KeOps

Seamless Kernel Operations on GPU, with auto-differentiation and without memory overflows

B. Charlier (IMAG - Univ Montpellier)
J. Feydy (Imperial College, London)

G. Durif (CNRS - IMAG - Univ Montpellier)
J. Glaunès (MAP5 - Univ Paris Descartes)

October 9th 2019 – *Journées Calcul et Données* (JCAD), Toulouse

`http://www.kernel-operations.io/`
`ghislain.durif@umontpellier.fr`

Outline

1. Introduction
2. Matrix reduction and kernel operations
3. Computation on GPU
4. Implementation
5. Using KeOps
6. Conclusion

Introduction

What KeOps can do?

- Compute generic reductions of very large arrays/matrices

$$\sum_{i=1}^{M} a_{ij} \quad \text{or} \quad \sum_{j=1}^{N} a_{ij}$$

for some large matrix $\mathbf{A} = [a_{ij}] \in \mathbb{R}^{M \times N}$

- Compute kernel dot products and the associated gradients

$$\sum_{i=1}^{M} K(\mathbf{x}_i, \mathbf{y}_j) \quad \text{or} \quad \sum_{j=1}^{N} K(\mathbf{x}_i, \mathbf{y}_j)$$

for a kernel function K and some vectors $\mathbf{x}_i, \mathbf{y}_j \in \mathbb{R}^D$

What KeOps can do?

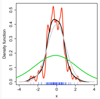
- Compute generic reductions of very large arrays/matrices
- Compute kernel dot products and the associated gradients

$\rightarrow$ large dimensions M and N ($\approx 10^4$ ou 10^6)

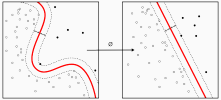
$\rightarrow$ fast computation on GPU without memory overflow

Kernel spaces in statistics and Learning

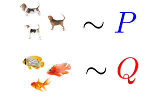
- Kernel density estimation:



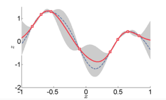
- Classification/Regression: SVM, K-NN, etc...



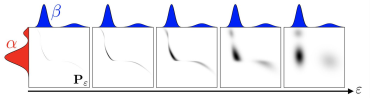
- Kernel embeddings to compare distribution:



- Interpolation and Kriging



- Optimal Transport



Motivations

- GPU user-friendly computing: development effort oriented for deep learning
  - → PyTorch or TensorFlow provide **GPU** implementation of common operations, together with **automatic differentiation**.
- GPU computing can be used for general purpose computations, not only neural networks
  - → Generic codes to use GPU computing require low-level tools (CUDA, OpenCL)
- Needs: provide an effortless tool for GPU computing (application: statistics, machine learning and more)

Matrix reduction and kernel operations

Matrix reduction

- Simple row or column-wise matrix reduction

$$\left[\sum_{i=1}^{M} a_{ij}\right]_{j=1,\ldots,N} \in \mathbb{R}^{N} \quad \text{or} \quad \left[\sum_{j=1}^{N} a_{ij}\right]_{i=1,\ldots,M} \in \mathbb{R}^{M}$$

for a matrix $\mathbf{A} = [a_{ij}] \in \mathbb{R}^{M \times N}$

- Vector/matrix or matrix/matrix product

$$\left[\sum_{i=1}^{M} a_{ij}\,\beta_j\right]_{j=1,\ldots,N} \in \mathbb{R}^{N} \quad \text{or} \quad \left[\sum_{j=1}^{N} a_{ij}\,\beta_j\right]_{i=1,\ldots,M} \in \mathbb{R}^{M}$$

for a matrix $\mathbf{A} = [a_{ij}] \in \mathbb{R}^{M \times N}$ and a vector $\boldsymbol{\beta} = [\beta_j] \in \mathbb{R}^{N}$

Matrix reduction

$$
\begin{bmatrix}
\times & \times & \times & \times & \times \\
\times & \times & \times & \times & \times \\
\times & \times & a_{ij} & \times & \times \\
\times & \times & \times & \times & \times \\
\times & \times & \times & \times & \times
\end{bmatrix}_{M \times N}
$$

$$\downarrow$$

$$
\begin{bmatrix}
\cdots & \cdots & \sum_{i=1}^{M} a_{ij} & \cdots & \cdots
\end{bmatrix}_{1 \times N}
$$

Matrix reduction

$$
\begin{bmatrix}
\times & \times & \times & \times & \times \\
\times & \times & \times & \times & \times \\
\times & \times & a_{ij} & \times & \times \\
\times & \times & \times & \times & \times \\
\times & \times & \times & \times & \times
\end{bmatrix}_{M \times N}
\rightarrow
\begin{bmatrix}
\vdots \\
\vdots \\
\sum_{j=1}^{N} a_{ij} \\
\vdots \\
\vdots
\end{bmatrix}_{M \times 1}
$$

Kernel operator

Considering some data vector $\mathbf{x}_i$ and $\mathbf{y}_j$ in $\mathbb{R}^D$

- (Intuitevely) a kernel function is an application $K : \mathbb{R}^D \times \mathbb{R}^D \to \mathbb{R}$

$$(\mathbf{x}_i, \mathbf{y}_i) \mapsto K(\mathbf{x}_i, \mathbf{y}_i)$$

  corresponding to a scalar product between $\mathbf{x}_i$ and $\mathbf{y}_j$ in a different space

- Example

$$\text{Linear kernel:} \qquad K(\mathbf{x}_i, \mathbf{y}_j) = \langle \mathbf{x}_i \,,\, \mathbf{y}_j \rangle = \mathbf{x}_i^T \mathbf{y}_j = \sum_{k=1}^{D} x_{ik}\, y_{jk}$$

$$\text{Gaussian kernel:} \qquad K(\mathbf{x}_i, \mathbf{y}_j) = \exp\left(-\frac{1}{2\sigma^2} \left\| \mathbf{x}_i - \mathbf{y}_j \right\|_2^2 \right)$$

Kernel reduction

- Convolution-like operation

$$\left[\sum_{i=1}^{M} K(\mathbf{x}_i, \mathbf{y}_j)\, \beta_j\right]_{j=1,\dots,N} \in \mathbb{R}^N \quad \text{or} \quad \left[\sum_{j=1}^{N} K(\mathbf{x}_i, \mathbf{y}_j)\, \beta_j\right]_{i=1,\dots,M} \in \mathbb{R}^M$$

for some D-vectors $(\mathbf{x}_i)_{i=1,\dots,M} \in \mathbb{R}^{M\times D}$, $(\mathbf{y}_j)_{j=1,\dots,N} \in \mathbb{R}^{N\times D}$ and $\boldsymbol{\beta} = [\beta_j] \in \mathbb{R}^N$

$\rightarrow$ Row-wise or column-wise reduction on the matrix $\mathbf{K} = \left[K(\mathbf{x}_i, \mathbf{y}_j)\right] \in \mathbb{R}^{M\times N}$

Kernel reduction

$$\begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & K(\mathbf{x}_i, \mathbf{y}_j) & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \end{bmatrix}_{M \times N}$$

$$\downarrow$$

$$\begin{bmatrix} \dots & \dots & \sum_{i=1}^{M} K(\mathbf{x}_i, \mathbf{y}_j) & \dots & \dots \end{bmatrix}_{1 \times N}$$

Kernel reduction

$$\begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & K(\mathbf{x}_i, \mathbf{y}_j) & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \end{bmatrix}_{M \times N} \rightarrow \begin{bmatrix} \vdots \\ \vdots \\ \sum_{j=1}^{N} K(\mathbf{x}_i, \mathbf{y}_j) \\ \vdots \\ \vdots \end{bmatrix}_{M \times 1}$$

Kernel reduction

- More complex operation

$$\sum_{i=1}^{M} K_1(\mathbf{x}_i, \mathbf{y}_j)\, K_2(\mathbf{u}_i, \mathbf{v}_j)\, \langle \boldsymbol{\alpha}_i \,;\, \boldsymbol{\beta}_j \rangle \quad \text{or} \quad \sum_{j=1}^{N} K_1(\mathbf{x}_i, \mathbf{y}_j)\, K_2(\mathbf{u}_i, \mathbf{v}_j)\, \langle \boldsymbol{\alpha}_i \,;\, \boldsymbol{\beta}_j \rangle$$

for some kernel K_1 and K_2, and some D-vectors $(\mathbf{x}_i)_i, (\mathbf{u}_i)_i, (\boldsymbol{\alpha}_i)_i \in \mathbb{R}^{M\times D}$ and $(\mathbf{y}_j)_j, (\mathbf{v}_j)_j, (\boldsymbol{\beta}_j)_j \in \mathbb{R}^{N\times D}$

Generic reduction in KeOps

$1 \leq i \leq N$ et $1 \leq j \leq M$ avec $N, M \approx 10^4$ ou 10^6

- A generic case:

$$\left[\sum_j F(\sigma_1, \cdots, \sigma_\ell, X_i^1, \cdots, X_i^k, Y_j^1, \cdots, Y_j^m)\right]_{i=1,\ldots,M} \in \mathbb{R}^M$$

- ...an even more generic case:

$$\left[\mathop{\ast}_j F(\sigma_1, \cdots, \sigma_\ell, X_i^1, \cdots, X_i^k, Y_j^1, \cdots, Y_j^m)\right]_{i=1,\ldots,M} \in \mathbb{R}^M$$

where $\ast$ can be any reduction (sum, max, min, etc.) over a dimension

Why GPU computing

- Matrix/kernel reduction = combination of generic matrix operations

- GPU are good for matrix computations

- **Problem:** the matrix $\mathbf{K} = \left[K(\mathbf{x}_i, \mathbf{y}_j)\right] \in \mathbb{R}^{M \times N}$ is very large ($M, N \approx 10^4$ ou 10^6)

  $\rightarrow$ how to store it in memory

  $\rightarrow$ how to iterate through rows/columns to do computations

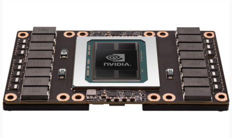
Computation on GPU

The GPU Market by Nvidia

Target:

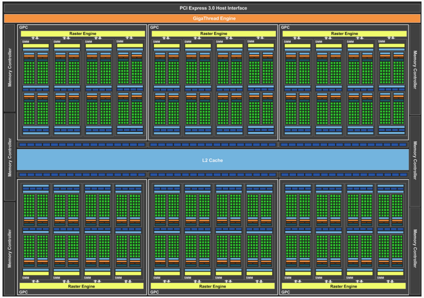
- Gamers: 1000 euros

- Scientific computing: 3000 – 9000 euros



Under the hood: similar chipsets with few enhancements (ECC, float64,...)

GPU = massively parallel architecture



Nividia GTX XXXX architecture

A GPU architecture

→ scalable array of multithreaded *Streaming Multiprocessors* (*SMs*)

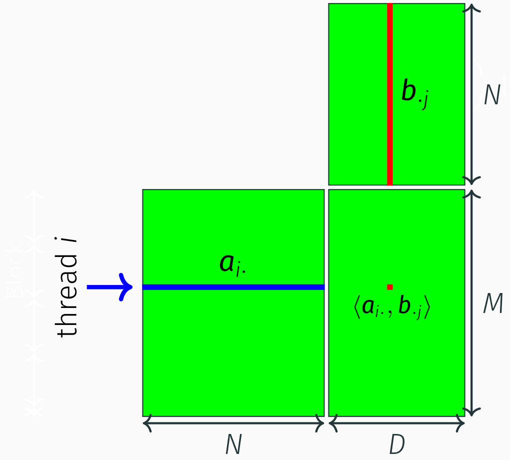
→ each single processor (called a *thread*) is able to execute an independent set of instructions.

1000's of cores inside a single GPU

(multi-CPU architecure = at best 10's – 100's of cores)

MatMult: A first naive implementation

$\mathbf{A} \in \mathbb{R}^{M \times N}$ and $\mathbf{B} \in \mathbb{R}^{N \times D}$



A matrix multiplication

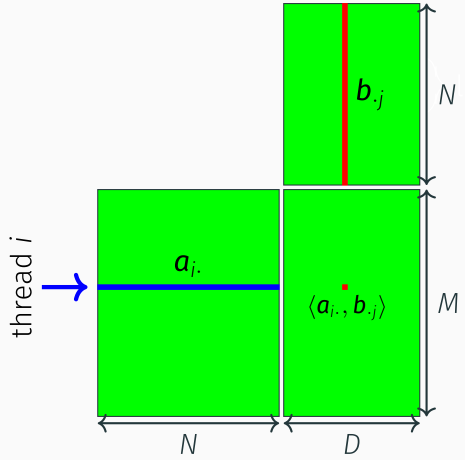
$$\mathbf{A}\,\mathbf{B} = \left[\sum_k a_{ik}\, b_{kj}\right]_{M \times D}$$

$\rightarrow$ a set of $N \times D$ scalar products

Parallel computing

- each thread computes D scalar products, i.e. $\langle \mathbf{a}_{i\cdot}, \mathbf{b}_{\cdot j} \rangle$ for all j

$\mathbf{A} \in \mathbb{R}^{M \times N}$ and $\mathbf{B} \in \mathbb{R}^{N \times D}$



Thread i needs to access

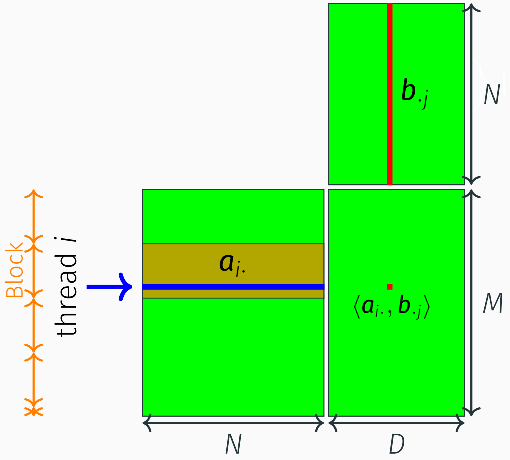
- row $\mathbf{a}_{i\cdot} \in \mathbb{R}^N$
- all columns $(\mathbf{b}_{\cdot j})_{j=1,\ldots,D}$ i.e. the full matrix **B**

→ potential memory overflow

→ no mutualisation of memory access between threads

MatMult: A first naive implementation

$\mathbf{A} \in \mathbb{R}^{M \times N}$ and $\mathbf{B} \in \mathbb{R}^{N \times D}$

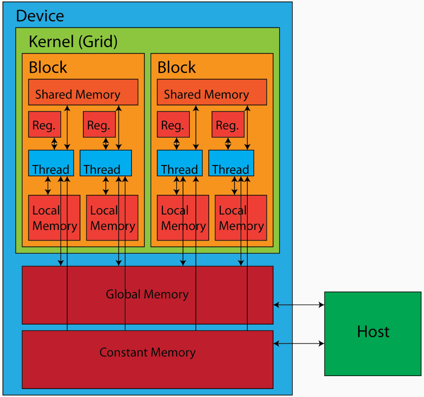


Assign a block of rows i to a thread

- mutualise the memory access to each $\mathbf{B}_{\cdot j}$ to compute all rows i in the block

→ each thread still requires to access the full matrix **B** to finish the computations for a row i

Memory management on GPU



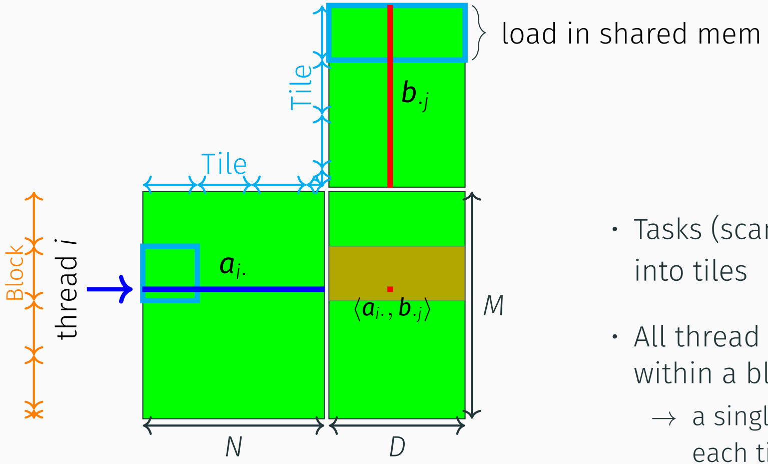
- Data initially stored on the host (in RAM)
  - → should be transfer to the device (GPU) to be treated (bottleneck)
- Different kinds of memory
  - → local vs shared memory

Smart use of the shared memory

→ less transfer between device and host

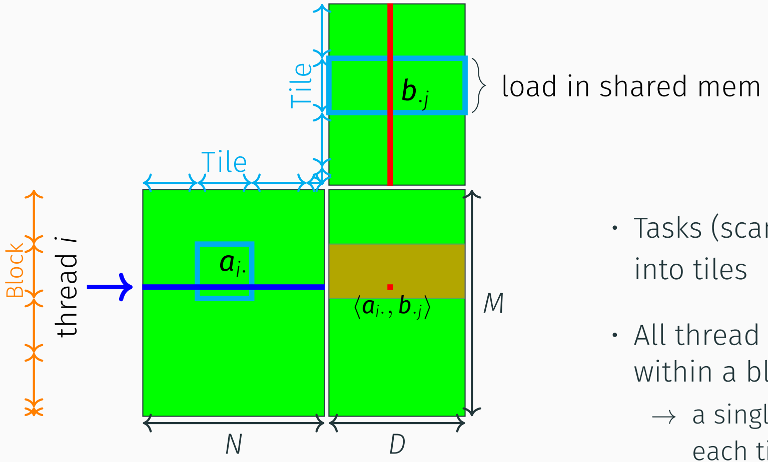
→ key to provide an efficient code in term of computational time

MatMult: Tiled implementation (decomposition with block sub-matrix product)



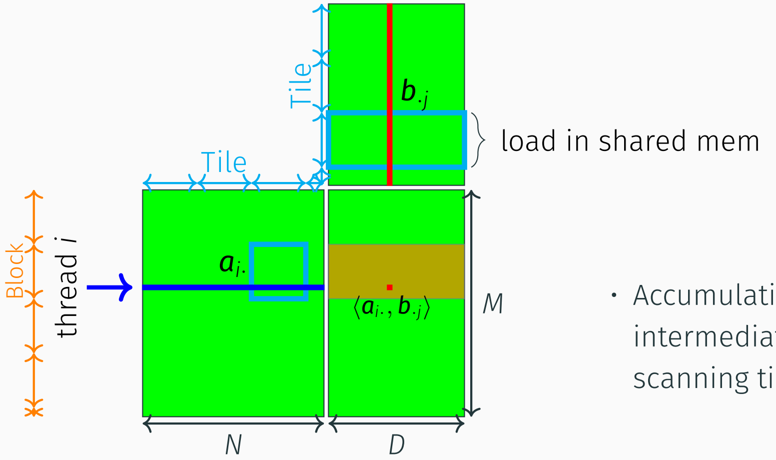
- Tasks (scanning rows $\mathbf{a}_i$) divided into tiles
- All thread use the shared memory within a block
  - → a single memory transfered of each tile in **B** for all threads

MatMult: Tiled implementation (decomposition with block sub-matrix product)



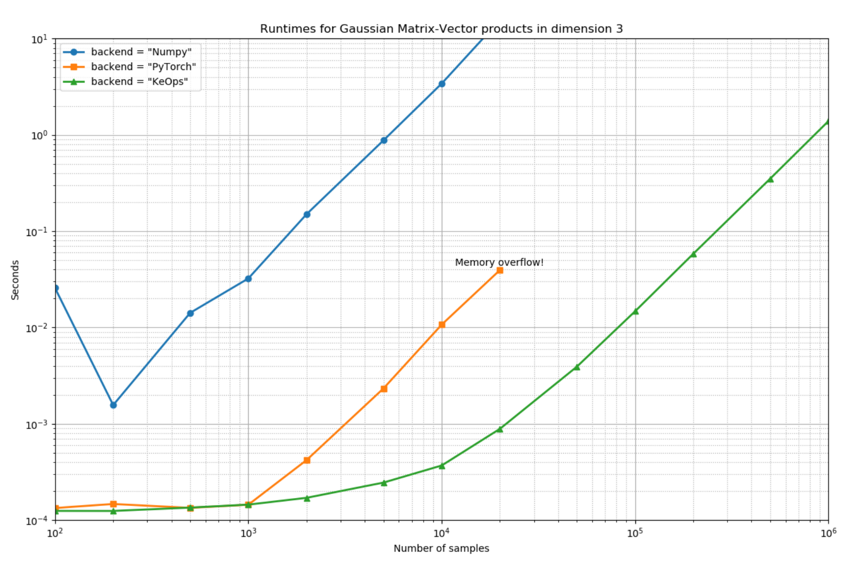
- Tasks (scanning rows $\mathbf{a}_i$) divided into tiles
- All thread use the shared memory within a block
  - $\rightarrow$ a single memory transfered of each tile in **B** for all threads

MatMult: Tiled implementation (decomposition with block sub-matrix product)



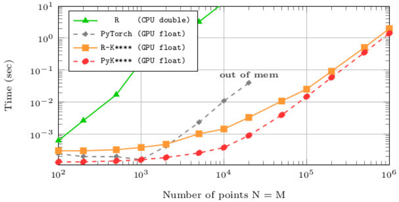
- Accumulation (addition of the intermediate results) when scanning tiles across **A**

Benchmark I

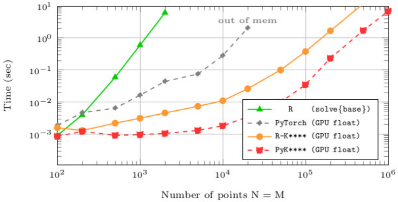


Runtimes for Gaussian Matrix-Vector products in dimension 3
backend = "Numpy"
backend = "PyTorch"
backend = "KeOps"
Memory overflow!
Seconds
Number of samples
10^1
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^2
10^3
10^4
10^5
10^6

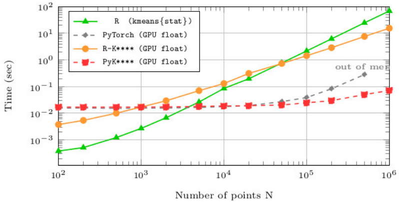
Benchmark II



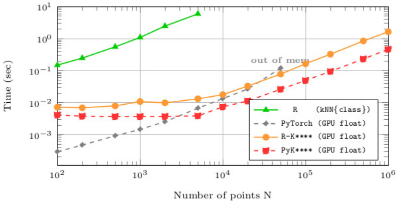
(a) Matrix-vector products with N-by-N Gaussian kernel matrices built from point clouds in dimension D = 3.



(b) Solving an N-by-N Gaussian kernel linear system with ridge regularization (constant diagonal weights).



(c) 10 iterations of K-means (Lloyd's algorithm) with N points in dimension D = 10 and $K = \lfloor\sqrt{N}\rfloor$ clusters.



(d) Exact (K = 10)-nearest neighbor search: 10k queries in dimension D = 100 with a database of N samples.

Implementation

Coding generic formulas with KeOps

- Mathematical formula with two vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^D$:

$$(\mathbf{x}, \mathbf{y}) \mapsto \exp\left(\langle \mathbf{x}, \mathbf{y} \rangle\right)$$

- A formula F in KeOps is first encoded as a string using combinations of elementary operations

```
"Exp(Scalprod(x,y))"
```

- Then it is expanded internally in the C++ code using templates:

```
F=Exp<Scalprod<X,Y>>
```

→ A formula is an instantiation of a variadic recursively defined templated class

→ KeOps is able to generate shared objects that compute on a GPU (compilation on the fly)

Coding generic formulas with KeOps

- Mathematical formula with two vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^D$:

$$(\mathrm{x}, \mathrm{y}) \mapsto \exp\left(\langle \mathrm{x}, \mathrm{y} \rangle\right)$$

- A formula F in KeOps is first encoded as a string using combinations of elementary operations

```
"Exp(Scalprod(x,y))"
```

- Then it is expanded internally in the C++ code using templates:

```
F=Exp<Scalprod<X,Y>>
```

→ A formula is an instantiation of a variadic recursively defined templated class

→ KeOps is able to generate shared objects that compute on a GPU (compilation on the fly)

Coding generic formulas with KeOps

- Mathematical formula with two vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^D$:

$$(\mathbf{x}, \mathbf{y}) \mapsto \exp\left(\langle \mathbf{x}, \mathbf{y} \rangle\right)$$

- A formula F in KeOps is first encoded as a string using combinations of elementary operations

```
"Exp(Scalprod(x,y))"
```

- Then it is expanded internally in the C++ code using templates:

```
F=Exp<Scalprod<X,Y>>
```

→ A formula is an instantiation of a variadic recursively defined templated class

→ KeOps is able to generate shared objects that compute on a GPU (compilation on the fly)

Coding generic formulas with KeOps

- Mathematical formula with two vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^D$:

$$(\mathbf{x}, \mathbf{y}) \mapsto \exp\left(\langle \mathbf{x}, \mathbf{y} \rangle\right)$$

- A formula F in KeOps is first encoded as a string using combinations of elementary operations

```
"Exp(Scalprod(x,y))"
```

- Then it is expanded internally in the C++ code using templates:

```
F=Exp<Scalprod<X,Y>>
```

→ A formula is an instantiation of a variadic recursively defined templated class

→ KeOps is able to generate shared objects that compute on a GPU (compilation on the fly)

Coding generic formulas with KeOps

- Mathematical formula with two vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^D$:

$$(\mathbf{x}, \mathbf{y}) \mapsto \exp\left(\langle \mathbf{x}, \mathbf{y} \rangle\right)$$

- A formula F in KeOps is first encoded as a string using combinations of elementary operations

```
"Exp(Scalprod(x,y))"
```

- Then it is expanded internally in the C++ code using templates:

```
F=Exp<Scalprod<X,Y>>
```

→ A formula is an instantiation of a variadic recursively defined templated class

→ KeOps is able to generate shared objects that compute on a GPU (compilation on the fly)

A typical KeOps (unary) operation is a `struct` that looks like:

```
template<class F>
struct Exp : UnaryOp<Exp, F> {
///////////////// dimension of the output
  static const int DIM = F::DIM;
```

Implementation of the operation:

```
///////////////// inlined function in the final cuda code
  static DEVICE INLINE void Operation(TYPE *out, TYPE *in) {
#pragma unroll
    for (int k = 0; k < DIM; k++) {  out[k] = exp(in[k]); }
   }
```

Under the hood: C++ encoding of maths operations in KeOps I

Gradient computation:

```
////////////////  Autodiff!
   template<class V, class GRADIN>
   using DiffT = typename F::template DiffT<V, Mult<Exp<F>, GRADIN>>;
 };
```

String encoding:

```
////////////////  Macro providing high level syntax
 #define Exp(f) Exp<decltype(f)>()
```

Under the hood: C++ encoding of maths operations in KeOps II

A typical KeOps (binary) operation is a `struct` that looks like:

```
template < class FA, class FB >
struct Add : BinaryOp< Add, FA, FB > {
//////////////// dimension of the output ... and (compile time) checks
  static const int DIM = FA::DIM; // Output dim = FA::DIM = FB::DIM
  static_assert(DIM == FB::DIM, "Dimensions must be the same for Add");
```

Implementation of the operation:

```
///////////////// inlined function in the final cuda code
  static DEVICE INLINE void Operation(TYPE *out, TYPE *inA, TYPE *inB) {
  for (int k = 0; k < DIM; k++) {out[k] = inA[k] + inB[k];}
  }
```

Under the hood: C++ encoding of maths operations in KeOps II

Gradient computation:

```
/////////////////  Autodiff!
  template < class V, class GRADIN >
  using DiffT = Add< typename FA::template DiffT< V, GRADIN >,
                     typename FB::template DiffT< V, GRADIN > >;
};
```

Simplification rule:

```
////////////////  Simplification rules: e.g.
template < class F >
struct Add_Alias0< F, F > { using type = Scal< IntConstant< 2 >, F >; };
```

Combining elementary operations

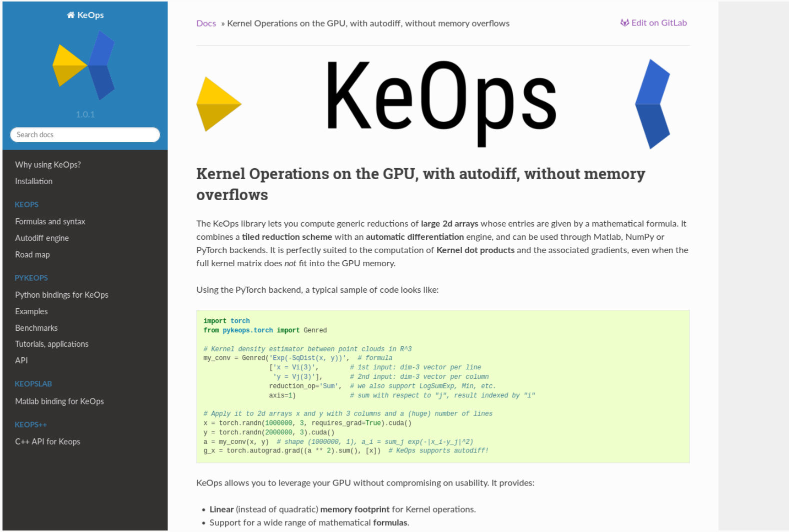
KeOps proposes a wide range of elementary operations

- **Simple vector operations:** scalar product, norm, distance, normalization, vector/vector element-wise operation $(+,-,*,/)$, etc.
- **Elementary $\mathbb{R} \to \mathbb{R}$ functions:** exp, log, inverse, abs, pow, sqrt, sin, cos, etc.
- **Simple matrix operations:** matrix product, tensor product (in Python), etc.
- **Matrix reduction:** sum, min, max, argmin, argmax, etc.

$\to$ a formula = a combination of these operations

Using KeOps

http://www.kernel-operations.io/



KeOps

1.0.1

Search docs

Why using KeOps?
Installation

KEOPS
Formulas and syntax
Autodiff engine
Road map

PYKEOPS
Python bindings for KeOps
Examples
Benchmarks
Tutorials, applications
API

KEOPSLAB
Matlab binding for KeOps

KEOPS++
C++ API for Keops

Docs » Kernel Operations on the GPU, with autodiff, without memory overflows — Edit on GitLab

KeOps

Kernel Operations on the GPU, with autodiff, without memory overflows

The KeOps library lets you compute generic reductions of **large 2d arrays** whose entries are given by a mathematical formula. It combines a **tiled reduction scheme** with an **automatic differentiation** engine, and can be used through Matlab, NumPy or PyTorch backends. It is perfectly suited to the computation of **Kernel dot products** and the associated gradients, even when the full kernel matrix does *not* fit into the GPU memory.

Using the PyTorch backend, a typical sample of code looks like:

```
import torch
from pykeops.torch import Genred

# Kernel density estimator between point clouds in R^3
my_conv = Genred('Exp(-SqDist(x, y))',  # formula
                 ['x = Vi(3)',           # 1st input: dim-3 vector per line
                  'y = Vj(3)'],          # 2nd input: dim-3 vector per column
                 reduction_op='Sum',     # we also support LogSumExp, Min, etc.
                 axis=1)                 # sum with respect to "j", result indexed by "i"

# Apply it to 2d arrays x and y with 3 columns and a (huge) number of lines
x = torch.randn(1000000, 3, requires_grad=True).cuda()
y = torch.randn(2000000, 3).cuda()
a = my_conv(x, y)  # shape (1000000, 1), a_i = sum_j exp(-|x_i-y_j|^2)
g_x = torch.autograd.grad((a ** 2).sum(), [x])  # KeOps supports autodiff!
```

KeOps allows you to leverage your GPU without compromising on usability. It provides:

- **Linear** (instead of quadratic) **memory footprint** for Kernel operations.
- Support for a wide range of mathematical **formulas**.

- doc
- install instructions
- examples

KeOps stack

- Dependencies: `Cmake` ($\leq$3.10), `C++` compiler[1] (g++ $\geq$ 7 or clang) or `cuda` compiler (nvcc $\geq$10) and CUDA libs (for GPU computing)
- Open source (MIT licence): `github.com/getkeops/keops`
- Continuous integration (tested on linux distros and MacOs): Jenkins at `ci.inria.fr`
- Sphinx based documentation on `http://www.kernel-operations.io/`

[1] for CPU computing

KeOps user interface

- PyKeOps: `Python` (`numpy` and `pytorch`)
- KeOpsLab: `Matlab`
- RKeOps: **R** (beta version)
- **C++** API

Example in Python: single Gaussian convolution

We want to compute

$$\gamma_i = \sum_{j=1}^{N} \exp\Big(- s\|\mathrm{x}_i - \mathrm{y}_j\|_2^2 \Big)\, \mathrm{b}_j$$

with $s \in \mathbb{R}$, $[\mathrm{x}_i]_{i=1,\ldots,M} \in \mathbb{R}^{M\times 3}$, $[\mathrm{y}_j]_{j=1,\ldots,N} \in \mathbb{R}^{N\times 3}$ and $[\mathrm{b}_j]_{j=1,\ldots,N} \in \mathbb{R}^{N\times 6}$

Example in Python: single Gaussian convolution

From Python using Numpy (similar in R or Matlab)

```python
from pykeops.numpy import Genred

## compilation on the fly (user-friendly syntax)
my_conv = Genred(
            formula="Sum_Reduction(Exp(-s * SqNorm2(x - y)) * b, 0)",
            aliases=["s = Pm(1)",      # parameter (scalar)
                     "x = Vi(3)",      # vector indexed by i (of dim 3)
                     "y = Vj(3)",      # vector indexed by j (of dim 3)
                     "b = Vj(6)"],     # vector indexed by j (of dim 6)
            dtype='float32')

# assuming s, x, y and b are Numpy arrays (data and parameter values)

## compute directly on the GPU
gamma = my_conv(s, x, y, b)
```

Example in Python (LazyTensor)

Mathematical formula (standard Gaussian kernel)

$$\gamma_i = \sum_{j=1}^{N} \exp\left(\|x_i - y_j\|_2^2\right)$$

with $[x_i]_{i=1,\ldots,M} \in \mathbb{R}^{M\times 3}$, $[y_j]_{j=1,\ldots,N} \in \mathbb{R}^{N\times 3}$

Example in Python (LazyTensor)

Create two arrays with 3 columns and a (huge) number of lines, on the GPU

```
import torch
x = torch.randn(1000000, 3, requires_grad=True).cuda()
y = torch.randn(2000000, 3).cuda()
```

Given the same data tensors `x` and `y`. Use a decorator to turn tensors into KeOps symbolic variables:

```
from pykeops.torch import LazyTensor
x_i = LazyTensor( x[:,None,:] )  # x_i.shape = (1e6, 1, 3)
y_j = LazyTensor( y[None,:,:] )  # y_j.shape = ( 1, 2e6,3)
```

Example in Python (LazyTensor)

```
## Perform symbolic large-scale computations

# Symbolic (1e6,2e6,1) matrix of squared distances
D_ij = ((x_i - y_j)**2).sum(dim=2)

# Symbolic (1e6,2e6,1) Gaussian kernel matrix
K_ij = (- D_ij).exp()

## Get the result (computations on GPU are done here)
a_i = K_ij.sum(dim=1)  # Genuine torch.cuda.FloatTensor
# a_i.shape = (1e6, 1)

## KeOps supports autograd!
g_x = torch.autograd.grad((a_i ** 2).sum(), [x])
```

Example in R

```
formula = "Sum_Reduction(Exp(lambda*SqNorm2(x-y))*beta, 1)"
args = c("x=Vi(3)", "y=Vj(3)", "beta=Vj(3)", "lambda=Pm(1)")

op <- keops_kernel(formula, args) # compilation

# data and paramters
nx = 1000
ny = 1500
x <- matrix(runif(nx*3), ncol=nx)
y <- matrix(runif(ny*3), ncol=ny)
beta <- matrix(runif(ny*3), ncol=ny)
lambda <- as.matrix(5)

# computation
res <- op(args=list(x, y, beta, lambda), nx=ncol(x), ny=ncol(y))
```

Example in R

- beta version
- Gradient computation not available for the moment
- Specific branch `rkeops`

```
git clone https://github.com/getkeops/keops
git checkout rkeops
```

- See `rkeops/REAMD.md` for install instructions

More features (not presented today)

- `PyKeOps (Numpy)`, `KeOpsLab`: formula gradient computation
- `PyKeOps (PyTorch)`: automatic differentiation engine (compatible with PyTorch autograd)
- **In the near future**
  - gradient computation and lazy evaluation in `Rkeops`
  - possible to add new generic operations upon request (responsive user support via Github issues)
  - and more...

Conclusion

Take-home message

KeOps:

Seamless Kernel Operations...

$\rightarrow$ write formulas with simple matrix operations (Python, Matlab, R)

...on GPU...

$\rightarrow$ fast computations

...with auto-differentiation...

$\rightarrow$ automatic gradient computation

...and without memory overflows

$\rightarrow$ implementation with tiling for efficient memory usage on GPU

Thank you for you attention

Questions?

`http://www.kernel-operations.io/keops/index.html`

`https://github.com/getkeops/keops`