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.

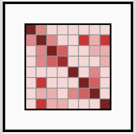
2021+ Public health.

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

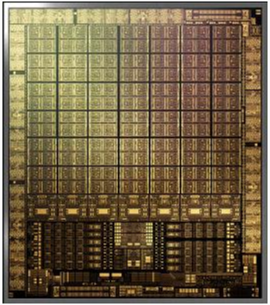
Target. Allow scientists to work with **tailor-made** models as **efficiently** as possible.

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

- Incredible **value for money**:

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

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

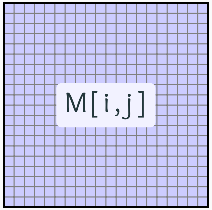
Computing libraries represent most objects as tensors

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

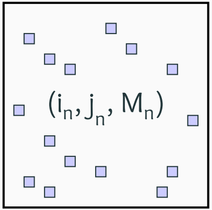
- **Long access times** to the registers penalize the use of large **dense** arrays.
- Hard-wired **contiguous** memory accesses penalize the use of **sparse** matrices.

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.

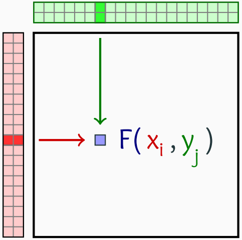
If the formula "F" is simple ($\leqslant$ 100 arithmetic operations):

"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**!

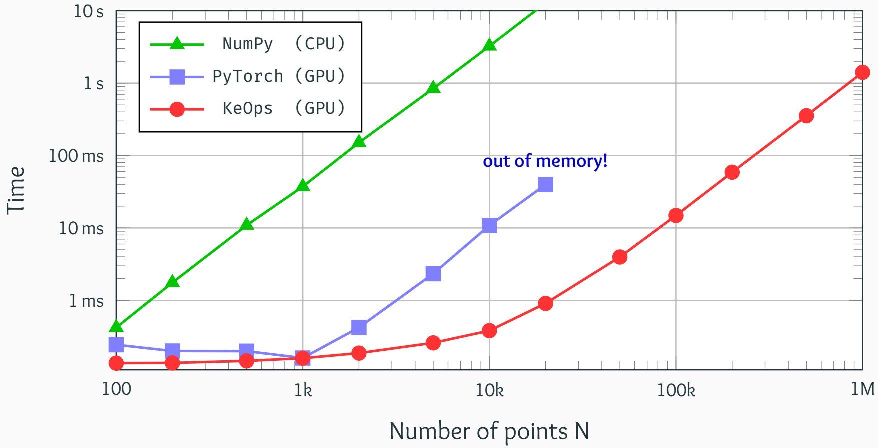
```
D_ij = ((x_i - x_j) ** 2).sum(dim=2)      # Euclidean
M_ij =  (x_i - x_j).abs().sum(dim=2)      # Manhattan
C_ij = 1 - (x_i | x_j)                    # Cosine
H_ij = D_ij / (x_i[...,0] * x_j[...,0])  # Hyperbolic
```

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.

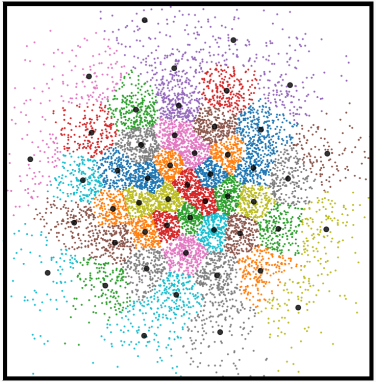
KeOps lets users work with millions of points at a time

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

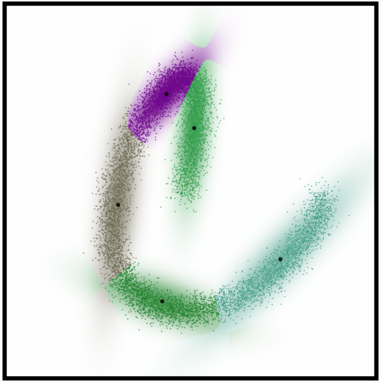


Applications

KeOps is a good fit for machine learning research



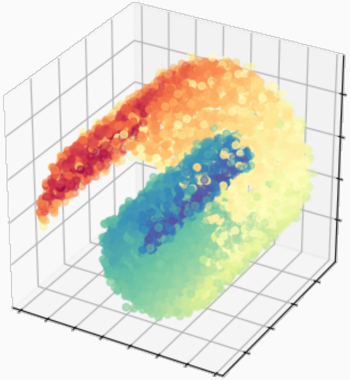
K-Means.



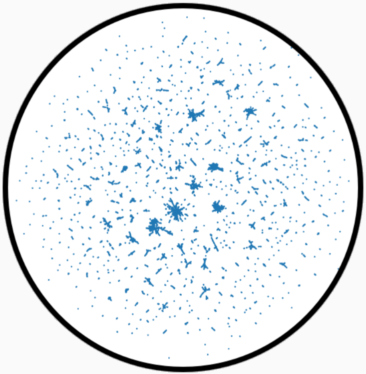
Gaussian Mixture Model.

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

KeOps is a good fit for machine learning research



Spectral analysis.

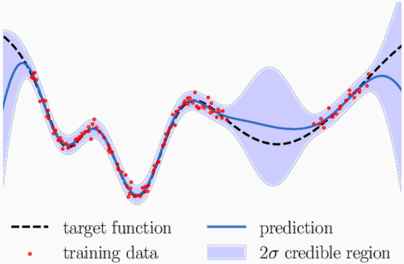


UMAP in hyperbolic space.

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 with 8 GPUs $\longrightarrow$ **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.

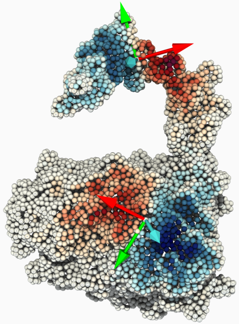
Challenge. In spite of growing interest in the industry, these models still **lack support** on the numerical side. C++/CUDA is (often) required to reach top performance.

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.

2. Fast optimal transport solvers

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

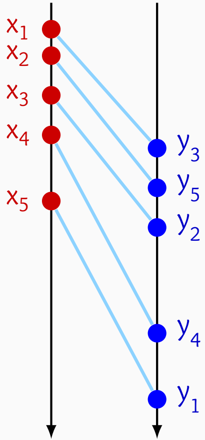
Context. If $A = (x_1, \ldots, x_N)$ and $B = (y_1, \ldots, y_N)$ are two clouds of N points in $\mathbb{R}^D$, we define:

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

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

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

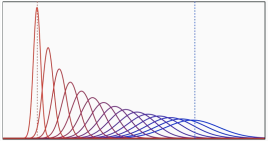
Optimal transport has two main uses in data sciences

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

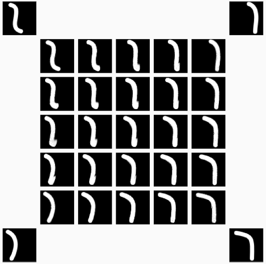
- A **nearest neighbor** projection subject to a **bijectivity** constraint.
- A fundamental operation in 3D shape analysis.
- A staple of operations research.

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:

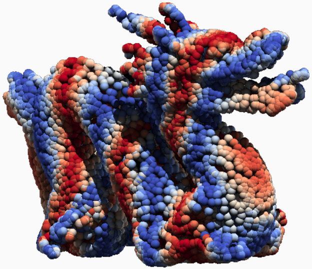
`pip install geomloss`

+

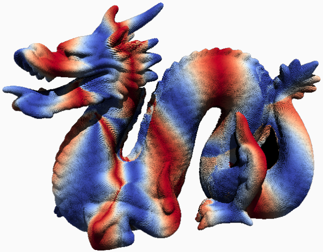
modern GPU

(1 000 €)

$\Longrightarrow$



10k points in 30-50ms



100k points in 100-200ms

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.

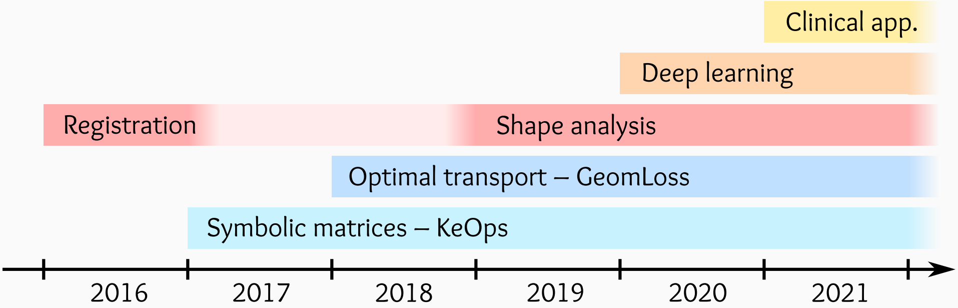
- Optimal Transport = **generalized sorting** :
  $\longrightarrow$ Simple registration for shapes that are close to each other.
  $\longrightarrow$ Super-fast $O(\text{N} \log \text{N})$ solvers.

- These tools open **new paths** for geometers and statisticians:
  $\longrightarrow$ GPUs are more **versatile** than 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

Alain Trouvé

Thibault Séjourné

F.-X. Vialard

Gabriel Peyré

Benjamin Charlier

Joan Glaunès

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 (130k+ downloads).
The target is now to **go beyond "expert users"**.

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

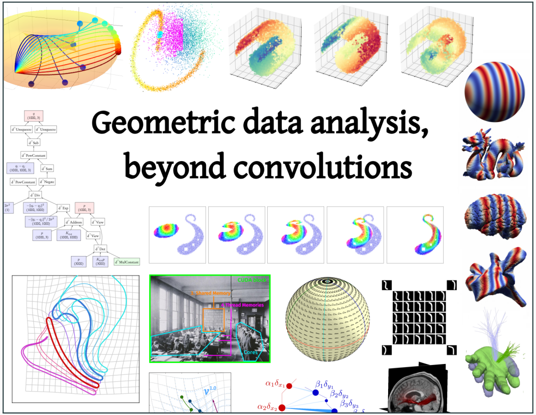
We are now working on:

- 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 the SNDS
  with Anne-Sophie Jannot, Alexis Van Straaten and Pierre Sabatier.

I hope that we'll have nice results to show you after the summer :-)

Documentation and tutorials are available online

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



www.jeanfeydy.com/geometric_data_analysis.pdf

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