KeOps

Seamless Kernel Operations on GPU without memory overflows

B. Charlier[1] J. Feydy[2] J. Glaunès[3] **G. Durif**[1] F.-D. Collin[1]

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[1]IMAG - CNRS - Univ Montpellier, France, [2]Imperial College, London, UK, [3]MAP5 - Univ Paris Descartes, France

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

Outline

1. Introduction
2. Kernel operations and reductions
3. Computation on GPU
4. Implementation
5. Using KeOps

Introduction

What is KeOps?

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

KeOps = “Kernel Operations”

RKeOps

RKeOps = **R** package interfacing KeOps library

What KeOps can do?

Compute **generic reductions** of very large arrays

e.g. row-wise or column-wise matrix sum

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

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

What KeOps can do?

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

$$\downarrow$$

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

What KeOps can do?

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

What KeOps can do?

Compute **kernel reduction**

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

and the associated **gradients**

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

$\rightarrow$ **Intuitively:** $\big[K(\mathbf{x}_i, \mathbf{y}_j)\big] \in \mathbb{R}^{M \times N}$ = matrix whose elements are given by a **formula**

What KeOps can do?

→ manage large dimensions

- even larger than GPU memory
- M and $N \approx 10^4, 10^5, 10^6$

→ fast computation on GPU without memory overflow

Kernels in Statistics and Learning

- Kernel density estimation
- Classification/Regression: SVM, K-NN, etc...
- Kernel embeddings to compare distributions
- Interpolation and Kriging
- Optimal Transport

Motivations

GPU user-friendly computing?

Only a few solution for specific tasks in `R`

See `https://CRAN.R-project.org/view=HighPerformanceComputing` (section GPUs)

Motivations

Over the past 5 years: GPU computing development effort oriented toward deep learning

→ e.g. PyTorch or TensorFlow provide **GPU** implementation of common operations, together with **automatic differentiation**.

Motivations

GPU computing can be used for general purpose computations and not only neural networks

$\rightarrow$ Generic codes to use GPU computing require **low-level tools** (CUDA, OpenCL)

Motivations

Needs: provide an effortless tool for GPU computing

Application: statistics, machine learning and more...

Kernel operations and reductions

Kernel operator

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

(Intuitively)

a **kernel** function = 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 than usual $\mathbb{R}^D$

Kernel operator

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

(Very intuitively)

a kernel function $\approx$ "*similarity measure*"

between $\mathbf{x}_i$ and $\mathbf{y}_j$

(different from Euclidean distance)

Example

Linear kernel

$$K(\mathbf{x}_i, \mathbf{y}_j) = \left\langle \mathbf{x}_i\,,\ \mathbf{y}_j \right\rangle = \mathbf{x}_i^T \mathbf{y}_j = \sum_{k=1}^{D} x_{ik}\, y_{jk}$$

Gaussian kernel

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

Kernel reduction

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

- And more complex operations

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

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 $(\mathbf{y}_j)_j, (\mathbf{v}_j)_j, (\boldsymbol{\beta}_j)_j \in \mathbb{R}^{N \times D}$

Kernel reduction

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

- And more complex operations

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

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 $(\mathbf{y}_j)_j, (\mathbf{v}_j)_j, (\boldsymbol{\beta}_j)_j \in \mathbb{R}^{N \times D}$

Why GPU computing?

Matrix/kernel reduction = combination of generic matrix operations

$\rightarrow$ GPU are good for matrix computations

Computation on GPU

GPUs

PLUS: thousands of computing units

$\rightarrow$ fast with heavily parallelized computations

MINUS: relatively small memory
(compared to the number of computing units)

$\rightarrow$ issue to process large data

Challenge

$$\text{Matrix } \mathbf{K} = \Big[K(\mathbf{x}_i, \mathbf{y}_j)\Big] \in \mathbb{R}^{M \times N} \text{ is very large}$$

$$(M, N \approx 10^4, 10^5, 10^6)$$

$\rightarrow$ store it in memory? **NO!**

$\rightarrow$ how to iterate through rows/columns?

Memory management on GPU

Data initially stored on the host (in RAM)

$\rightarrow$ should be transfered to the device (GPU) for computations (bottleneck)

Different kinds of memory inside the GPU

$\rightarrow$ local (smaller) vs shared (bigger) memory

Memory management on GPU

Smart use of the shared memory

→ less transfer between device and host

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

Tiling implementation

skip example

Tiled implementation

Computations are divided into steps

Data are divided into blocks (called tiles)

Use of accumulators to combine intermediate results from each step on each block

Tiled implementation

Objective for massive parallel computing:

- Shared memory stores data commonly used by all threads during a computation step

  $\rightarrow$ reduce transfers between host and GPU

- Size of data only used by a single thread during a step is reduced (in local memory)

  $\rightarrow$ data locality

Example: matrix product

$$\mathsf{A} = [a_{ij}] \in \mathbb{R}^{M \times N} \text{ and } \mathsf{B} = [b_{jk}] \in \mathbb{R}^{N \times P}$$

$$\mathsf{C} = \mathsf{A}\,\mathsf{B}$$

$$\mathsf{C} = [c_{ik}] \in \mathbb{R}^{M \times P} \text{ and } c_{ik} = \sum_j a_{ij}\, b_{jk} = \langle \mathbf{a}_{i\cdot}, \mathbf{b}_{\cdot k} \rangle$$

Example: matrix product

$$\begin{bmatrix} \cdot & \cdot & \cdot \\ \hline & \mathbf{a}_{i\cdot} & \\ \hline \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}_{M \times N} \times \left[\begin{array}{c|c|c} \cdot & & \cdot \\ \cdot & \mathbf{b}_{\cdot k} & \cdot \\ \cdot & & \cdot \end{array}\right]_{N \times P}$$

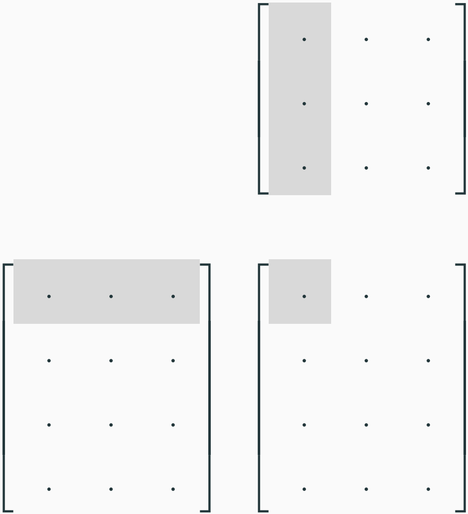
$$= \begin{bmatrix} \cdot & \cdot & \cdot \\ \cdot & \sum_j a_{ij} b_{jk} & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}_{M \times P}$$

Example: matrix product

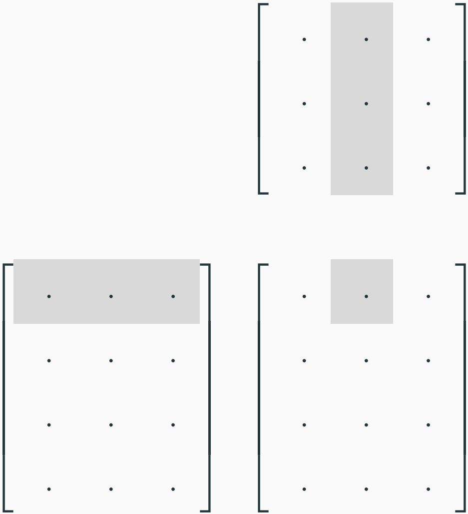
$$
\left[\begin{array}{c|c|c}
\cdot & & \cdot \\
\cdot & \mathbf{b}_{\cdot k} & \cdot \\
\cdot & & \cdot
\end{array}\right]_{N\times P}
$$

$$
\left[\begin{array}{ccc}
\cdot & \cdot & \cdot \\
\hline
 & \mathbf{a}_{i\cdot} & \\
\hline
\cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot
\end{array}\right]_{M\times N}
\qquad
\left[\begin{array}{ccc}
\cdot & \cdot & \cdot \\
\cdot & \sum_j a_{ij} b_{jk} & \cdot \\
\cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot
\end{array}\right]_{M\times P}
$$

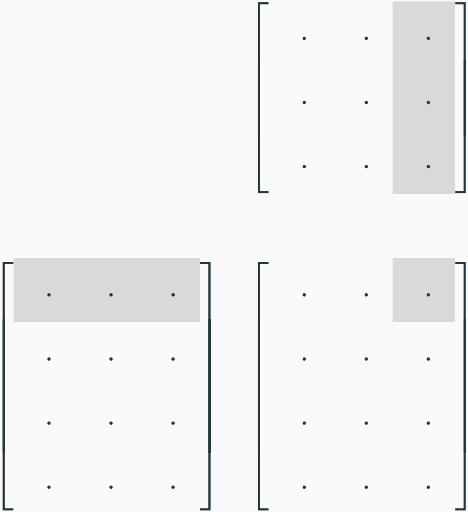
Iterating through rows and columns



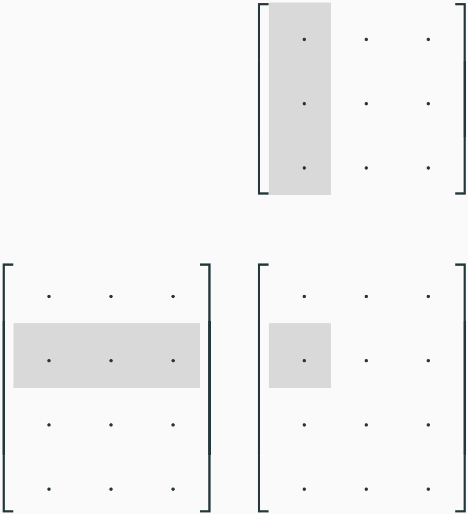
Iterating through rows and columns



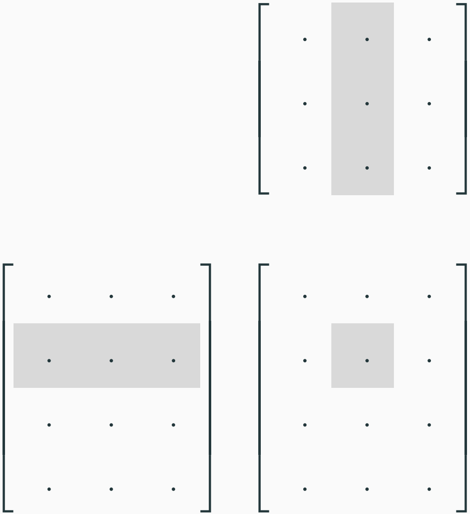
Iterating through rows and columns



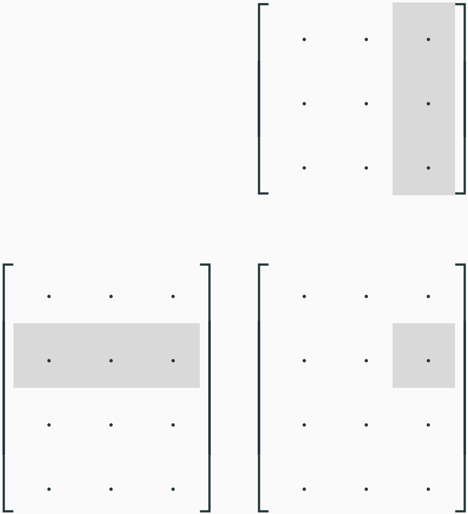
Iterating through rows and columns



Iterating through rows and columns



Iterating through rows and columns



Iterating through rows and columns

and so on…

Parallel matrix product

Thread 1 and thread 2 **work in parallel**

$$\begin{bmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

$$\begin{array}{rc} \text{thread 1 computes } T_1 & \rightarrow \\ \text{thread 2 computes } T_2 & \rightarrow \\ & \\ & \end{array} \begin{bmatrix} \boxdot & \boxdot & \boxdot \\ \triangle & \triangle & \triangle \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix} \begin{bmatrix} T_1 & \cdot & \cdot \\ T_2 & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

= shared data between threads

$\boxdot$ = data only used by thread 1

$\triangle$ = data only used by thread 2

Parallel matrix product

Thread 1 and thread 2 **work in parallel**

$$\begin{bmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

$$\begin{array}{rc} & \\ & \\ \text{thread 1 computes } T_1 \quad \rightarrow & \\ \text{thread 2 computes } T_2 \quad \rightarrow & \end{array} \begin{bmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \boxdot & \boxdot & \boxdot \\ \triangle & \triangle & \triangle \end{bmatrix} \begin{bmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ T_1 & \cdot & \cdot \\ T_2 & \cdot & \cdot \end{bmatrix}$$

= shared data between threads

$\boxdot$ = data only used by thread 1
$\triangle$ = data only used by thread 2

Parallel matrix product

Potential issues if dimension N is large (nb. of columns in matrix **A**)

- $\rightarrow$ parallel threads are asynchronous and have to wait each other before updating shared memory (= using next column of matrix **B**)
- $\rightarrow$ rows of **A** are too large to fit into local memory used by each thread, hence numerous memory transfer

Tiled implementation

Thread 1 and thread 2 **work in parallel**

$$\begin{bmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

thread 1 accumulates over T_{1k}'s $\rightarrow$

thread 2 accumulates over T_{2k}'s $\rightarrow$

$$\begin{bmatrix} \boxdot & \cdot & \cdot \\ \triangle & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix} \begin{bmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

= shared "tile" between threads

$\boxdot$ = "tile" only used by thread 1

$\triangle$ = "tile" only used by thread 2

Tiled implementation

Thread 1 and thread 2 **work in parallel**

$$\begin{bmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

$$\begin{array}{l} \text{thread 1 accumulates over } T_{1k}\text{'s} \quad \rightarrow \\ \text{thread 2 accumulates over } T_{2k}\text{'s} \quad \rightarrow \\ \\ \\ \end{array} \begin{bmatrix} \cdot & \boxdot & \cdot \\ \cdot & \triangle & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix} \quad \begin{bmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

= shared "tile" between threads

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Tiled implementation

Thread 1 and thread 2 **work in parallel**

$$\begin{bmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

$$\begin{array}{ll} \text{thread 1 accumulates over } T_{1k}\text{'s} & \rightarrow \\ \text{thread 2 accumulates over } T_{2k}\text{'s} & \rightarrow \\ & \\ & \end{array} \begin{bmatrix} \cdot & \cdot & \boxdot \\ \cdot & \cdot & \triangle \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix} \begin{bmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

= shared “tile” between threads

$\boxdot$ = “tile” only used by thread 1

$\triangle$ = “tile” only used by thread 2

Tiled implementation

- Tasks (scanning rows $\mathbf{a}_{i\cdot}$) divided into tiles
- All threads use the shared memory within a block
  - $\rightarrow$ a single memory transfer of each tile in $\mathbf{B}$ for all threads
- Accumulation (addition of the intermediate results) when scanning tiles across $\mathbf{A}$

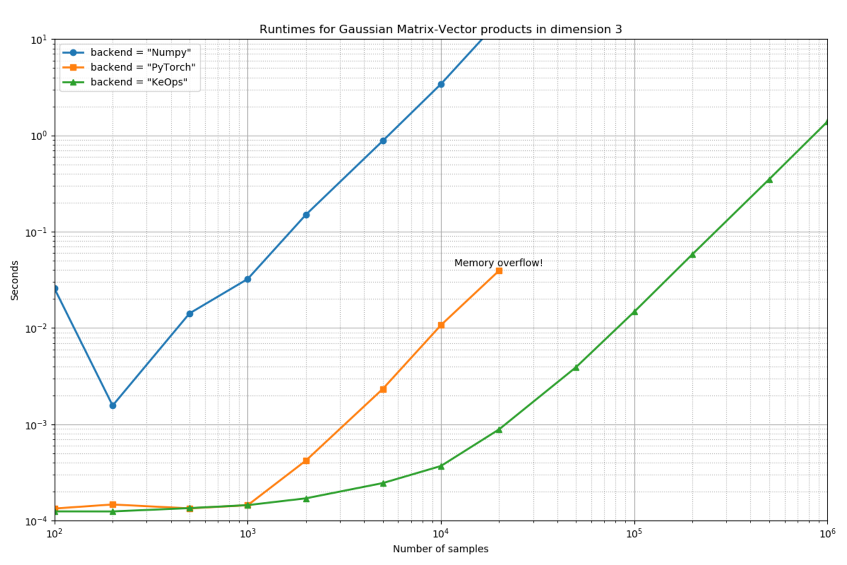
Benchmark

Runtime comparison for Gaussian matrix-vector product on GPU with different data size

- For small sample sizes (up to 10^3): similar performance for KeOps and PyTorch
- For larger sample sizes ($> 10^3$): **KeOps outperforms PyTorch**
- Memory overflow with PyTorch on large sample
- **KeOps** able to process data **larger than GPU memory**

skip benchmark II

Benchmark


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

R specific benchmarks

Runtime comparison between

- standard `R`
- `RKeOps`
- `PyKeOps`
- `PyTorch`

R specific benchmarks

Different tasks

- Matrix-vector product with Gaussian kernel
- Solving Gaussian kernel linear system
- 10-iterations of K-means algorithm
- Exact K-nearest neighbor search

R specific benchmarks

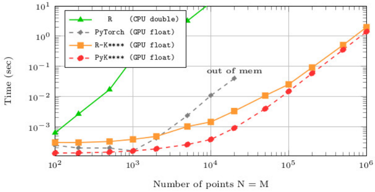
- *RKeOps* outperforms standard *R* and *PyTorch* with very large data sizes

  (except for *K*-means algorithm because of bad implementation)

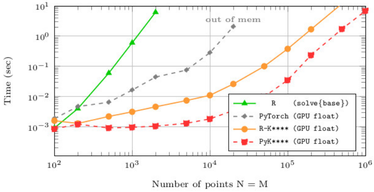
- Memory overflow with PyTorch on large sample

- RKeOps able to process data larger than GPU memory

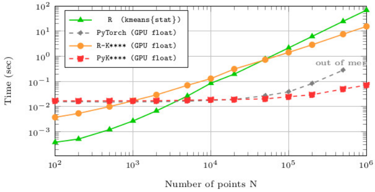
R specific benchmarks



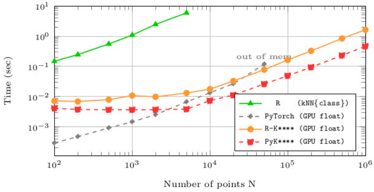
(a) Matrix-vector products with N-by-N Gaussian kernel matrices built from point clouds in dimension $D = 3$.



(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 $\mathbf{x}, \mathbf{y} \in \mathbb{R}^D$:

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

$\rightarrow$ what I want to compute

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

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

$\rightarrow$ what I have to write

Under the hood

The formula F 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

$\rightarrow$ KeOps compiles your operator on the fly to **compute on GPU**

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.

Combining elementary operations

KeOps proposes a wide range of elementary operations

- **Simple matrix operations:** matrix product, etc.
- **Matrix reduction:** sum, min, max, argmin, argmax, etc.

Combining elementary operations

KeOps proposes a wide range of elementary operations

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

Using KeOps

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

- Complete documentation
- Installation instructions (available on CRAN)

```
install.packages("rkeops")
```

- Examples

KeOps stack

https://github.com/getkeops/keops

Open source (MIT licence)

Example in R: single Gaussian convolution

We want to compute

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

with $s \in \mathbb{R}$,

$[\mathbf{x}_i]_{i=1,\dots,M} \in \mathbb{R}^{M\times 3}$, $[\mathbf{y}_j]_{j=1,\dots,N} \in \mathbb{R}^{N\times 3}$

and $[\mathbf{b}_j]_{j=1,\dots,N} \in \mathbb{R}^{N\times 6}$

Example in R: single Gaussian convolution

Compilation on the fly of the operator

```r
library(rkeops)

# implementation of a convolution with a Gaussian kernel
formula = "Sum_Reduction(Exp(-s * SqNorm2(x - y)) * b, 0)"

# definition of input arguments
args = c("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)
         "s = Pm(1)")      # parameter (scalar)

# compilation
op <- keops_kernel(formula, args)
```

Example in R: single Gaussian convolution

Some data

```r
# data and parameter values
nx <- 100
ny <- 150
X <- matrix(runif(nx*3), nrow=nx)   # matrix 100 x 3
Y <- matrix(runif(ny*3), nrow=ny)   # matrix 150 x 3
B <- matrix(runif(ny*6), nrow=ny)   # matrix 150 x 6
s <- 0.2
```

Example in R: single Gaussian convolution

Run computations

```r
# run computations on GPU (optional)
use_gpu()


# computation
# (order of input list similar to `args`)
res <- op(list(X, Y, B, s))
```

Example in R: single Gaussian convolution

Gradient

```
# compile gradient regarding 'x' variable
grad_op <- keops_grad(op, var="x")
```

Conclusion

Take-home message: KeOps

Seamless Kernel Operations...

$\rightarrow$ write formulas with simple matrix operations in R

...on GPU...

$\rightarrow$ fast computations

...with auto-differentiation...

$\rightarrow$ automatic gradient computation

...and without memory overflows

$\rightarrow$ tiling implementation

In the future?

Lazy evaluation in R (example below with PyKeOps)

```
# Symbolic representation of data
x_i = LazyTensor( x[:,None,:] )  # shape (1e6, 1, 3)
y_j = LazyTensor( y[None,:,:] )  # shape ( 1, 2e6,3)

# 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()

## Result (computations on GPU are done here)
a_i = K_ij.sum(dim=1)  # shape (1e6, 1)
```

Thank you for you attention

`https://arxiv.org/abs/2004.11127`
(pending publication)

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

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