

Comparison between a sequential and multi-thread version of the k-Nearest Neighbors problem

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Abstract—Retrieving the *k*-Nearest Neighbors in a given dataset is a very common problem. Due to the inherent highly parallelizable structure of the problem, it's possible to speed up the search by using a multi-core CPU or a GPU. In this study, we try to investigate how much we can speed up the search task when implementing the algorithm in OpenMP/CUDA, compared to the C++ sequential version. We discuss the results for different dataset sizes and different threads number.

Index Terms—k-Nearest Neighbors, parallel computing, OpenMP, CUDA

I. INTRODUCTION

Given a dataset \mathcal{D} of N points $x_i \in \mathbb{R}^n$, a test point $q \in \mathbb{R}^n$ and a distance measure d , the *k*-Nearest Neighbors problem (k-NN) is to find the k points closest to q in \mathcal{D} , i.e. find an ordered subset \mathcal{S} of \mathcal{D} such that:

- $\mathcal{S} = \{x_{i_1}, x_{i_2}, \dots, x_{i_k}\}$
- $j < h \implies d(q, x_{i_j}) \leq d(q, x_{i_h})$
- $d(q, x_{i_j}) \leq d(q, x_m), \forall x_{i_j} \in \mathcal{S}, \forall x_m \in \mathcal{D} \setminus \mathcal{S}$

Such a problem is very common in pattern recognition: an algorithm that solves k-NN can be used as a subroutine inside a method that addresses a *classification* or a *regression* task.

In other words, in the case where each dataset point x_i is associated with a value y_i , the correspondences obtained with k-NN can be used to learn how to approximate the unknown function $f: x \rightarrow y$, for any x .

Approaches

There are many possible approaches to solve the k-NN problem: the simplest one (naive approach) consists in calculate distances of all dataset points from the query, and select only the smallest distances after sorting; other approaches like [1] [2] or something that try construct data structures (such as k-d trees) that allow reducing the number of points from which it is necessary to calculate the distance [3]. In this study, we use the naive version because we are not interested in obtaining the state of the art performance, but only in seeing the potential of implementing highly parallelizable algorithms on GPU.

Variants

The k-NN problem formulation can be slightly relaxed to reduce even more the execution times of the searches. One example is *Approximate Nearest Neighbors* (a-NN): in this variant, we allow the finding of k-Near Neighbors, which don't

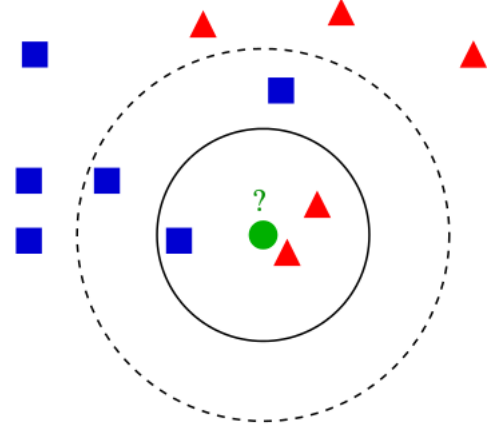


Fig. 1. Example of a k-NN problem: the circle represents the query of which find nearest neighbors. All the others are the dataset points. In this case, every dataset point is associated with information (shape/color) that can be used for other tasks, after finding the nearest neighbors.

have to be the *nearest*. The algorithms that solve ANN take advantage of techniques and data structures (such as *locality-sensitive hashing*) that make the search stochastic. For these type of algorithms is also important the *quality* of the search results, measured ad example with the *recall* metric.

We do not investigate these types of algorithms in this paper.

II. IMPLEMENTATIONS

A. Sequential Version

For the sequential version of the k-NN problem we use the simple (naive) implementation: given a query, we calculate the euclidean distance from each point in the dataset. After that, we sort the array of points by increasing distance: finally, the first k elements in the ordered array are the nearest neighbors of the query.

As sorting algorithm we use *qsort*, the implementation of quicksort included in *stdlib*.

The pseudocode is reported in Algorithm 1.

B. Parallel OpenMP Version

The OpenMP [6] version is similar to the sequential one. The differences are the parallelization of the calculation of the distances and the sorting. The parallelization of the sorting implies a subsequent merge procedure.

Algorithm 1: k-Nearest Neighbors - Sequential version

Input : dataset, query, k
Output: nearestNeighbors

```
1 // init
2 indexes = new int[dataset.size]
3 distances = new float[dataset.size]
4 // calculate distances
5 for p from 0 to dataset.size-1 do
6   indexes[p] = p
7   distances[p] = euclideanDistance(query, dataset[p])
8 end
9 // sort by increasing distance
10 sortByKey(indexes, keys=distances)
11 // slice
12 nearestNeighbors = indexes[:k]
```

The pseudo-code is reported in Algorithm 2: here, details about border effects (due to data split among threads) are omitted; furthermore, it is intended that all assignments of arrays are deep copies.

Algorithm 2: k-Nearest Neighbors - OpenMP version

Input : dataset, query, k, numThreads
Output: nearestNeighbors

```
1 // init
2 indexes = new int[dataset.size]
3 distances = new float[dataset.size]
4 chunkSize = dataset.size / numThreads
5 // calculate distances
6 # pragma omp parallel for
7 for p from 0 to dataset.size-1 do
8   indexes[p] = p
9   distances[p] = euclideanDistance(query, dataset[p])
10 end
11 // sort chunks by increasing distance
12 # pragma omp parallel for
13 for j from 0 to numThreads-1 do
14   s = j * chunkSize
15   e = s + chunkSize
16   sortByKey(indexes[s:e], keys=distances[s:e])
17 end
18 // merge sorted chunks
19 for j from 1 to numThreads-1 do
20   i, d = indexes[:k], distances[:k]
21   s = j * chunkSize
22   e = s + k
23   indexes[:k], distances[:k]
24   =merge(i,d,indexes[s:e],distances[s:e])
25 end
26 // slice
27 nearestNeighbors = indexes[:k]
```

C. Parallel CUDA Version

The CUDA version differs from the previous mainly because we need to take care of memory transfers between CPU and GPU. Moreover, since GPU threads are very efficient, we launch the kernel that calculates the distances with as many threads as many elements in the dataset: each thread is responsible to calculate the distance from the query to one single dataset element.

As sorting algorithm we use *sort_by_key*, a sorting algorithm included in *thrust* that allows ordering on GPU.

The pseudo-code is reported in Algorithm 3.

Algorithm 3: k-Nearest Neighbors - CUDA version

Input : dataset, query as q, k, bSize
Output: nearestNeighbors

```
1 // init
2 indexes = new int[dataset.size]
3 distances = new float[dataset.size]
4 // move query to GPU memory
5 q = toGPU(q)
6 // determine the number of blocks
7 blocks = (datasetSize + bSize - 1) / bSize
8 // calculate the distances
9 idxs,dists=cudaDistances<<<blocks,bSize>>>(dataset,q)
10 // sort by increasing distance on GPU
11 sortByKeyOnGPU(idxs, keys=dists)
12 // slice and move results to CPU memory
13 nearestNeighbors = toCPU(idxs[:k])
```

III. SETUP

All the experiments are done in C++14, the output is a csv file. The graphs are obtained with Python3 using the matplotlib library.

A. Test configuration

We test our code in a laptop with this configuration:

- CPU: Intel Core i7-8750H, 6 cores / 12 threads
- GPU: NVIDIA GeForce GTX 1050 Ti (Notebook), 768 CUDA cores, 4 GiB video RAM
- RAM: 16 GiB
- CUDA: 10.0
- OpenMP: 4.5

B. Compilation

A full compilation requires the use of the *nvcc* compiler and the *OpenMP* library. However, if one or both of them aren't available, our *CMakeLists.txt* automatically allows a partial compilation.

For the experiments, we compile the code using all available compiler optimizations (-O3) to achieve better performances, taking advantage of techniques like loop vectorization when possible.

IV. EXPERIMENT

We set k (number of *Nearest Neighbors*) to 100 for all tests. When calculating the wall clock time of the algorithms, we distinguish between *initialization time* (required only once) and the time needed to answer all queries (*evaluation time*).

As comparison metrics, we calculate the **wall clock time** for all three algorithms and we report the **speedup** obtained by the parallel versions compared to the sequential version. The *speedup* S is defined as the ratio between the evaluation time of the sequential version t_S and the evaluation time of the parallel version t_P , i.e. $S = t_S/t_P$.

We calculate these metrics in many different configurations: distinct configurations have a different *number of dataset examples* and/or a different *number of threads* for the parallel versions. In particular, the number of threads goes from 1 to 6 for the *OpenMP* version, while for *CUDA* we try different setting (32, 64, 128, 256, 512, 1024) of the number of threads per block (a.k.a. *block size*).

When varying the number of threads, we use all dataset examples. When varying the number of dataset examples, we use the maximum number of threads for the *OpenMP* version, and the best block size setting for the *CUDA* version.

The output of the experiment is a *.csv* file that contains a row for each different configuration. Then, this file is read by a Python script that generates the plots reported in the *Results* section.

A. Dataset

The experiments are made on two SIFT datasets [4], which are sets of 128-dimensional vectors. Each of these vectors is a feature vector that describes local properties in an image.

This dataset is usually used in pattern recognition: keypoints of objects are first extracted from a set of reference images; for each keypoint, the SIFT descriptor is calculated and stored in a database. Objects in a new image are recognized by individually comparing each feature from the new image to this database and finding candidate matching features based on Euclidean distance of their feature vectors: here is where k-NN comes into play.

Each of the two SIFT datasets used in our tests comprises 3 main components:

- *query*: the vectors of which to find nearest neighbors
- *base*: the vectors in which the search is performed
- *groundtruth*: indexes of true nearest neighbors for queries

The first dataset (*siftsmall*) has 10000 base vectors and 100 query vectors each of them with its 100 nearest neighbors. The second dataset (*sift*) has 1000000 base vectors and 10000 query vectors each of them with its 10000 nearest neighbors.

We use the small dataset to verify the correctness of our algorithms. Then we switched to the bigger dataset to run all the tests.

V. RESULTS

Table I reports the results of the experiment: for each different setting, are reported the processing unit, the number of threads (intended per block for the GPU), the dataset size

TABLE I
RESULTS OF THE EXPERIMENT (TIMES IN SECONDS)

hw	threads	dataset_size	init_time	eval_time	total_time
cpu	1	10000	0.001	17.387	17.389
cpu	6	10000	0.001	4.345	4.346
gpu	16	10000	0.439	2.802	3.241
gpu	32	10000	0.034	2.656	2.690
gpu	64	10000	0.034	2.730	2.764
gpu	128	10000	0.034	2.770	2.804
gpu	256	10000	0.044	2.758	2.802
gpu	512	10000	0.062	2.822	2.885
gpu	1024	10000	0.034	2.822	2.856
cpu	1	50000	0.007	93.854	93.861
cpu	6	50000	0.006	19.909	19.915
gpu	16	50000	0.176	9.061	9.238
gpu	32	50000	0.171	8.449	8.620
gpu	64	50000	0.171	8.643	8.814
gpu	128	50000	0.172	8.607	8.780
gpu	256	50000	0.191	8.630	8.821
gpu	512	50000	0.204	8.729	8.933
gpu	1024	50000	0.203	8.852	9.054
cpu	1	150000	0.021	293.606	293.627
cpu	6	150000	0.021	69.687	69.708
gpu	16	150000	0.526	26.279	26.805
gpu	32	150000	0.556	24.368	24.924
gpu	64	150000	0.564	25.010	25.574
gpu	128	150000	0.594	25.021	25.615
gpu	256	150000	0.534	25.005	25.539
gpu	512	150000	0.562	24.930	25.492
gpu	1024	150000	0.532	24.970	25.502
cpu	1	450000	0.064	914.098	914.163
cpu	6	450000	0.063	193.692	193.755
gpu	16	450000	1.740	74.733	76.473
gpu	32	450000	1.648	69.471	71.120
gpu	64	450000	1.645	71.850	73.495
gpu	128	450000	1.659	71.807	73.466
gpu	256	450000	1.639	71.343	72.982
gpu	512	450000	1.644	71.175	72.819
gpu	1024	450000	1.670	70.966	72.635
cpu	1	1000000	0.144	2087.270	2087.410
cpu	2	1000000	0.139	1087.240	1087.380
cpu	3	1000000	0.140	767.498	767.638
cpu	4	1000000	0.139	613.098	613.237
cpu	5	1000000	0.141	508.506	508.647
cpu	6	1000000	0.138	461.747	461.885
gpu	16	1000000	3.610	164.362	167.972
gpu	32	1000000	3.533	153.298	156.831
gpu	64	1000000	3.552	158.413	161.964
gpu	128	1000000	3.577	157.963	161.540
gpu	256	1000000	3.564	157.053	160.617
gpu	512	1000000	3.538	157.434	160.972
gpu	1024	1000000	3.569	156.956	160.525

(number of vectors in the search space) and elapsed times to answer all the queries (divided into *init_time* and *eval_time*). From these data, we generate the subsequent plots to better visualize the results. To create the plots, we consider only the evaluation time, whereas the initialization time it's not used.

A. OpenMP

In Figure 2 we show the evaluation time for the OpenMP version of k-NN when the number of threads is varying. We observe that the evaluation time for the parallel OpenMP version decreases when the number of threads increases, as expected.

In Figure 3 we show the speedup of the OpenMP version of k-NN (w.r.t. the sequential version) when the number

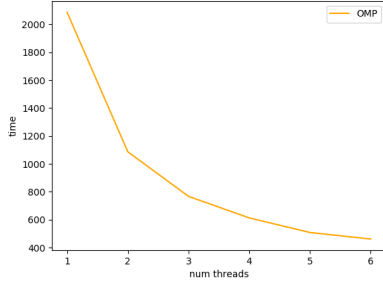


Fig. 2. Evaluation time for the OpenMP version of k-NN, in function of the number of threads.

of threads is varying. The speedup of the parallel OpenMP version increases when the number of threads increases, as expected. The speedup we got is sub-linear.

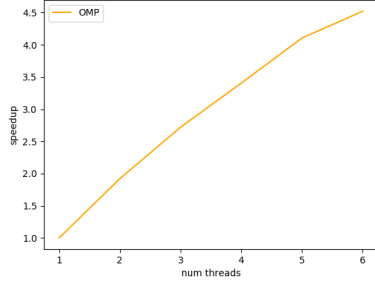


Fig. 3. Speedup of the OpenMP version of k-NN, in function of the number of threads.

B. CUDA

In Figure 4 we show the evaluation time for the CUDA version of k-NN when the number of threads per block is varying.

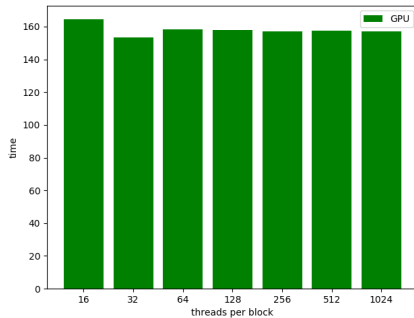


Fig. 4. Evaluation time for the CUDA version of k-NN, in function of the number of threads per block.

In Figure 5 we show the speedup of the CUDA version of k-NN (w.r.t. the sequential version) when the number of threads per block is varying.

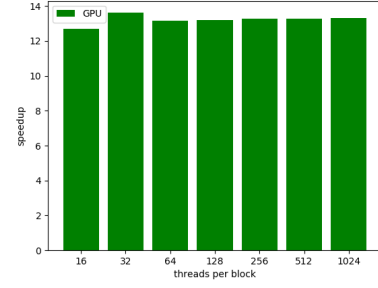


Fig. 5. Speedup of the CUDA version of k-NN, in function of the number of threads per block.

We can observe that the block size in the CUDA k-NN is not much relevant for the evaluation time in the test we have done. In our opinion, the reason why the time does not change very much is that the GPU used in our tests has 6 Streaming Multiprocessors only: even with a big block size (and so a not very big number of blocks), it's easy to occupy all the Streaming Multiprocessors.

However, the kernel that calculates the distances requires a bigger time compared to sorting time and time for data transfer + synchronization between CPU and GPU. We verify this using Valgrind tools (in particular *Callgrind* and *KCachegrind*) [5], this tool show the elapsed time in every *statement* of our code.

C. Comparison

In this comparison, we set the maximum number of threads (6) for the OpenMP version and the best blockSize (1024) for the CUDA version. In Figure 6 we show the comparison between the evaluation time of the three versions (sequential, OpenMP, CUDA) of k-NN when the dataset size is varying.

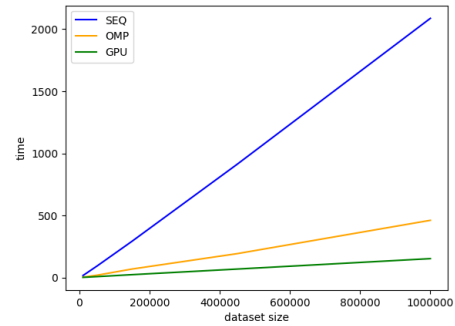


Fig. 6. Comparison between the evaluation time of the three versions (sequential, OpenMP, CUDA) of k-NN, in function of the dataset size.

As expected, we can observe that the *Evaluation time* increases almost linearly in function of the dataset size. The asymptotic computational complexity of the sequential version is $\Theta(n \log(n))$: $\Theta(n)$ for the calculation of Euclidean distances from every query node to all the dataset nodes, and $\Theta(n \log(n))$ for the subsequent sorting.

In Figure 7 we show the comparison between the speedup of the two parallel versions (OpenMP, CUDA) of k-NN (w.r.t. the sequential version) when the dataset size is varying.

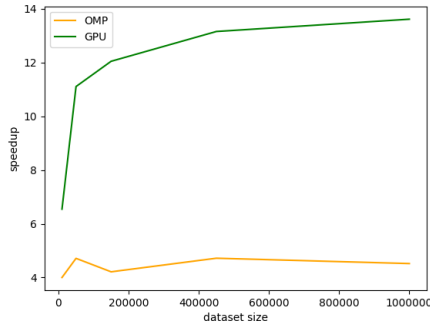


Fig. 7. Comparison between the speedup of the two parallel versions (OpenMP, CUDA) of k-NN, in function of the dataset size.

In particular, the CUDA version performs better than the OpenMP version even when the dataset is very small, and when varying the dataset size the difference in performance is even more pronounced.

VI. CONCLUSION

In this study, we evaluate the performance of different implementations of the *k-Nearest Neighbors* algorithm to better understand the potentiality of parallel computing. We observed that substantial performance gain can be obtained with both the OpenMP and CUDA parallel version, w.r.t. the simple sequential algorithm.

We obtained a sublinear speedup with OpenMP: the time of the sequential version turned out to be 4.5 times bigger than that of the OpenMP version with 6 threads (equal to the number of cores of the CPU used).

With CUDA, the speedup obtained was about 13.5 times, therefore much higher than that obtained with OpenMP.

Parallelizing with OpenMP is a relatively simple task, and it doesn't have much impact on the general structure of the code, so we believe there is no reason not to parallelize the code whenever possible. Parallelizing with CUDA requires greater and specific technical knowledge but allows to obtain potentially higher speedups: this is especially useful in contexts where performance is a crucial requirement of the software, for example in the analysis of large quantities of data in realtime.

Parallelism is gaining broader interest due to the need for processing an increasing quantity/dimension of data. Substantially improve single-core performance is difficult and therefore we believe that in the future more and more applications will take advantage of parallelism techniques to exploit the full performance of the computational resources.

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- [5] Valgrind is an instrumentation framework for building dynamic analysis tools. There are Valgrind tools that can automatically detect many memory management and threading bugs, and profile your programs in detail. You can also use Valgrind to build new tools. Url: <https://valgrind.org>
- [6] OpenMP <https://www.openmp.org>
- [7] CUDA <https://developer.nvidia.com/cuda-zone>