K-Means clustering

OpenMP and CUDA

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Final-term assignment

Introduction

Abstract

The goal of this project is to parallelize the K-Means Clustering algorithm and analyze the performance gain with respect to the sequential version.

One parallel versions has been created using the **OpenMP** framework and another using **CUDA** to run on the GPU.

The performance gain is measured in terms of

$$\text{speed-up} = \frac{\text{sequential time}}{\text{parallel time}}$$

Pseudocode

Algorithm 1: K-Means Clustering

Data: k, $max\_iterations$, $observations$
Result: $centroids$, $labels$
1. Select k random $observations$ as starting $centroids$;
while *not* $max\_iterations$ **do**
  foreach $observation$ **do**
    2. Compute the distance between each $centroid$ and $observation$;
    3. Assign $observation$ to closest $centroid$;
  end
  4. Compute new $centroids$ (mean of $observations$ in a cluster);
end

The algorithm can be divided in 4 steps.

The **embarassingly parallel** portion of the algorithm is the **FOR** loop (steps 2. and 3.), every iterarion is independent from one another.

Observations can be distributed among any number of threads.

Implementation

Sequential

The sequential implementation is basically a C++ translation of the pseudocode, with some nuances:

1. o*bservations* and *centroids* are organized as **Structure of Arrays** to improve the alignment with cache lines and benefit of the memory bursts when accessing the various coordinates;

2. step 4. is partially executed in the for loop, in particular the sum required to compute the mean is updated as soon as a point is assigned to a centroid. This avoids having to loop again on every observation.

OpenMP

The directive **#pragma omp parallel for** allows splitting observation indices among threads, so that each one will be assigned a different subset of the dataset.

N = **coresNumber** threads

Thread 1
for (int i=0;
i<datasetSize/N; i++) {
- assign point[i] to centroid
- **update local partial sum**

}

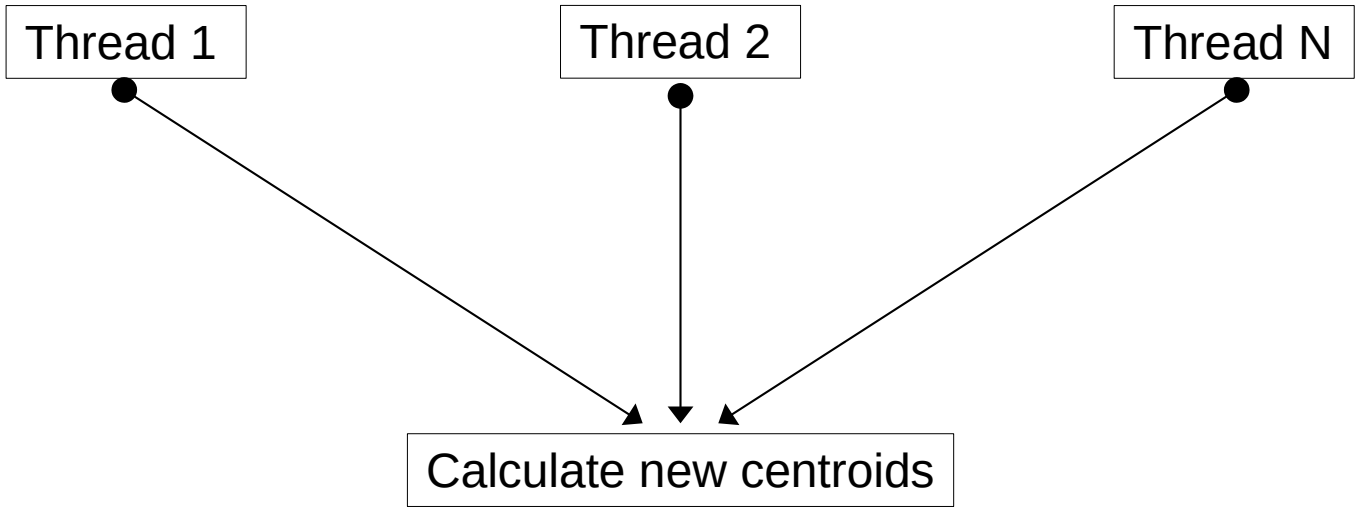
Thread 2
for (int i=datasetSize/N;
i<datasetSize*2/N; i++) {
- assign point[i] to centroid
- **update local partial sum**

}

Thread N
for (int i=datasetSize*(N-1)/N;
i<datasetSize; i++) {
- assign point[i] to centroid
- **update local partial sum**

}

Since a partial sum of points in a cluster is maintained in each thread, a final **reduction** is needed to extract the total sum and be able to compute the mean; this is accomplished with the directive **#pragma omp declare reduction(...)** which allows to specify a reduction function to conglomerate the data of each thread.



CUDA

Each thread is assigned a **single** *observation*, this way, the FOR loop can be removed and so the maximum parallelization possible is achieved.

N = **datasetSize** threads

Thread idx=1 • assign point[idx] to centroid • **atomically update global partial sum**	Thread idx=2 • assign point[idx] to centroid • **atomically update global partial sum**	Thread idx=N • assign point[idx] to centroid • **atomically update global partial sum**

Step 1. is done on the host.
Two kernels are used to complete step 2., 3. and 4.

```
Kernel 1:
   assign points to centroids
   update partial sums

cudaDeviceSynchronize();

Kernel 2:
   use final sums to calculate new centroids
```

Two kernels are necessary because the whole *grid* needs to be synchronized to get final sums.

The memory management is as follows:

• *observations* and *centroids* are copied from host to device global memory

At each kernel execution:
• *centroids* are pulled by threads into shared memory
• threads atomically update sums into global memory

• When final *centroids* are found, structures are copied back to host.

Tests

Hardware:

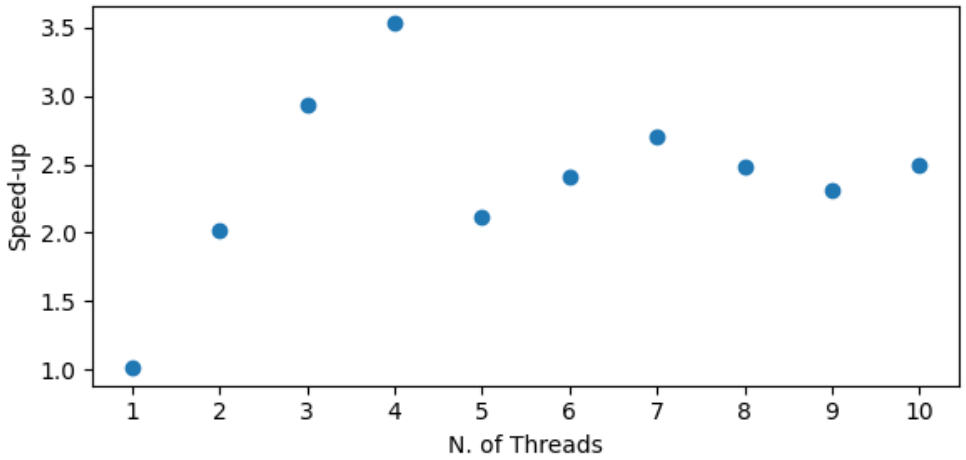
- CPU Intel Core i5-4670 (4-core)
- GPU Nvidia GeForce GTX 770 (compute capability 3.0)

Dataset:

- Number of elements: 100,000
- Points dimension: 2

OpenMP

The parallel program was run with varying number of threads with the purpose to find the optimum value.

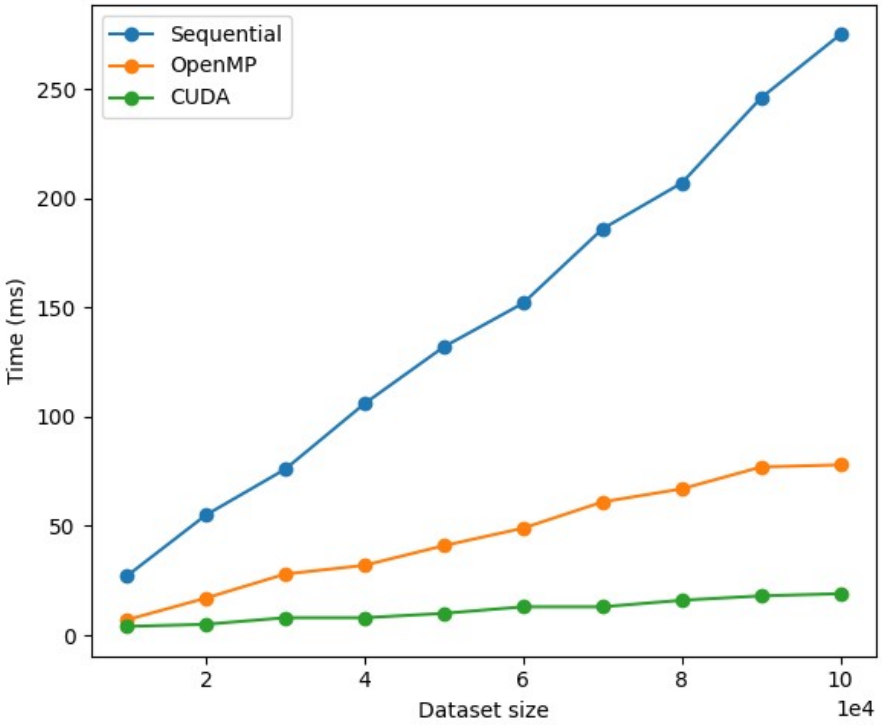


Max speed-up: **3.53** with **4** threads

Around **2.4** with more threads

CUDA

Tests have been made with increasing dataset size to appreciate the scaling of the various parallelization methods.



Max speed-up: **14.47**
with 100k elements

Scaling to dataset size:
- Sequential: **linear**
- OpenMP: **linear**
- CUDA: **sub-linear**