Optimal transport: mature tools and open problems

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

14th of June, 2022
Curves and Surfaces 2022
Arcachon

My motivation: speeding up core computations for healthcare

Computational anatomy. 3D medical scans are orders of magnitude heavier than natural 2D images:

- 100k triangles to represent a brain surface.
- 512x512x512 $\simeq$ 130M voxels for a typical 3D image.

Public health. Over the last decade, medical datasets have **blown up**:

- Clinical trials: **1k patients**, controlled environment.
- UK Biobank: **500k people**, curated data.
- French Health Data Hub: **70M people**, full social security data since ~2000.

Medical doctors, pharmacists and governments need scalable methods.

A field that is moving fast

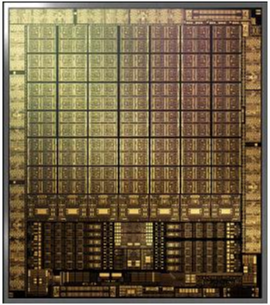
Target. Scale up models that combine medical **expertise** with modern **datasets**.

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

- Incredible **value for money**:

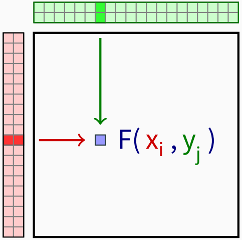
  $1\,000€ \simeq 1\,000$ cores $\simeq 10^{12}$ operations/s.
- **Bottleneck**: constraints on **register** usage.

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



7,000 cores
in a single GPU.

The KeOps library: efficient support for symbolic matrices



Symbolic matrix

Formula + data

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

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.

A long-term investment in the foundations of our field

Since 2016, I've been working on speeding up:

- Geometric **machine learning**: K-Nearest Neighbors, kernel methods.
- Geometric **statistics**: Gaussian processes, Maximum Mean Discrepancies.
- Geometric **deep learning**: point convolutions, attention layers.
- **Survival** analysis: CoxPH solvers, time-varying features.
- **Optimal transport**: our focus today!

Today's talk

1. What is Optimal Transport, and **why does it matter**?
2. **Computational** advances.
3. How people use OT **today**.
4. What about the **future**?

Optimal transport?

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

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:

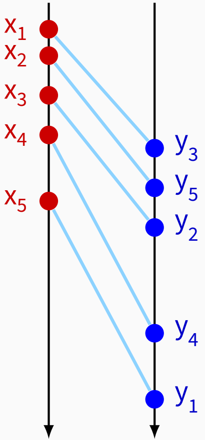
$$\mathrm{OT}(A, B) \;=\; \min_{\sigma \in \mathcal{S}_N} \frac{1}{2N} \sum_{i=1}^{N} \| x_i - y_{\sigma(i)} \|^2$$

Generalizes **sorting** to metric spaces.

Linear problem on the permutation matrix P:

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

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



assignment

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

Practical use

Alternatively, we understand OT as:

- Nearest neighbor **projection** + **incompressibility** constraint.
- Fundamental example of **linear optimization** over the transport plan $\mathsf{P}_{i,j}$.

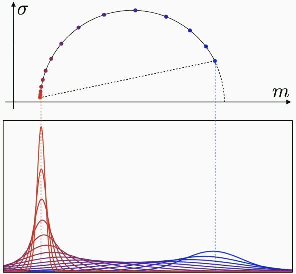
This theory induces two main quantities:

- The transport plan $\mathsf{P}_{i,j} \simeq$ the optimal mapping $x_i \mapsto y_{\sigma(i)}$.
- The "Wasserstein" distance $\sqrt{\mathrm{OT}(\mathsf{A}, \mathsf{B})}$.

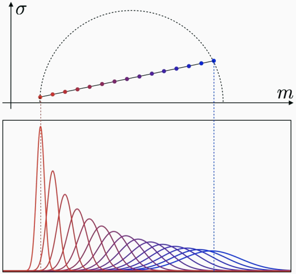
OT induces a geometry-aware distance between probability distributions [PC18]

Gauss map $\mathcal{N} : (m, \sigma) \in \mathbb{R} \times \mathbb{R}_{\geqslant 0} \;\mapsto\; \mathcal{N}(m, \sigma) \in \mathbb{P}(\mathbb{R})$.

If the space of **probability distributions** $\mathbb{P}(\mathbb{R})$ is endowed with a given metric, what is the “pull-back” geometry on the space of **parameters** (m, σ)?



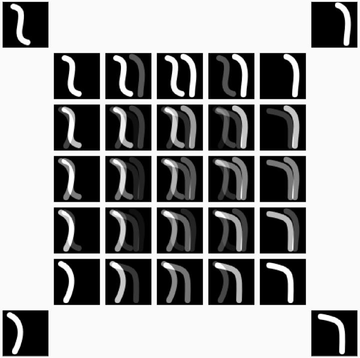
Fisher-Rao ($\simeq$ relative entropy) on $\mathcal{N}(m, \sigma)$
$\to$ Hyperbolic Poincaré metric on (m, σ).



OT on $\mathcal{N}(m, \sigma)$
$\to$ Flat Euclidean metric on (m, σ).

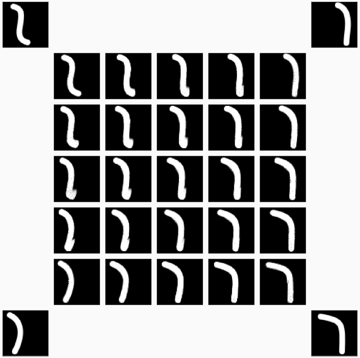
Geometric solutions to least square problems [AC11]

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



Euclidean barycenters.

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



Wasserstein barycenters.

$$\mathrm{Loss}({\color{red}\mathsf{A}}, {\color{blue}\mathsf{B}}) \;=\; \mathrm{OT}({\color{red}\mathsf{A}}, {\color{blue}\mathsf{B}})$$

How should we solve the OT problem?

A fundamental problem in applied mathematics

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 gaming GPU:

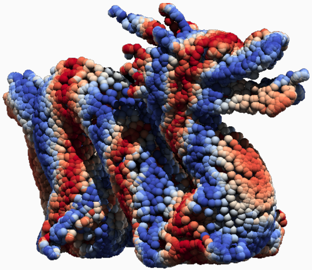
`pip install geomloss`

+

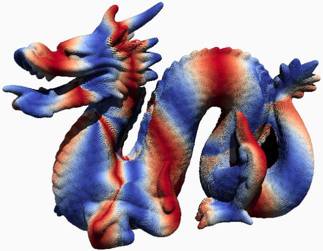
modern GPU

(1 000 €)

$\Longrightarrow$



10k points in 30-50ms



100k points in 100-200ms

How do people use OT in 2022?

1. Physics and simulation of Partial Differential Equations

Since the 1990s, OT is an essential tool to deal with flows:

- Fundamental models have an **appealing form** when seen through the OT lense:
  the incompressible **Euler flow** is a **geodesic** trajectory,
  heat diffusion is a gradient **descent**…
- This framework allows mathematicians to design and study new models **effectively**.
- **Implementations** in 2D and 3D are now becoming mature.
- Lots of cool simulations of **crowds**, **water** or the **early universe**!

Pointers: MoKaPlan Inria team, Bruno Lévy, Quentin Mérigot,
Filippo Santambrogio, Yann Brenier, Felix Otto…

2. An intriguing tool in machine learning

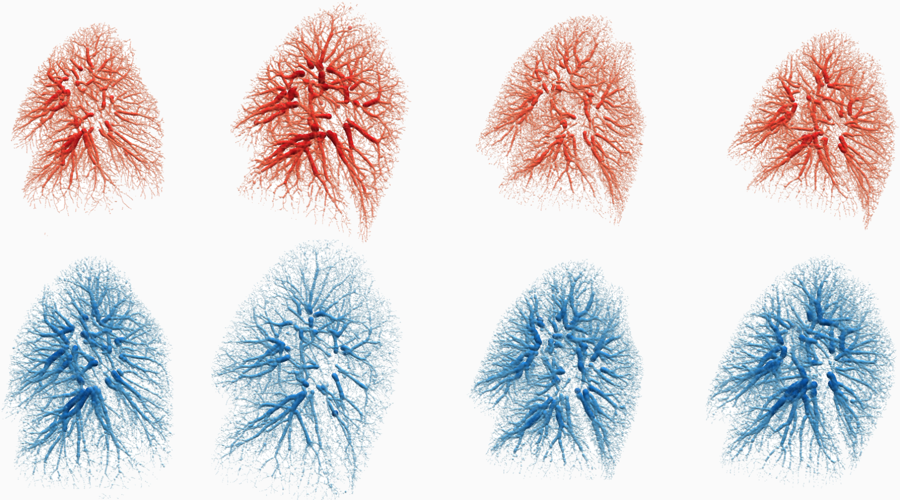
OT **lifts to probability distributions** the geometry of the sample space $\|x_i - y_j\|$.

This is relevant at the intersection between geometry and statistics in order to:

- Design **2-sample tests** : do these two samples come from the same distribution?
- Quantify the **discrepancy** between a synthetic sample and the data distribution.
- Study the convergence of **particle-based optimization** schemes, from simple neural networks to MCMC samplers.

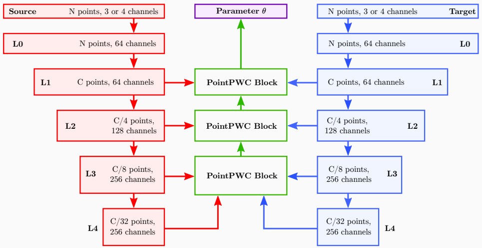
Pointers: Python Optimal Transport (Flamary, Courty et al.),
Computational Optimal Transport (Peyré and Cuturi),
Jonathan Weed, Justin Solomon, Philippe Rigollet, Lenaïc Chizat, Anna Korba…

3. A typical example in shape analysis: 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**:

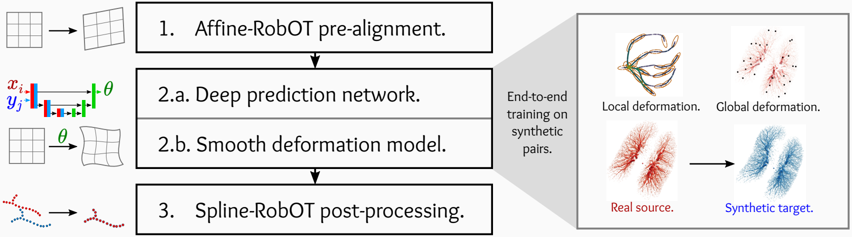
- Compute **descriptors** at all scales.
- **Match** them using geometric layers.
- Train on **synthetic** deformations.

Strengths and weaknesses:

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

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

Three-steps registration with Robust OT (RobOT)



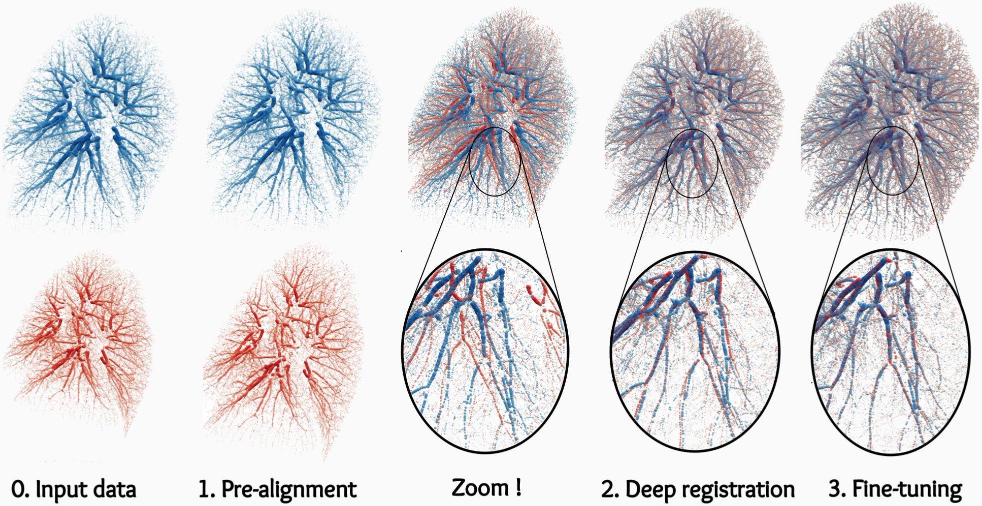
This **pragmatic** method:

- 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



What about the future?

Some open problems

1. Can we generalize standard ML algorithms from **vector spaces** to a (non-linear) space of **probability** distributions?

2. What about distances on **graphs**?
   What about **non-convex** costs, e.g. $\sqrt{\|x_i - y_j\|}$?

3. Can we enforce some **spatial regularity** while keeping super-fast solvers?

4. OT as a source of inspiration in **high-dimension**:
   can we design robust geometric distances between distributions?

My job: pave the way for a new generation of researchers

1. **Secure** a permanent position.
   $\longrightarrow$ Inria researcher since Dec. 2021.

2. Shore up the **GPU foundations** of the field.
   $\longrightarrow$ KeOps v2.0 released in March 2022, now seamless to install.

3. **Re-write GeomLoss** with a better interface and full support for 2D/3D images.
   $\longrightarrow$ WIP with the Python Optimal Transport devs, first release very soon.

4. Maintain an **open benchmarking platform** for the community,
   following the example of www.ann-benchmarks.com for nearest neighbor search.
   $\longrightarrow$ WIP, release this Fall.

Conclusion

Genuine team work


Alain Trouvé


Thibault Séjourné


F.-X. Vialard


Gabriel Peyré


Benjamin Charlier


Joan Glaunès


Marc Niethammer


Shen Zhengyang

We’re hiring!

Job opportunities at Inria Paris:

- Research **engineer**: Deformetrica/scikit-shapes, Sep. 2022 – Feb. 2024.
- Paid M2 **internship**: social security data, Apr. 2023 – Aug. 2023.
- **PhD thesis**: geometric data analysis, Sep. 2023 – Aug. 2026.

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** = **incompressibility** prior:

  $\longrightarrow$ Super-fast solvers on simple domains (especially 2D/3D spaces).

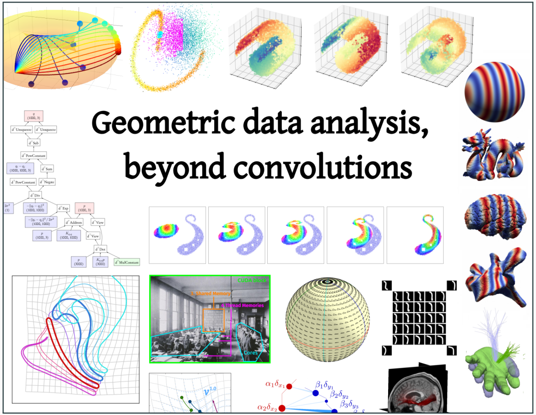
  $\longrightarrow$ Fundamental tool at the intersection of geometry and statistics.

- 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.

Documentation and tutorials are available online

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



www.jeanfeydy.com/geometric_data_analysis.pdf

References

References i

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.

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.

Marco Cuturi.

Sinkhorn distances: Lightspeed computation of optimal transport.

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

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.

References v

Bruno Lévy.

A numerical algorithm for l2 semi-discrete optimal transport in 3d.

ESAIM: Mathematical Modelling and Numerical Analysis, 49(6):1693–1715, 2015.

Quentin Mérigot.

A multiscale approach to optimal transport.

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

Gabriel Peyré and Marco Cuturi.

Computational optimal transport.

arXiv preprint arXiv:1803.00567, 2018.

Bernhard Schmitzer.

Stabilized sparse scaling algorithms for entropy regularized transport problems.

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