Seamless Kernel Operations on GPU without memory overflows

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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 $A = [a_{ij}] \in \mathbb{R}^{M \times N}$)
What KeOps can do?

\[ \sum_{i=1}^{M} a_{ij} \]

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

\[
\begin{bmatrix}
  \cdots & \cdots & \sum_{i=1}^{M} a_{ij} & \cdots & \cdots \\
\end{bmatrix}_{1 \times N}
What KeOps can do?

\[
\begin{bmatrix}
\times & \times & \times & \times & \times & \times & \times \\
\times & \times & \times & \times & \times & \times & \times \\
\times & \times & \times & \times & \times & \times & \times \\
\times & \times & \times & \times & \times & \times & \times \\
\times & \times & \times & \times & \times & \times & \times \\
\times & \times & \times & \times & \times & \times & \times \\
\times & \times & \times & \times & \times & \times & \times \\
\times & \times & \times & \times & \times & \times & \times \\
\end{bmatrix}
\rightarrow
\begin{bmatrix}
\vdots \\
\vdots \\
\vdots \\
\sum_{j=1}^{N} a_{ij} \\
\vdots \\
\vdots \\
\end{bmatrix}
\begin{bmatrix}
M \times N \\
M \times 1 \\
\end{bmatrix}
\]
What KeOps can do?

Compute kernel reduction

\[ \sum_{i=1}^{M} K(x_i, y_j) \quad \text{or} \quad \sum_{j=1}^{N} K(x_i, y_j) \]

and the associated gradients

(for a kernel function \( K \) and some data vectors \( x_i, y_j \in \mathbb{R}^D \))

\( \rightarrow \) Intuitively: \[ [K(x_i, y_j)] \in \mathbb{R}^{M \times N} = \text{matrix whose elements are given by a formula} \]
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?

In R: only a few solution for specific tasks

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

→ 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 \( x_i \) and \( y_j \) in \( \mathbb{R}^D \)

(Intuitively)

a **kernel** function = an application \( K : \mathbb{R}^D \times \mathbb{R}^D \rightarrow \mathbb{R} \)

\[
(x_i, y_i) \mapsto K(x_i, y_i)
\]

corresponding to a **scalar product** between \( x_i \) and \( y_j \) in a different space than usual \( \mathbb{R}^D \)
Kernel operator

Considering some data vector $x_i$ and $y_j$ in $\mathbb{R}^D$

(Very intuitively)

a **kernel** function $\approx \text{“similarity measure”}$

between $x_i$ and $y_j$

(different from Euclidean distance)
Example

**Linear kernel**

\[ K(x_i, y_j) = \langle x_i , y_j \rangle = x_i^T y_j = \sum_{k=1}^{D} x_{ik} y_{jk} \]

**Gaussian kernel**

\[ K(x_i, y_j) = \exp \left( -\frac{1}{2\sigma^2} \| x_i - y_j \|_2^2 \right) \]
Kernel reduction

- **Row-wise or column-wise reduction** on the matrix \( K = [K(x_i, y_j)] \in \mathbb{R}^{M \times N} \)

- And more complex operations

Example:

\[
\sum_{i=1}^{M} K_1(x_i, y_j) K_2(u_i, v_j) \langle \alpha_i ; \beta_j \rangle
\]

for some kernel \( K_1 \) and \( K_2 \), and some \( D \)-vectors \((x_i)_i, (u_i)_i \)
\((\alpha_i)_i \in \mathbb{R}^{M \times D} \) and \((y_j)_j, (v_j)_j, (\beta_j)_j \in \mathbb{R}^{N \times D} \)
Kernel reduction

- **Row-wise or column-wise reduction** on the matrix \( K = \left[ K(x_i, y_j) \right] \in \mathbb{R}^{M \times N} \)

- And more complex operations

Example:

\[
\sum_{j=1}^{N} K_1(x_i, y_j) K_2(u_i, v_j) \langle \alpha_i ; \beta_j \rangle
\]

for some kernel \( K_1 \) and \( K_2 \), and some \( D \)-vectors \((x_i)_i, (u_i)_i\)
\((\alpha_i)_i \in \mathbb{R}^{M \times D} \) and \((y_j)_j, (v_j)_j, (\beta_j)_j \in \mathbb{R}^{N \times D} \)
Matrix/kernel reduction = combination of generic matrix operations

→ GPU are good for matrix computations
Computation on GPU
GPUs

**PLUS**: thousands of computing units

→ fast with heavily parallelized computations

**MINUS**: relatively small memory

(compared to the number of computing units)

→ issue to process large data
Matrix $K = \left[ K(x_i, y_j) \right] \in \mathbb{R}^{M \times N}$ is very large

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

→ store it in memory? NO!

→ how to iterate through rows/columns?
Memory management on GPU

Data initially stored on the host (in RAM)

→ should be transferred to the device (GPU) for computations *(bottleneck)*

Different kinds of memory inside the GPU

→ 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
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
  → reduce transfers between host and GPU

- Size of data only used by a single thread during a step is reduced (in local memory)
  → data locality
Example: matrix product

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

\[ C = A \times B \]

\[ C = [c_{ik}] \in \mathbb{R}^{M \times P} \text{ and } c_{ik} = \sum_j a_{ij} b_{jk} = \langle a_{i.}, b_{.k} \rangle \]
Example: matrix product

\[
\begin{bmatrix}
\ddots & \ddots & \ddots \\
\vdots & a_{ij} & \ddots \\
\vdots & \ddots & \ddots \\
\end{bmatrix}_{M \times N} \times 
\begin{bmatrix}
\vdots & \vdots & \ddots \\
\vdots & b_{jk} & \ddots \\
\vdots & \ddots & \ddots \\
\end{bmatrix}_{N \times P}
\]

= 
\[
\begin{bmatrix}
\ddots & \ddots & \ddots \\
\vdots & \sum_j a_{ij} b_{jk} & \ddots \\
\vdots & \ddots & \ddots \\
\end{bmatrix}_{M \times P}
\]
Example: matrix product

\[
\begin{bmatrix}
\cdots \\
a_{ij} \\
\cdots \\
\end{bmatrix}_{M \times N}
\]

\[
\begin{bmatrix}
\cdots \\
b_{jk} \\
\cdots \\
\end{bmatrix}_{N \times P}
\]

\[
\begin{bmatrix}
\cdots \\
\sum_j a_{ij} b_{jk} \\
\cdots \\
\end{bmatrix}_{M \times P}
\]
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

\[
\begin{bmatrix}
  \cdot & \cdot & \cdot \\
  \cdot & \cdot & \cdot \\
  \cdot & \cdot & \cdot \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
  \cdot & \cdot & \cdot & \cdot \\
  \cdot & \cdot & \cdot & \cdot \\
  \cdot & \cdot & \cdot & \cdot \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
  \cdot & \cdot & \cdot & \cdot \\
  \cdot & \cdot & \cdot & \cdot \\
  \cdot & \cdot & \cdot & \cdot \\
  \cdot & \cdot & \cdot & \cdot \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
  \cdot & \cdot & \cdot & \cdot \\
  \cdot & \cdot & \cdot & \cdot \\
  \cdot & \cdot & \cdot & \cdot \\
  \cdot & \cdot & \cdot & \cdot \\
\end{bmatrix}
\]

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Iterating through rows and columns

and so on...
Parallel matrix product

Thread 1 and thread 2 work in parallel

thread 1 computes $T_1$ → $\begin{bmatrix} \Box & \Box & \Box \\ \Delta & \Delta & \Delta \\ . & . & . \end{bmatrix}$ → $\begin{bmatrix} T_1 & . & . \\ . & . & . \\ . & . & . \end{bmatrix}$

thread 2 computes $T_2$ → $\begin{bmatrix} \Box & \Box & \Box \\ \Delta & \Delta & \Delta \\ . & . & . \end{bmatrix}$ → $\begin{bmatrix} T_2 & . & . \\ . & . & . \\ . & . & . \end{bmatrix}$

= shared data between threads

= data only used by thread 1

= data only used by thread 2
Parallel matrix product

Thread 1 and thread 2 work in parallel

- thread 1 computes $T_1$
- thread 2 computes $T_2$

= shared data between threads

= data only used by thread 1

= data only used by thread 2
Potential issues if dimension $N$ is large (nb. of columns in matrix $A$)

→ parallel threads are asynchronous and have to wait each other before updating shared memory (= using next column of matrix $B$)

→ 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

thread 1 accumulates over $T_{1k}$’s $\rightarrow$ 
thread 2 accumulates over $T_{2k}$’s $\rightarrow$

$\square$ = “tile” only used by thread 1
$\triangle$ = “tile” only used by thread 2

= shared “tile” between threads
Tiled implementation

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

thread 1 accumulates over $T_{1k}$'s  →  \[ \begin{array}{ccc} . & \Box & . \\ . & \triangle & . \\ . & . & . \end{array} \]

thread 2 accumulates over $T_{2k}$'s  →  \[ \begin{array}{ccc} . & . & . \\ T_{21} & T_{22} & T_{23} \\ . & . & . \end{array} \]

= shared “tile” between threads

\(\Box\) = “tile” only used by thread 1
\(\triangle\) = “tile” only used by thread 2
Tiled implementation

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

- Thread 1 accumulates over $T_{1k}$’s
- Thread 2 accumulates over $T_{2k}$’s

= shared “tile” between threads

= “tile” only used by thread 1

= “tile” only used by thread 2
Tiled implementation

- Tasks (scanning rows $a_i$) divided into tiles
- All threads use the shared memory within a block
  - a single memory transfer of each tile in $B$ for all threads
- Accumulation (addition of the intermediate results) when scanning tiles across $A$
Benchmark I

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
Benchmark I

Runtimes for Gaussian Matrix-Vector products in dimension 3

- backend = "Numpy"
- backend = "PyTorch"
- backend = "KeOps"

Memory overflow!
Benchmark II

Runtime comparison between

- standard R
- RKeOps
- PyKeOps
- PyTorch
Different tasks

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

- *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
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 \( \mathbf{x}, \mathbf{y} \in \mathbb{R}^D \):

\[
(x, y) \mapsto \exp\left(\langle x, y \rangle\right)
\]

→ 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))"

→ what I have to write
Under the hood

The formula $F$ is expanded internally in the C++ code using templates:

$$F = \text{Exp}<\text{Scalprod}<X,Y>>$$

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

→ 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

→ a formula = *a combination of these operations*
Using KeOps
• 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

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

with \( s \in \mathbb{R} \),

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

and \( [b_j]_{j=1, \ldots, N} \in \mathbb{R}^{N \times 6} \)
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

```r
# compile gradient regarding 'x' variable
grad_op <- keops_grad(op, var="x")
```
Conclusion
Take-home message: KeOps

Seamless Kernel Operations...

→ write formulas with simple matrix operations in R

...on GPU...

→ fast computations

...with auto-differentiation...

→ automatic gradient computation

...and without memory overflows

→ tiling implementation
In the future?

**Lazy evaluation in R** (example below with PyKeOps)

```r
# 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 your attention

(pending publication)

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

https://github.com/getkeops/keops