

In-memory k Nearest Neighbor GPU-based Query Processing

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Abstract: The k Nearest Neighbor (k -NN) algorithm is widely used for classification in several application domains (medicine, economy, entertainment, etc.). Let a group of query points, for each of which we need to compute the k -NNs within a reference dataset to derive the dominating feature class. When the reference points volume is extremely big, it can be proved challenging to deliver low latency results. Furthermore, when the query points are originating from streams, the need for new methods arises to address the computational overhead. We propose and implement two in-memory GPU-based algorithms for the k -NN query, using the CUDA API and the Thrust library. The first one is based on a Brute Force approach and the second one is using heuristics to minimize the reference points near a query point. We also present an extensive experimental comparison against existing algorithms, using synthetic and real datasets. The results show that both of our algorithms outperform these algorithms, in terms of execution time as well as total volume of in-memory reference points that can be handled.

1 INTRODUCTION

Modern applications utilize big spatial or multidimensional data. Processing of these data is demanding and the use of parallel processing plays a crucial role. Parallelism based on GPU devices is gaining popularity during last years (Barlas, 2014). A GPU device can host a very large number of threads accessing the same device memory. In most cases, GPU devices have much larger numbers of processing cores than CPUs and faster device memory than main memory accessed by CPUs, thus, providing higher computing power. GPU devices that have general computing capabilities appear in many modern commodity computers. Therefore, GPU-devices can be widely used to efficiently compute demanding spatial queries.

Since GPU device memory is expensive in comparison to main memory, it is important to take advantage of this memory as much as possible and scale-up to larger datasets and avoid the need for costly distributed processing. Distributed processing suffers from excessive network cost which sometimes overcomes the benefits of distributed parallel execution.

The k Nearest Neighbor (k -NN) algorithm is widely used for classification in many problems areas (medicine, economy, entertainment, etc.). For example, k -NN classification has been used for economic

forecasting, including bankruptcy prediction. (Chen et al., 2011) present a model for bankruptcy prediction using adaptive fuzzy k -NN, where k and the fuzzy strength parameter are adaptively specified by particle swarm optimization, while (Cheng et al., 2019) use k -NN for predicting financial distress (a key factor for bankruptcy).

Let a group of query points, for each of which we need to compute the k -NNs within a reference dataset to derive the dominating feature class. When the reference points volume is extremely big, it can be proved challenging to deliver low latency results and GPU-based techniques may improve efficiency. Furthermore, when the query points are originating fast from streams, the computational overhead is even larger and the need for new parallel methods arises.

In this paper, We propose and implement two in-memory GPU-based algorithms for the k -NN query, using the CUDA API (NVIDIA, 2020) and the Thrust library (Barlas, 2014). The first one is Brute-force based and the second one is using heuristics to minimize the reference points near a query point.

We also present an extensive experimental comparison against existing algorithms, using synthetic and real datasets. The results show that both of our algorithms outperform these algorithms, in terms of execution time as well as total volume of in-memory

reference points that can be handled.

The rest of this paper is organized as follows. In Section 2, we review related work and present the motivation for our work. Next, in Section 3, we present the new algorithms that we developed for the k -NN GPU-based Processing and in Section 4, we present the experimental study that we performed for studying the performance of our algorithms and for comparing them to their predecessors. Finally, in Section 5, we present the conclusions arising from our work and discuss our future plans.

2 RELATED WORK AND MOTIVATION

In this section, we review the most representative algorithms to solve k -NN queries in GPU. k -NN is typically implemented on GPUs using *brute force* (BF) methods applying a two-stage scheme: (1) the computation of distances and (2) the selection of the nearest neighbors. For the first stage, a distance matrix is built grouping the distance array to each query point. In the second stage, several selections are performed in parallel on the different rows of the matrix.

There are different approaches for these two stages. In (Kuang and Zhao, 2009), the distance matrix is split into blocks of rows and each matrix row is sorted using radix sort method. In (Garcia et al., 2010), the previous distance matrix calculation scheme is used, but insertion sort method is applied instead of radix sort. (Liang et al., 2009) uses the same approach as (Kuang and Zhao, 2009) and (Garcia et al., 2010) to compute the distance matrix and, for the selection phase, they calculate a local k -NN for each block of threads and obtain a global k -NN by merging. In (Komarov et al., 2014), for the matrix computation uses the (Kuang and Zhao, 2009) and (Garcia et al., 2010) scheme and modifies the selection phase with a quicksort-based selection. Each block performs a selection operation with a large number of threads per block. In (Sismanis et al., 2012), the truncated sort algorithm was introduced in the selection phase.

In (Arefin et al., 2012), the *GPU-FS-kNN* algorithm was presented. It divides the computation of the distance matrix into squared chunks. Each chunk is computed using a different kernel call, reusing the allocated GPU-memory. A selection phase is performed after each chunk is processed.

In (Gutiérrez et al., 2016), an incremental neighborhood computation that eliminates the dependencies between dataset size and memory is presented. The iterative process copies several reference point

subsets into the GPU. Then, the algorithm runs the local neighborhood search to find the k nearest neighbors from the query points to the reference point subsets. Merging candidate result sets with new reference point subsets is used to reach the final solution.

In (Barrientos et al., 2011), a GPU heap-based algorithm (called Batch Heap-Reduction) is presented. Since it requires large shared memory, it is not able to solve k -NN queries for high k values. In (Barrientos et al., 2017), new approaches to solving k -NN queries in GPU using exhaustive algorithms based on the selection sort, quicksort and state-of-the-art heaps-based algorithms are presented.

(Kato and Hosino, 2012) proposes a new algorithm that is also suitable for several GPU devices. The distance matrix is split into blocks of rows. Each thread computes the distances for a row. Parallel threads push new candidates to a max-heap using atomic operations. (Masek et al., 2015) presents a multi-GPU implementation of a k -NN algorithm.

In (Li and Amenta, 2015), a new BF k -NN implementation is proposed by using a modified inner loop of the SGEMM kernel in MAGMA library, a well-optimized open source matrix multiplication kernel. This brute force k -NN approach has been used in (Singh et al., 2017) to accelerate calibration process of a k -nearest neighbors classifier using GPU.

Some of these algorithms (like the ones of (Garcia et al., 2010) and their improved implementations (Garcia et al., 2018)) consume a lot of device memory, since a Cartesian product matrix, containing the distances of reference points to the query points, is stored. In this paper, we present alternative algorithms that focus on maximizing the total reference points stored in the device memory, which could accelerate execution by avoiding the creation of extra (unnecessary) data chunks and could scale-up to larger reference datasets.

3 k -NN GPU-BASED ALGORITHMS

In this section, we present the two new algorithms that we developed and implemented using this library.

3.1 Thrust Brute-force

The first method is based on a “brute force” algorithm (Fig.1), using the Thrust library (denoted by T-BF). Brute force algorithms are highly efficient when executed in parallel. The algorithm has two input parameters, a dataset R consisting of m reference points $R = \{r_1, r_2, r_3, \dots, r_m\}$ in a 3d space and a dataset Q of

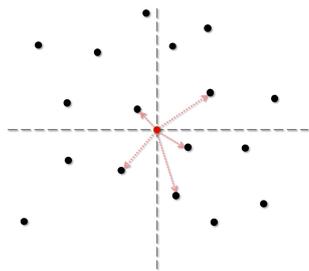


Figure 1: Query point (red), $k = 5$ nearest neighbors (black).

n query points $Q = \{q_1, q_2, q_3 \dots q_n\}$ also in a three-dimensional space. For every query point $q \in Q$, the following steps are executed:

1. Calculate all the Euclidean distances between the query point q and the reference points $r \in R$. Store the calculated distances in a dataset D consisting of m distances $D = \{d_1, d_2, d_3 \dots d_m\}$
2. Sort the distances D dataset
3. Create the KNN dataset K of the k nearest neighbor points
 $K = \{k_1, k_2, k_3 \dots k_k\}$. These points contain the sorted distances as well as the R dataset indices.

After n repetitions, all the KNN points will be calculated. Although the BF is perfectly suitable for a GPU implementation, we noticed that the sorting step is extremely GPU computationally bound. The CUDA profiler revealed the 90% (or more in large datasets) of the GPU computation is dedicated to sorting.

3.2 Thrust Distance Refinement

The aforementioned method T-BF is memory efficient and well-performing but when the reference dataset is extremely big, the distance sorting step deteriorates the overall performance. This observation led us to our next implementation, which radically refines the nearest reference points.

The main concept of distance refinement method (denoted by T-DS) is that we can calculate the number of reference points by searching in concentric ranges. We count the reference points of each concentric range until the total points counted exceed the needed k points.

Our first approach was to search in concentric rings of equal width. The width of the ring l is constant and is calculated as k times double the maximum width of reference points area $tmax$, divided by the number of reference points tp .

$$l = k * 2t * tmax / tp$$

Experimentation revealed that this approach was only efficient in dense and uniformly distributed reference

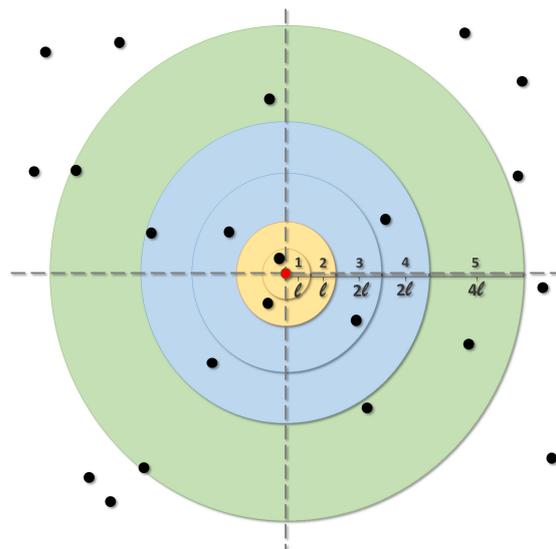


Figure 2: Distance Refinement, query point in red, reference points in black, $k = 10$.

points without gaps. When we used synthetic or real data, the results were the same or only a bit better than the T-BF method. The problem was that the search area did not scale quickly enough.

On our second approach, we used a hybrid area incrementation step. Every two search rings, we doubled the search ring width (Fig.2). This way the search increment was semi-exponential. The algorithm can scale quickly and produce excellent results for all kinds of datasets.

By refining the initial dataset, we create a very small intermediate dataset that contains at least k reference points. This dataset will be used in the costly sorting part of the algorithm and will speed up the execution time (as we will experimentally show).

The algorithm has two input parameters, a dataset R consisting of m reference points $R = \{r_1, r_2, r_3 \dots r_m\}$ in a three-dimensional space and a dataset Q of n query points $Q = \{q_1, q_2, q_3 \dots q_n\}$ also in a three-dimensional space. For every query point $q \in Q$, the following steps are executed:

1. Calculate the starting ring width l
2. Calculate all the Euclidean distances between the query point q and the reference points $r \in R$. Store the calculated distances in a dataset D consisting of m distances $D = \{d_1, d_2, d_3 \dots d_m\}$
3. While the count of reference points c is less than equal of k repeat
 - (a) If $repetition \% 2 = 0$, count the distance points of the area ring between the circles with radius $repetition * l$ and $(repetition + 1) * l$
 - (b) If $repetition \% 2 = 1$, count the distance points

of the area ring between the circles with radius $repetition * l$ and $(repetition + 1) * l$. Double the ring width $l = 2 * l$

4. Refine the distance points of less than or equal to distance $(repetition + 1) * wr$ and copy them to dataset DR consisting of c distances $DR = \{dr_1, dr_2, dr_3..dr_c\}$
5. Sort the distances DR dataset
6. Create the KNN dataset K of the k nearest neighbor points
 $K = \{k_1, k_2, k_3..k_k\}$. These points contain the sorted distances as well as the R dataset indices.

After n repetitions, all the KNN points will be calculated. For example in Figure 2, we calculated a distance refinement of radius $4l$ resulting to a total of 12 distance points.

4 EXPERIMENTAL STUDY

We run a large set of experiments to compare the repetitive application of the existing algorithms and the newly implemented ones for processing batch KNN queries. All experiments query at least 100K reference points. We did not include less than 100K reference points because we target the maximum in-memory utilization and reference point less than 100K do not fit in this context. The maximum reference points limit is 200M, which only our algorithm T-DS achieved.

We have created random and synthetic clustered datasets of 100.000, 250.000, 500.000 and 1.000.000 points. All the existing methods could only be executed with 100.000 reference points and only one of them scaled to 1.000.000 points. Furthermore, in order to check our method scaling we also created random datasets of 10.000.000, 100.000.000 and 200.000.000 reference points. We also used three big real datasets (Eldawy and Mokbel, 2015), which represent water resources of North America (Water Dataset) consisting of 5.836.360 line-segments and world parks or green areas (Parks Dataset) consisting of 11.503.925 polygons and world buildings (Buildings Dataset) consisting of 114.736.539 polygons. To create sets of points, we used the centers of the line-segment MBRs from Water and the centroids of polygons from Park and Build. For all datasets the 3-dimensional data space is normalized to have unit length (values [0, 1] in each axis).

We run a series of experiments searching for 20 Nearest Neighbors ($k = 20$), using the aforementioned datasets with groups of 1,10,100,250,500,750 random query points. Every experiment was run at least 10

times and the mean of the experiment results were calculated for every method.

All experiments were performed on a Dell Inspiron 7577 laptop, running Windows 10 64bit, equipped with a quad-core (8-thread) Intel I7 CPU, 16GB of main memory, a 256SSD disk used for the operating system, a 1TB 7.2K SATA-3 Seagate HDD storing our data and a NVIDIA Geforce 1060 (Mobile Max-Q) GPU with 6GB of memory.

We run experiments to compare the performance of batch KNN queries, regarding execution time as well as memory utilisation. We tested a total of five algorithms. Three of them are existing ones and the other two are the new algorithms we implemented. The list of algorithms is as follows:

1. BF-Global, Brute Force algorithm using the Global memory (Garcia et al., 2010)
2. BF-Texture, using the GPU texture memory (Garcia et al., 2018)
3. BF-Cublas, using CUBLAS (BLAS highly optimized linear algebra library) (Garcia et al., 2010)
4. T-BF, Brute Force algorithm using Thrust library
5. T-DS, Distance Refinement algorithm using Thrust library

4.1 Random Reference Points

In our first series of tests, we used random datasets for the reference points. We created the datasets in various volumes using normalized random points. The resulting datasets' density increased analogously to the reference points cardinality. The datasets created are near uniformly distributed.

In the first chart (Fig. 3) with one query point, we can see that our algorithms T-BF and T-DS are extremely faster than the other methods. For one query point T-BF finished in 0,53ms and T-DS in 0,59ms for the 100K reference points experiment. The best of the other methods was BF-Texture achieving 39,68ms. It worths mentioning that the 100K experiment was the only one that BF-Texture and BF-Cublas finished. These two methods (BF-Texture and BF-Cublas) could not scale at higher volumes of reference points, mainly due to execution exceptions regarding memory allocation problems. For the 1M reference points experiment the execution time difference is much greater, the BF-Global implementation finished in 369,18ms while T-BF finished in 3,61ms and T-DS in 0.92ms. The maximum speedup gain that T-DS achieved was 529 (times faster) than BF-Global, at 750K reference points (Table 1).

In the second chart with 10 query points, we can observe about the same results as with the one query

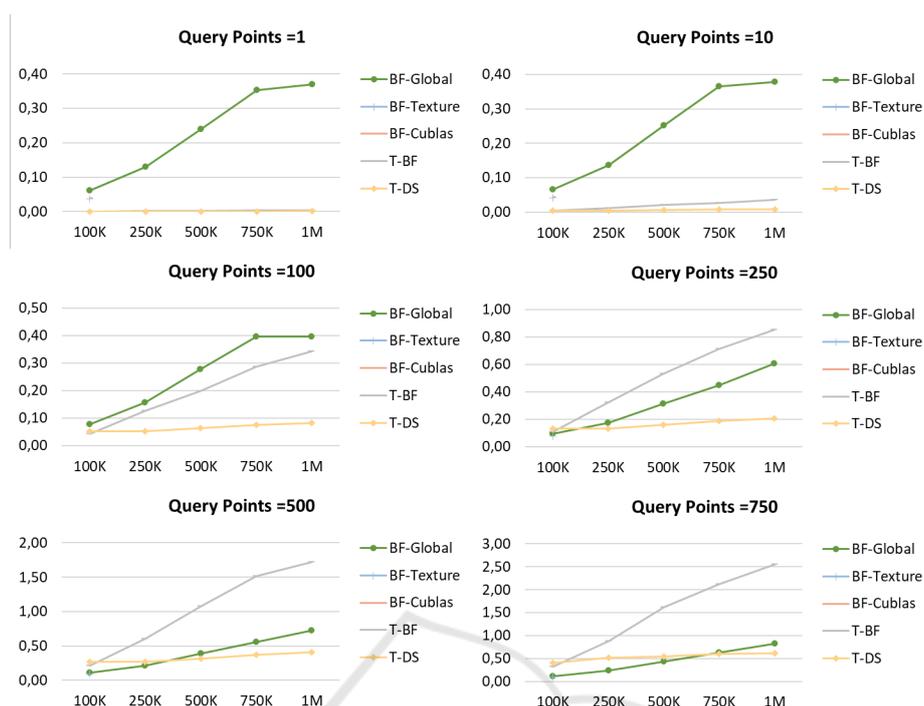


Figure 3: Random reference points, $k = 20$. X-axis: reference point cardinality, Y-axis: execution time measured in ms.

Table 1: Speedup gain of new methods T-BF, T-DS versus BF-Global, using Random dataset.

Algo-rithm	Query Points	Random Reference Points				
		100K	250K	500K	750K	1M
T-BF	1	117,27	101,69	123,58	122,25	102,41
T-DS	1	104,33	251,95	405,79	529,63	401,72
T-BF	10	15,36	11,62	11,98	13,82	10,47
T-DS	10	12,88	26,07	41,74	48,79	45,64
T-BF	100	1,80	1,24	1,40	1,38	1,15
T-DS	100	1,46	3,03	4,26	5,21	4,86
T-BF	250	0,86	0,54	0,59	0,63	0,71
T-DS	250	0,69	1,33	1,94	2,39	2,93

experiment. At 100K reference points, the best of existing algorithms was again BF-Texture, finishing at 40ms, while T-BF finished at 4.29ms and T-DS at 5.11ms. For the 1M reference points experiment the execution time difference is again much greater, the BF-Global implementation finished in 377,91ms while T-BF finished in 36.11ms and T-DS in 8.28ms. T-DS was 45 times faster than BF-Global.

When reaching the group of 100 query points, we can see that the execution time of T-BF is a slightly better than the BF-Global. The overhead of sorting large volumes of distance datasets begin to emerge. The T-DS on the other hand continued its excellent performance, finishing in 81.8ms at 1M reference points, while BF-Global finished in 397.42ms.

In the following experiments, using groups of

250,500 and 700 query points, T-BF performance was inferior compared to BF-Global. The T-DS algorithm kept on outperforming the other ones, especially on the large volumes of reference points.

In order to explore the limits of the algorithms, we created random datasets ranging from 10M to 200M reference points (Fig. 4). The existing algorithms could not scale higher than 1M reference points. The T-BF reached 100M reference points. The only algorithm that succeeded in 200M reference points is T-DS. T-BF using one query point, executed in 10M reference points in 28.96ms and T-DS in just 4.07ms. The T-DS finished in the 200M reference points experiment in 61.93ms. The 10 points query group, resulted analogously in 291.93ms for T-BF and 37.08ms for T-DS. All the other experiments resulted to close linear performance, in respect to query points groups. The T-DS implementation executed 10 times faster than the T-BF one, in extremely large volumes of reference datasets.

In terms of memory scaling the new algorithm T-DS can compute up to 200M reference points. The maximum reference points that other methods could achieve are 1M reference points, thus our methods can scale up to 200 times more than the other ones. It worths mentioning that T-DS is much faster than T-BF, because of the sorting overhead of T-BF.

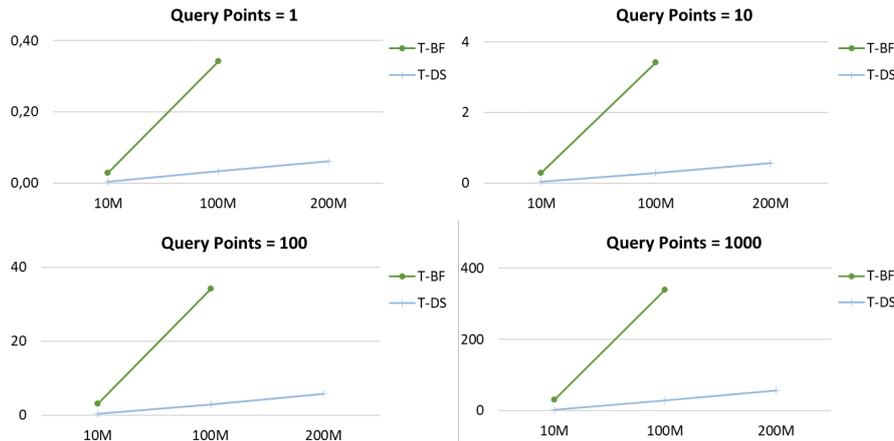


Figure 4: Maximum reference points, $k = 20$. X-axis: reference point cardinality, Y-axis: execution time measured in ms.

4.2 Synthetic Reference Points

We have also used synthetic datasets following different data distributions, and each data set contains 100,000, 250,000, 500,000, 750,000 and 1,000,000 points (Fig. 5). We have created these datasets because they are not uniformly distributed, like the random ones and they resemble real-life data distributions. The synthetic reference points datasets are created according to Zipf's law. The Zipf distribution is defined as follows, and the value of z that we have used is 0.7.

$$f(i) = \frac{\frac{1}{i^z}}{\sum_{j=1}^n \frac{1}{j^z}}, i = 1, 2, \dots, n$$

The random experiment results are confirmed in this experiment. In the one query point experiment, in ascending order, T-BF finished in 0.48ms, T-DS in 0.65ms, BF-Texture in 49,76ms, BF-Global in 62.04ms and BF-Cublas in 74.41ms, for the 100K reference dataset. The 1M experiment resulted to T-DS 2.18ms, T-BF 3.56ms and BF-Global 367.57ms. The maximum speedup gain that T-DS achieved was 270 (times faster) than BF-Global, at 750K reference points (Table 2).

The 10 query point experiment resulted to a similar outcome. The T-DS again was faster and outperformed BF-Global by 25 times. When the query points reached up to 100, we noticed that the performance of T-BF is similar and slightly better than BF-Global. On the other hand T-DS is still performing good, especially for $\geq 500K$ reference points. Finally in the 250 query points experiment, BF-Global surpasses T-BF, but is still slower than T-DS algorithm.

For one more time, T-DS is much faster than T-BF, because of the sorting advantage reduction, as documented in the previous section.

Table 2: Speedup gain of new methods T-BF,T-DS versus BF-Global, using Synthetic dataset.

Algo- rithm	Query Points	Synthetic Reference Points				
		100K	250K	500K	750K	1M
T-BF	1	128,45	89,87	101,04	118,75	103,25
T-DS	1	94,57	134,70	196,90	270,53	168,76
T-BF	10	15,64	9,02	9,52	13,22	10,86
T-DS	10	10,34	11,56	20,48	25,04	24,58
T-BF	100	1,82	1,06	1,02	1,44	1,10
T-DS	100	1,20	1,21	1,94	3,65	2,54
T-BF	250	0,82	0,58	0,64	0,68	0,70
T-DS	250	0,54	0,66	1,25	1,44	1,74

4.3 Real Reference Points Comparison

We conducted 6 experiments using three different real datasets using groups of query points of 10 and 100 points (Fig. 6). In order to compare all the algorithms we created two reference datasets of 100K and 1M points per every real dataset, by reducing them (the real datasets) uniformly.

The only experiment that all the algorithms completed, is the one with 100K reference points. The BF-Texture and BF-Cublas algorithm failed in all subsequent experiments. The fastest algorithm in the 100K case was T-BF, finishing in 4.53ms (Water), 4.38ms (Parks) and 4.36ms (Buildings), while querying 10 points and 43.78ms (Water), 43.99ms (Parks) and 41.1ms (Buildings) while querying 100 points. In the case of 1M reference points the T-DS was slightly faster than T-BF. When we queried the hole datasets the T-DS was about 2 times faster than T-BF.

The maximum speedup gain that T-DS achieved was 391 (times faster) than BF-Global, at 1M water reference points, using one query point (Table 3). Furthermore, in the real dataset example, we certify once more that T-DS is much faster than T-BF, because of the sorting advantage.

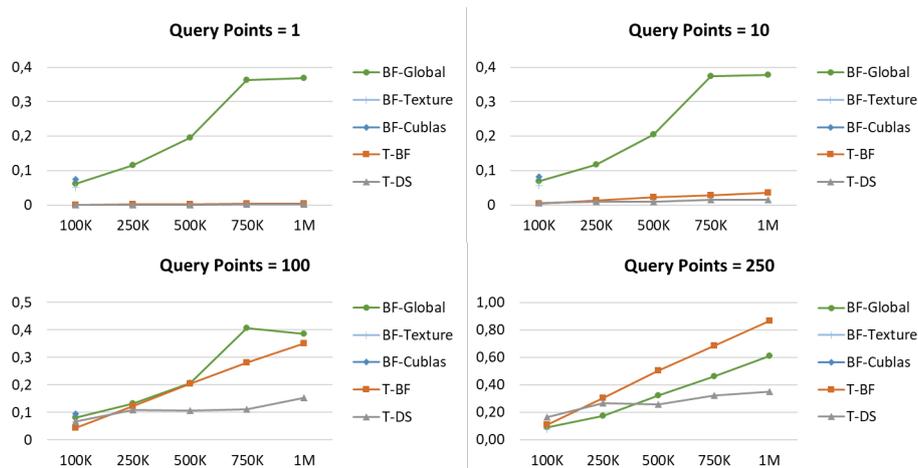


Figure 5: Synthetic reference points, $k = 20$. X-axis: reference point cardinality, Y-axis: execution time measured in ms.

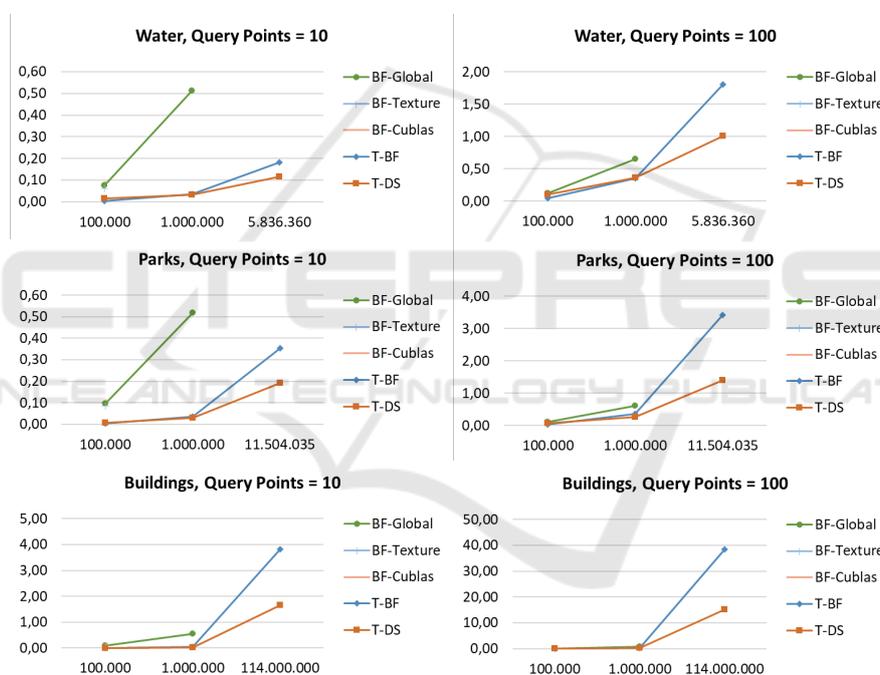


Figure 6: Real reference points, $k = 20$. X-axis: reference point cardinality, Y-axis: execution time measured in ms.

Table 3: Speedup gain of new methods T-BF,T-DS versus BF-Global, using Real datasets.

Algorithm	Query Points	Water Ref. Points		Parks Ref. Points		Buildings Ref. Points	
		100K	1M	100K	1M	100K	1M
T-BF	1	120,98	135,49	128,43	131,26	119,25	136,10
T-DS	1	38,31	391,19	74,74	102,16	78,85	352,03
T-BF	10	16,71	14,55	22,33	14,54	23,81	15,64
T-DS	10	5,55	15,73	11,07	16,95	10,97	32,28
T-BF	100	2,72	1,84	2,52	1,71	4,00	1,98
T-DS	100	1,14	1,81	1,53	2,31	2,19	3,22
T-BF	250	1,51	1,02	1,37	0,76	1,50	0,89
T-DS	250	0,61	1,08	0,79	1,04	0,80	1,47

5 CONCLUSIONS AND FUTURE PLANS

In this paper, we presented new algorithms for k -NN query processing in GPUs. These algorithms maximize the utilization of device memory, handling more reference points in the computation. Through an experimental evaluation on synthetic and real datasets, we concluded that these algorithms, not only work faster than existing methods for small groups of query points, but also scale-up to much larger reference datasets. Moreover we validated that T-DS algorithm is faster than T-BS, because of the extra refinement step minimizing the sorting overhead.

Future work plans include:

- Comparison of our algorithms to other algorithms in the literature, regarding execution time and scaling-up within the available device memory,
- Combination of GPU-based algorithms to data stored in SSDs, using smart transferring of data between the SSD, RAM and device memory (Roumelis et al., 2016) (without indexes), (Roumelis et al., 2019) (using indexes),
- Testing the effectiveness of our algorithms on data from other application domains, e.g. financial data (Cheng et al., 2019),
- Implementation of queries (like K -closest pairs), based techniques utilized in this paper.

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