Fast geometric learning with symbolic matrices

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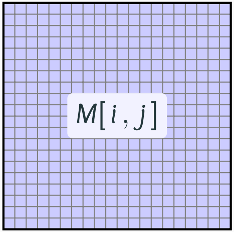
Machine learning libraries represent most objects as tensors



Dense matrix
Coefficients only

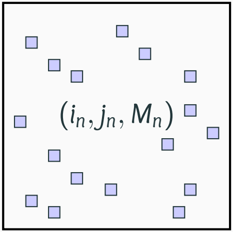
Dense matrices – large, contiguous **arrays** of numbers:

- \+ **Convenient** and well supported.
- – Heavy load on the **memories** of our GPUs, with **time-consuming transfers** taking place between layers of CUDA **registers.**

Machine learning libraries represent most objects as tensors

Dense matrix

Coefficients only



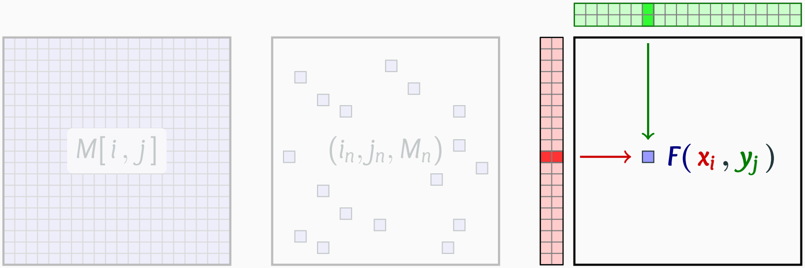
Sparse matrix

Coordinates + coeffs

Sparse matrices – tensors that have **few non-zero entries**:

+ Represent **large tensors** with a small memory footprint.
– Outside of **graph** processing, few objects are **sparse enough** to really benefit from this representation.

Machine learning libraries represent most objects as tensors



Dense matrix	**Sparse matrix**	**Symbolic matrix**
Coefficients only	Coordinates + coeffs	Formula + data

Distance and **kernel** matrices, **point** convolutions, **attention** layers:

- + **Linear** memory usage: no more **memory** overflows.
- + We can optimize the use of registers for a $\times$**10**-$\times$**100 speed-up** vs. a standard PyTorch GPU baseline.

We provide support for this “new abstraction” on the GPU

Our library comes with all the perks of a deep learning toolbox:

+ Transparent **array-like** interface.
+ Full support for automatic **differentiation**.
+ Comprehensive collection of **tutorials**, available online.

Under the hood: combines an optimized **C++** engine with high-level binders for **PyTorch**, **NumPy**, Matlab and R (thanks to Ghislain Durif). (We welcome **contributors** for JAX, Julia and other frameworks!)

To get started:

$\Longrightarrow$ `pip install pykeops` $\Longleftarrow$

`www.kernel-operations.io`

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
```

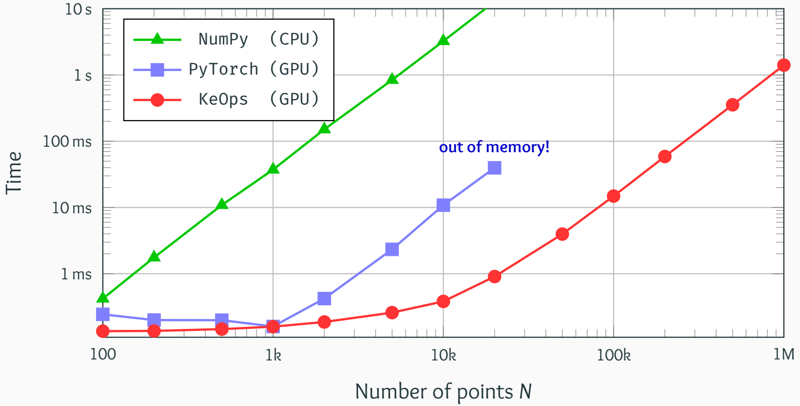
KeOps supports arbitrary **formulas** and **variables** with:

- **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 matrix-vector product with a N-by-N Gaussian kernel matrix between 3D point clouds.

We run NumPy, PyTorch and KeOps on a RTX 2080 Ti GPU.



KeOps lets users experiment freely with advanced methods

KeOps provides a **fast backend for research codes**:

- Interfaces well with **standard libraries**: SciPy, GPytorch, etc.

- Speeds up Gaussian process regression: see e.g. *Kernel methods through the roof: handling* ***billions of points*** *efficiently*, by G. Meanti, L. Carratino, L. Rosasco, A. Rudi (NeurIPS 2020).

- Speeds up **optimal transport** solvers and **point cloud convolutions** by one or two orders of magnitude.

- Much more in the **paper**!

Strengths and limitations of our library

KeOps **symbolic** tensors:

+ Have a negligible **memory** footprint.
+ Provide a sizeable **speed-up** for geometric computations.

– Always rely on **bruteforce** computations.
– Are less interesting when the formula $F(x_i, y_j)$ is **too large**.

Our top priority for **early 2021** is to mitigate these weaknesses: we will add support for **Tensor cores** and standard **approximation strategies** – e.g. using trees or the Nyström method.

Conclusion

Symbolic matrices are to **geometric** ML what
sparse matrices are to **graph** processing.

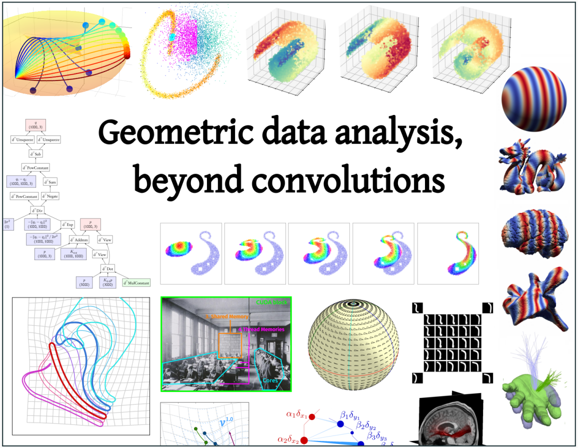
We believe that **KeOps** will stimulate research on:

- **Clustering** methods: fast K-Means and EM iterations.
- Data **representation**: UMAP, fast KNN graphs with any metric.
- **Kernel** methods: kernel matrices.
- **Gaussian** processes: covariance matrices.
- **Geometric** deep learning: point convolutions.
- Natural **language** processing: transformer networks?

We'll be happy to **discuss** these questions with you!

Documentation and tutorials are available online

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



`www.jeanfeydy.com/geometric_data_analysis.pdf`