on a protein surface.

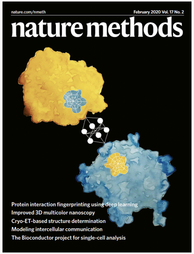
Applications to protein sciences [SFCB20]



(a) Raw protein data. **(b)** Interface. **(c)** Prediction.

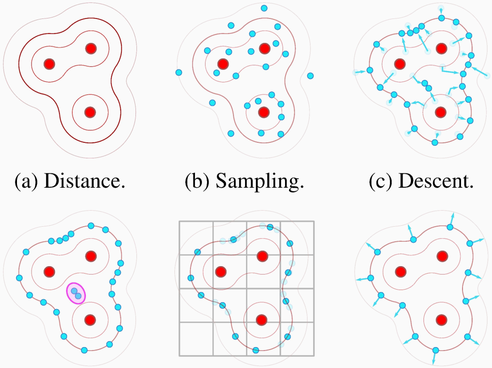
Fast end-to-end learning on protein surfaces





→ $\times$100 - $\times$1,000 faster, lighter and fully differentiable.

Idea 1: on-the-fly sampling of protein surfaces

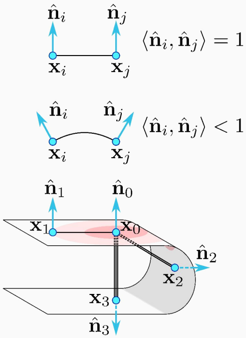


(a) Distance. (b) Sampling. (c) Descent.

(d) Cleaning. (e) Sub-sampling. (f) Normals.

Fast, fully **differentiable**, heterogeneous batches (without padding).

Idea 2: quasi-geodesic convolutions

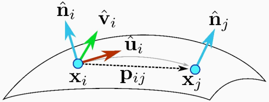


(a) Quasi-geodesic distance d_{ij}.

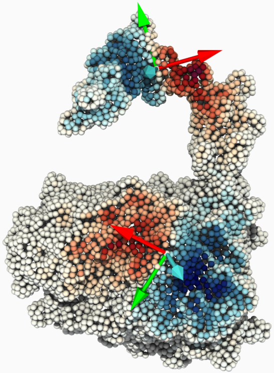
$$\mathbf{p}_{ij} = \underbrace{\left[\ (\mathbf{x}_j - \mathbf{x}_i)^\top\ \right]}_{\text{delta of positions}} \cdot \left[\ \hat{\mathbf{n}}_i \ \middle|\ \hat{\mathbf{u}}_i \ \middle|\ \hat{\mathbf{v}}_i\ \right]$$

$$\mathbf{q}_{ij} = \underbrace{\left[\ (\hat{\mathbf{n}}_j - \hat{\mathbf{n}}_i)^\top\ \right]}_{\text{delta of normals}} \cdot \underbrace{\left[\ \hat{\mathbf{n}}_i \ \middle|\ \hat{\mathbf{u}}_i \ \middle|\ \hat{\mathbf{v}}_i\ \right]}_{\text{local coordinate system}}$$

$$\mathrm{Conv}(\mathbf{x}_i, \mathbf{x}_j, \mathbf{f}_j) = \underbrace{\mathrm{Window}(\mathrm{d}_{ij})}_{\text{quasi-geodesic patch}} \cdot \underbrace{\mathrm{Filter}(\mathbf{p}_{ij}\ ,\ \mathbf{q}_{ij})}_{\text{oriented filter}} \cdot \mathbf{f}_j$$



(b) Quasi-geodesic convolution.



Fast, fully **differentiable**, heterogeneous batches (without padding).

Conclusion

KeOps lets us implement:

- **Custom** operations that best reflect a biological prior.
- Zero need to talk about CUDA blocks, threads, etc.
- Great tool for **prototyping with geometric ideas**.

Main limitation: beyond 16-32 channels per convolution, register spilling.

This is just **one example** of architecture that is equivariant to isometries.

(Some?) general E3NN layers could also be accelerated: **we can talk about it.**

2. Fast optimal transport solvers

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

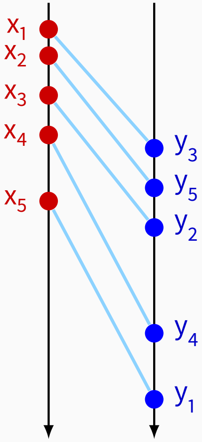
Context. If $A = (x_1, \dots, x_N)$ and $B = (y_1, \dots, y_N)$ are two clouds of N points in $\mathbb{R}^D$, we define:

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

Generalizes **sorting** to metric spaces.

We turn a **distance matrix** into a **permutation**.

We extend this definition to **weighted** samples, **continuous** distributions with **outliers**, etc.



assignment

$\sigma : [\![1, 5]\!] \to [\![1, 5]\!]$

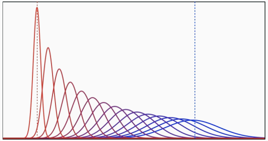
Optimal transport has two main uses in data sciences

The **optimal matching** $x_i \mapsto y_{\sigma(i)}$ is:

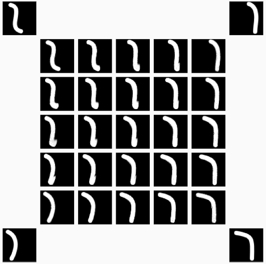
- A **nearest neighbor** projection subject to a **bijectivity** constraint.
- A fundamental operation in 3D shape analysis.
- A staple of operations research.

The **total cost** $\text{OT}(A, B)$ induces:

- A useful **distance** between probability distributions.
- Particle-based **interpolation** with $\arg\min_A \lambda_1 \text{OT}(A, B_1) + \cdots + \lambda_K \text{OT}(A, B_K)$.



OT geodesic



OT barycenters

But 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:

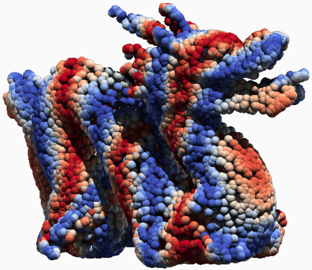
`pip install geomloss`

+

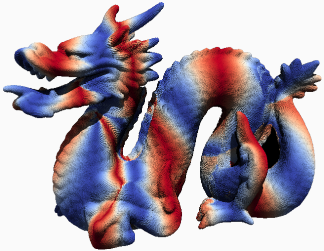
modern GPU

(1 000 €)

$\Longrightarrow$

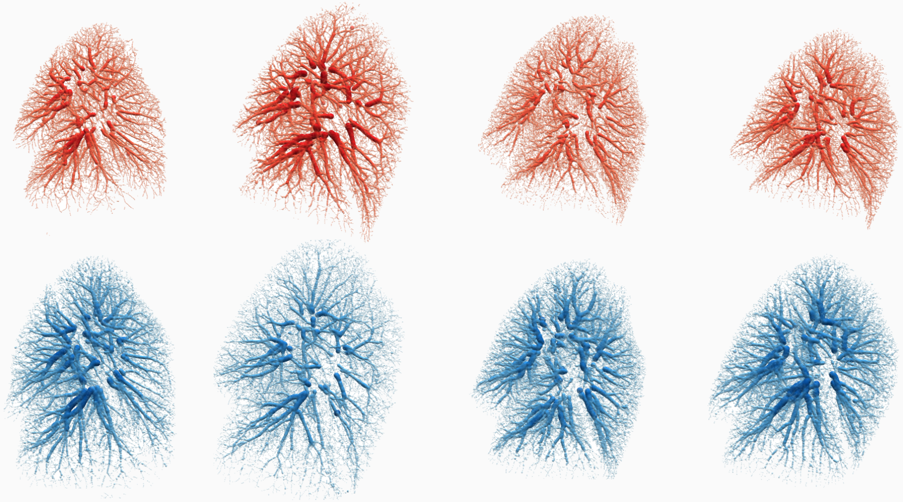


10k points in 30-50ms



100k points in 100-200ms

Lung registration “Exhale – Inhale”



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

State-of-the-art networks – and their limitations

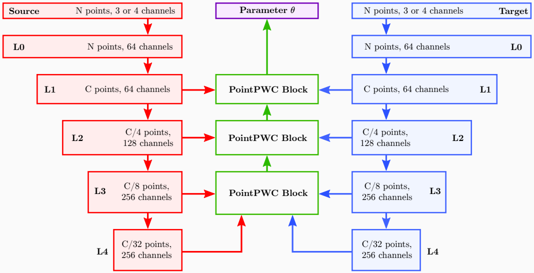
Point neural nets, **in practice**:

- Compute **descriptors** at all scales.
- **Match** them using geometric layers.
- Train on **synthetic** deformations.

Strengths and weaknesses:

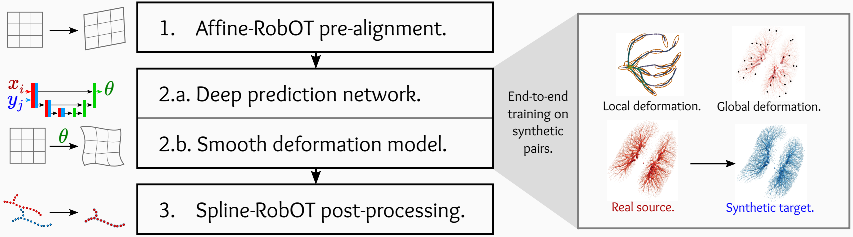
- Good at **pairing** branches.
- Hard to train to high **accuracy**.

$\Longrightarrow$ **Complementary** to OT.



Multi-scale convolutional point neural network.

Three-steps registration



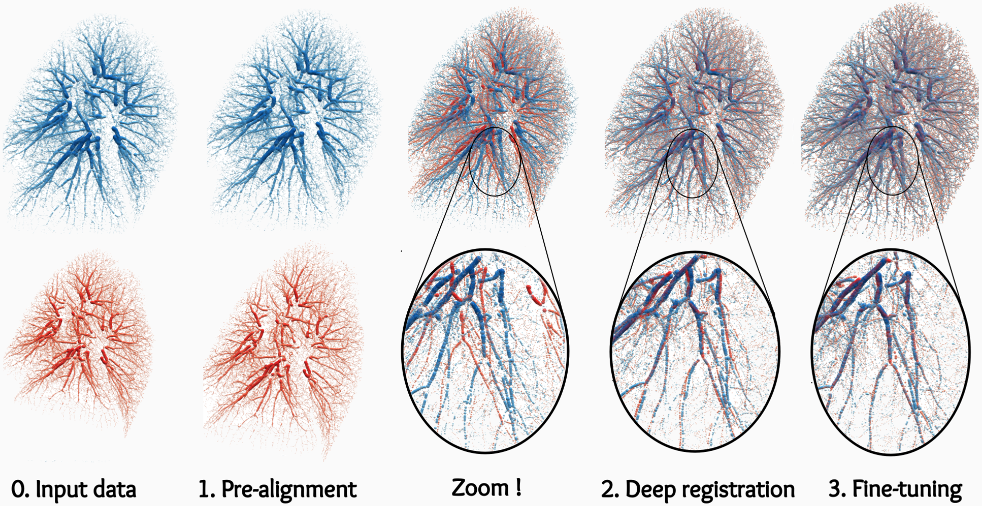
This **pragmatic** method:

- 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.

Three-steps registration



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** :

  $\longrightarrow$ Simple registration for shapes that are close to each other.

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

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

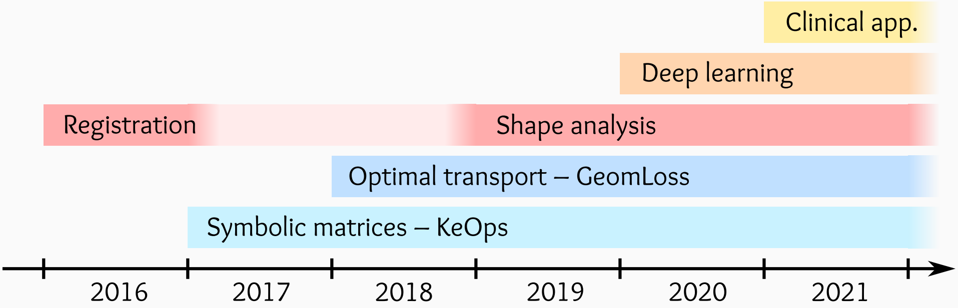
  $\longrightarrow$ GPUs are more **versatile** than people think.

  $\longrightarrow$ 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**.

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Freyr Sverrisson


Shen Zhengyang

+ Marc Niethammer, Bruno Correia, Michael Bronstein…

Going forward: the long road to genuine clinical impact

These tools are diffusing well in our research communities (500k+ downloads).
The target is now to **go beyond "expert users"**.

First step in March 2022: removed all problematic **dependencies** from KeOps 2.0.

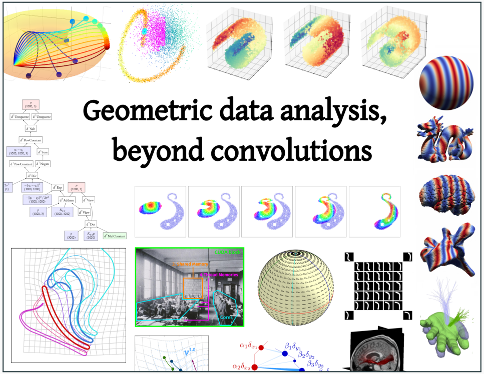
We are now working on:

- High performance on **CPU**.
- A 100% transparent and NumPy-compatible **API** for KeOps+GeomLoss.
- Standard **benchmarks** for kernel methods and optimal transport.
- Applications to **drug consumption** data from 70M French people with Anne-Sophie Jannot, Alexis Van Straaten and Pierre Sabatier.

I hope that we'll have nice results to show you soon :-)

Documentation and tutorials are available online

⟹ www.kernel-operations.io ⟸



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