Fast libraries for geometric data analysis

Jean Feydy
HeKA team, Inria Paris
Inserm, Université Paris-Cité

11th of July, 2022
discussion with Nvidia

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**:

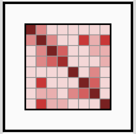
- **2015+** Medical imaging.
- **2016+** Computational anatomy.
- **2021+** Public health.

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**?

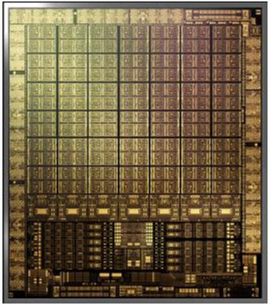
A field that is moving fast

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. **Survival analysis** on the French social security data.

1. Symbolic matrices

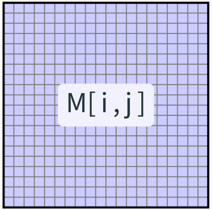
Computing libraries represent most objects as tensors

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

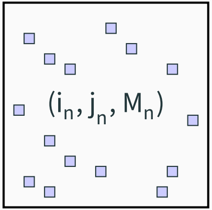
- **Long access times** to the registers penalize the use of large **dense** arrays.
- Hard-wired **contiguous** memory accesses penalize the use of **sparse** matrices.

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.

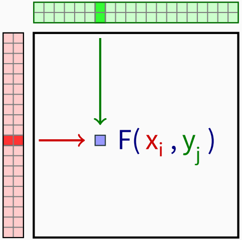
If the formula "F" is simple ($\leqslant$ 100 arithmetic operations):

"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**!

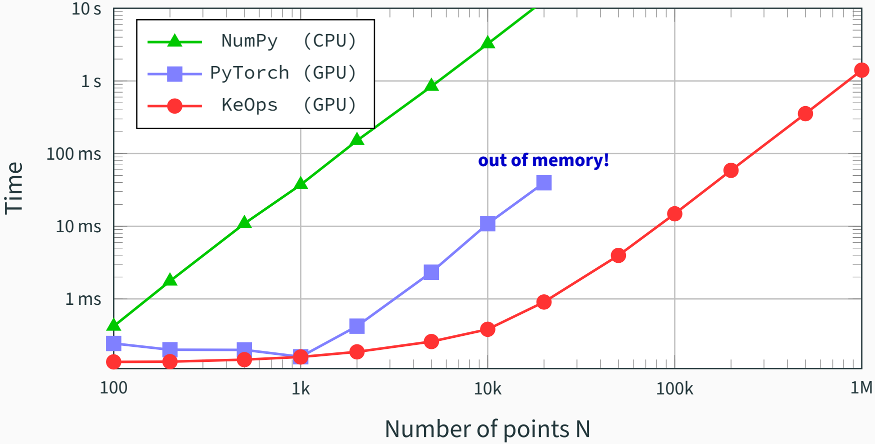
```
D_ij = ((x_i - x_j) ** 2).sum(dim=2)      # Euclidean
M_ij =  (x_i - x_j).abs().sum(dim=2)      # Manhattan
C_ij = 1 - (x_i | x_j)                    # Cosine
H_ij = D_ij / (x_i[...,0] * x_j[...,0])  # Hyperbolic
```

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.

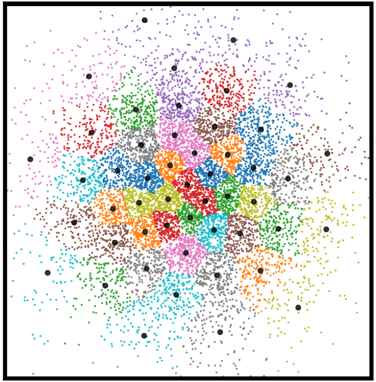
KeOps lets users work with millions of points at a time

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

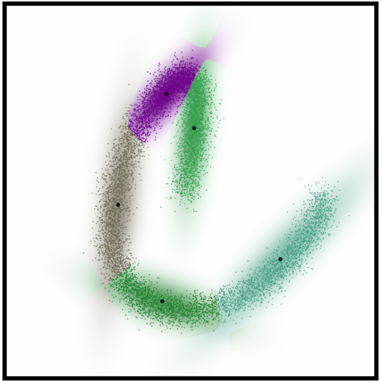


Applications

KeOps is a good fit for machine learning research



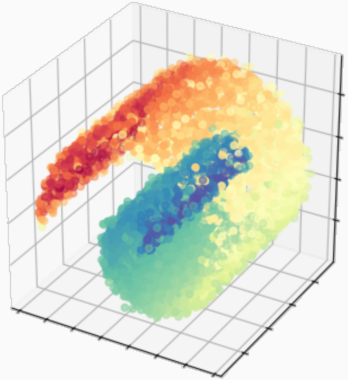
K-Means.



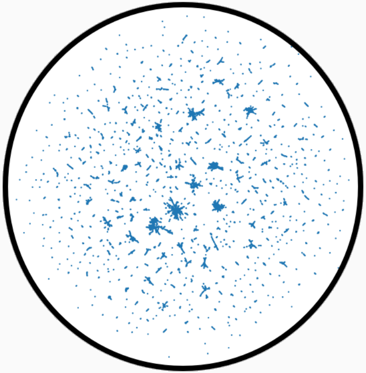
Gaussian Mixture Model.

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

KeOps is a good fit for machine learning research



Spectral analysis.

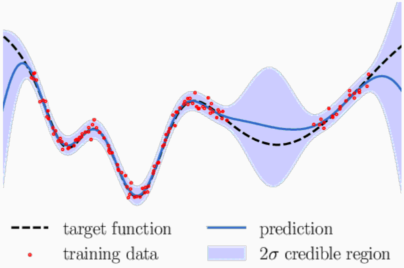


UMAP in hyperbolic space.

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.

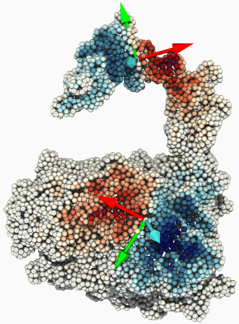
Challenge. In spite of growing interest in the industry, these models still **lack support** on the numerical side. C++/CUDA is (often) required to reach top performance.

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

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

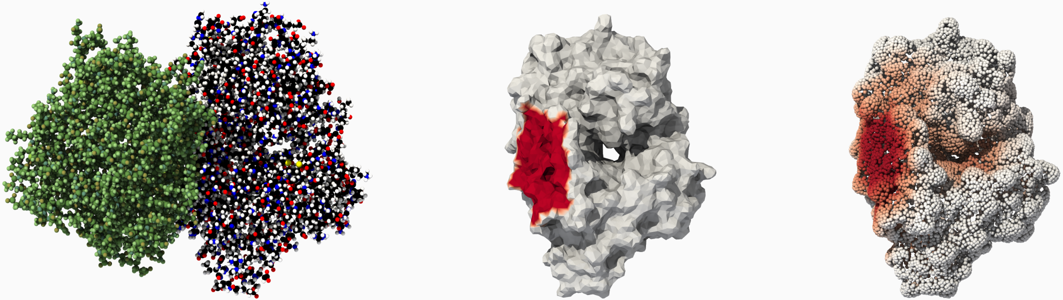
Modelling **freedom**

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



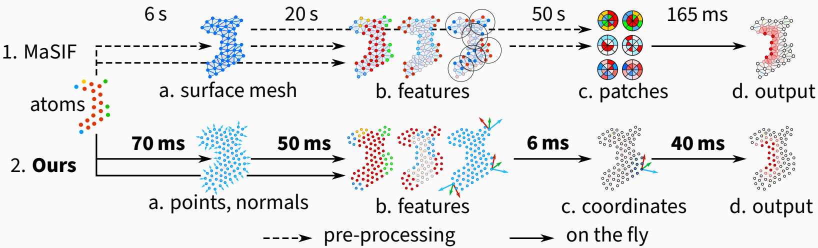
Quasi-geodesic convolution on a protein surface.

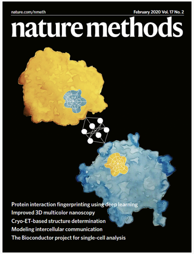
Applications to protein sciences [SFCB20]



(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.

2. Fast optimal transport solvers

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

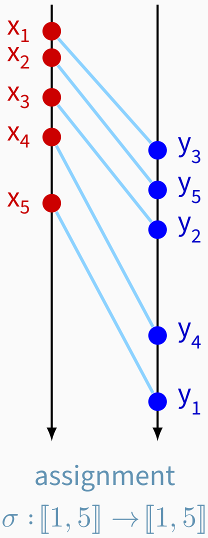
Context. If $A = (x_1, \dots, x_N)$ and $B = (y_1, \dots, y_N)$ are two clouds of N points in $\mathbb{R}^D$, we define:

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

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.



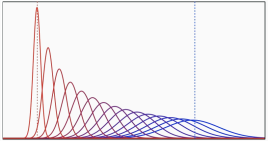
Optimal transport has two main uses in data sciences

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

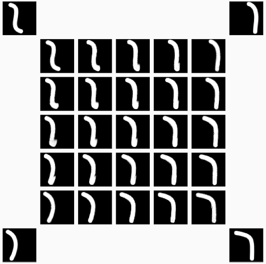
- A **nearest neighbor** projection subject to a **bijectivity** constraint.
- A fundamental operation in 3D shape analysis.
- A staple of operations research.

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:

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

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

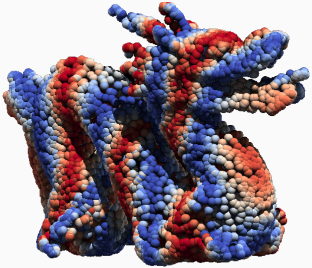
`pip install geomloss`

+

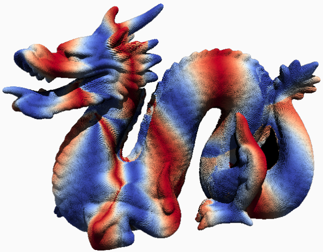
modern GPU

(1 000 €)

$\Longrightarrow$

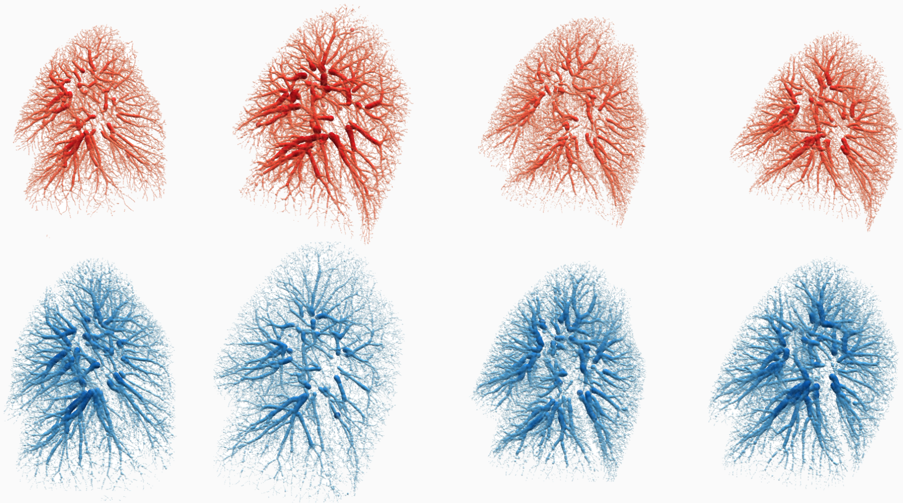


10k points in 30-50ms



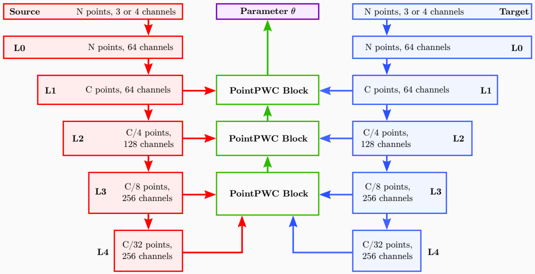
100k points in 100-200ms

Lung registration "Exhale – Inhale"



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

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



Multi-scale convolutional point neural network.

Point neural nets, **in practice**:

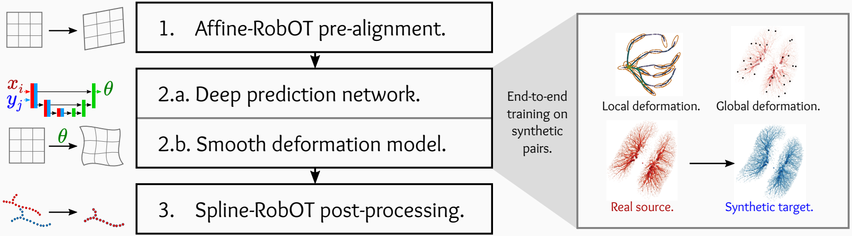
- Compute **descriptors** at all scales.
- **Match** them using geometric layers.
- Train on **synthetic** deformations.

Strengths and weaknesses:

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

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

Three-steps registration



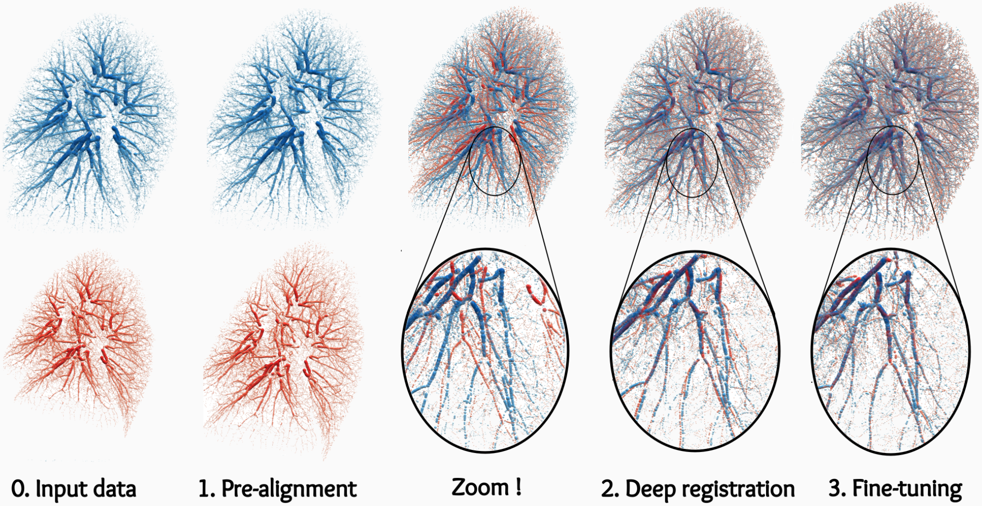
This **pragmatic** method:

- 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,

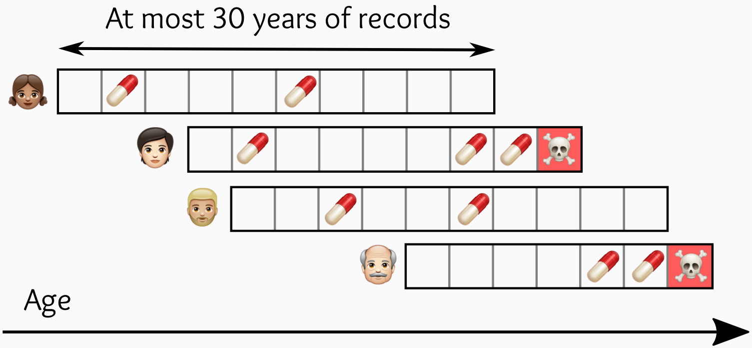
Shen, Feydy et al., NeurIPS 2021.

Three-steps registration



Survival analysis on GPUs

Survival analysis: a classification problem on time series



Fundamental problem for:

- **Factories**: why are components breaking?
- **Businesses**: why are customers leaving?
- **Public health**: why are patients getting cancer?

Survival analysis: implementations

Standard model: Cox Proportional Hazards,
with **time-dependent features** such as Weighted Cumulated Exposures (WCE).

Standard implementation: the `survival` and WCE packages for R (10M+ downloads).

Excellent packaging, but CPU only:

- this is OK for clinical trials (1k–10k patients),
- but prohibitively **slow** for large-scale studies.

Projet Epi-Phare - 150k€: scale up this method to **70M+ patients (SNDS)**.
Sep. 2021 – Aug. 2023: we are **halfway** through.

Step 1: leverage Graphics Processing Units (GPUs)

Striking similarities between survival and machine learning models:

- **Cox** model = **logistic** regression on a **graph** (1 node = 1 patient).
- Weighted Cumulated Exposures = **kernel** features.

I have implemented a **fast GPU solver** for these problems.
Alexis Van Straaten is packaging it as a R library.

survival-GPU (for R and Python) produces the exact same output
as the standard **survival** and **WCE** packages, but **x1,000 faster.**

Two main consequences:

- **Bootstrap**: we can repeat an experiment 1,000 times to estimate **uncertainties**.
- **Scalability**: we can process **millions** of patients in minutes.

Step 2: get access to the French social security data (SNDS)

- **Pierre Sabatier** (pharmacologist at the HEGP) has access to the SNDS.
- **Inria** received a security clearance for the SNDS in June 2021.
- Inria paid for my **week-long SNDS training** in May 2022 – thanks!

We are now starting to work on this data: clinical papers out soon.

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 $O(\mathrm{N} \log \mathrm{N})$ solvers.

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

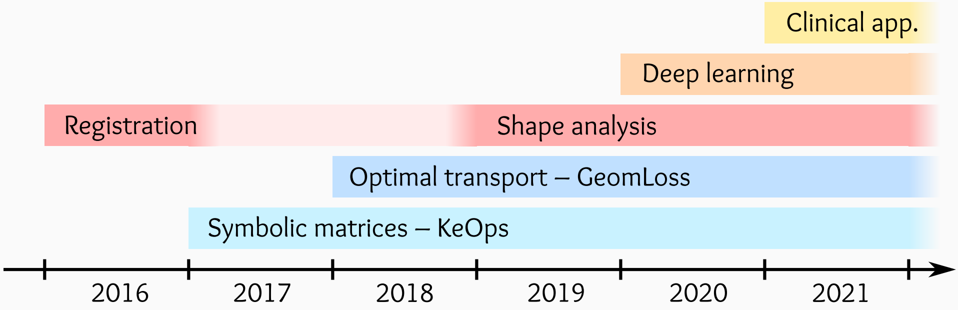
$\longrightarrow$ GPUs are more **versatile** than you think.

$\longrightarrow$ 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 > **10k** $\longrightarrow$ N > **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 (170k+ downloads).
The target is now to **go beyond "expert users"**.

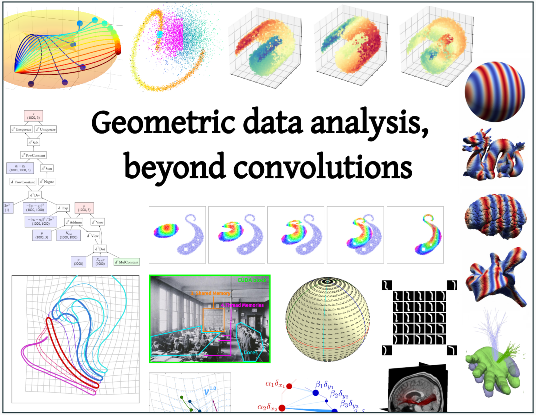
We are actively working on:

- High performance on **CPU**.
- Native support for **approximation** strategies.
- A 100% transparent and NumPy-compatible **API** for KeOps+GeomLoss.
- Standard **benchmarks** for kernel methods and optimal transport.
- Clinical application on **drug consumption** data from the SNDS.

Needless to say, we're very open to discussions :-)

Documentation and tutorials are available online

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



www.jeanfeydy.com/geometric_data_analysis.pdf

References

References i

Dimitri P Bertsekas.

A distributed algorithm for the assignment problem.

Lab. for Information and Decision Systems Working Paper, M.I.T., Cambridge, MA, 1979.

Grégoire Clarté, Antoine Diez, and Jean Feydy.

Collective proposal distributions for nonlinear MCMC samplers: Mean-field theory and fast implementation.

arXiv preprint arXiv:1909.08988, 2019.

References ii

Christophe Chnafa, Simon Mendez, and Franck Nicoud.

Image-based large-eddy simulation in a realistic left heart.

Computers & Fluids, 94:173–187, 2014.

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-care-0507, 2019.

MIT CSAIL.

Marco Cuturi.

Sinkhorn distances: Lightspeed computation of optimal transport.

In *Advances in Neural Information Processing Systems*, pages 2292–2300, 2013.

Pierre Degond, Amic Frouvelle, Sara Merino-Aceituno, and Ariane Trescases.

Alignment of self-propelled rigid bodies: from particle systems to macroscopic equations.

In *International workshop on Stochastic Dynamics out of Equilibrium*, pages 28–66. Springer, 2017.

Pierre Degond and Sébastien Motsch.

Continuum limit of self-driven particles with orientation interaction.

Mathematical Models and Methods in Applied Sciences, 18(supp01):1193–1215, 2008.

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.

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.

Florent Leclercq.

Bayesian optimization for likelihood-free cosmological inference.

Physical Review D, 98(6):063511, 2018.

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.

Quentin Mérigot.

A multiscale approach to optimal transport.

In *Computer Graphics Forum*, volume 30, pages 1583–1592. Wiley Online Library, 2011.

Bernhard Schmitzer.

Stabilized sparse scaling algorithms for entropy regularized transport problems.

SIAM Journal on Scientific Computing, 41(3):A1443–A1481, 2019.

Freyr Sverrisson, Jean Feydy, Bruno E. Correia, and Michael M. Bronstein.

Fast end-to-end learning on protein surfaces.

bioRxiv, 2020.