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Accelerating Nearest-Neighbours via KD-Trees on GPUs

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7.5 ECTS, Project Outside Course Scope

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May 1, 2020

Contents

1 Introduction

Computing KNN is the core of many applications in various fields, such as Computer Vision and Machine Learning. The naive approach of computing KNN is using brute force, and while brute force is efficient when dealing with small datasets, such as in the hundreds, it is inefficient for larger datasets due to its complexity $O(n \times m)$, where n is the size of the reference point dataset and m is the size of the query set.

The idea of computing KNN by k-d trees is to construct a spatial data-structure, which is a binary tree, where each internal node semantically corresponds to a subset of the reference points that can be reached through them, while keeping the number of comparisons asymptotically cheaper than the $O(n \times m)$.

The original direction of this project was inspired by (He & Sun, 2012) who propose a solution for efficiently computing approximate nearest-neighbours (ANN) computations using propagation-assisted k-d trees. While there exists other approaches, such as PatchMatch (Barnes, Shechtman, Finkelstein, & Goldman, 2009) and Coherency Sensitive Hashing (Korman & Avidan, 2016), currently (He & Sun, 2012) is proven to be the most efficient approximate solution.

The performance bottleneck is typically the search for K-nearest neighbours (KNN). Various methods have been used to solve this problem, such as using the k-means tree, the bbd-tree and the k-d tree, and while both the k-means tree and the bbd-tree are more accurate than the k-d tree, they have significantly more overhead in building the trees. For instance, the building time for the k-means tree is 10-20 times more than for the k-d tree (He & Sun, 2012).

We found that in order to implement such algorithms, we would still need all the components of the exact KNN computations by k-d trees as we would for the approximate solution. Thus, for this project, it was commonly agreed to concentrate on the exact KNN computation solution.

In our approach, the leaves contain a set of reference points in the hundreds, to which we apply brute force at the leaf level. Computing the KNN for a query requires traversing the tree in which each visit to each node determines whether it is necessary to visit the next node, or to skip it.

In principal, the k-d tree solution reduces the asymptotic work to a factor of $O(m\ lg\ n)$, but in practice, the efficiency of the solution depends fundamentally on the dimensionality and the size of K. While the solution offers a cheaper traversal it still suffers from the curse of high dimensionality.

To address the curse of high dimensionality, we present a more accurate test that, in several cases, allows to efficiently process queries of higher dimensionality, than the classical approach. While the typical solution decides to visit the second node by computing the distance between the query to the current median on one dimension, against the distance to the worst nearest-neighbour, this solution considers the upper and lower bounds of all dimensions.

Additional optimisation, such as improving temporal locality, have been done by sorting the queries such that they access the same leaves in the same order, when performing brute force.

In section 4, the performances of the optimisations are demonstrated. Here we see that using sorting to improve temporal locality, particularly achieves performance gains on large datasets of high dimensionality. In table 1, we experiment with dimensionality D=9 and datasets of roughly size 2 million, in which we achieve a speed-up of almost 5, regardless of the size of K.

The optimisations on the traversal are proven to increase the performance 4.3 times more on dimensionality D=12 as opposed to D=6, on datasets of roughly size 4 million, visible in figure 8. In table 2, we see a speed-up of 4.5 for D=12, K=5 on a dataset of roughly size 1 million, and if we increase K=17, the speed-up is 4.3.

When comparing how many leaves are visited for each of the traversal solutions in section 4.2.1, we see that the optimised version performs much fewer visits to additional leaves. Thus it explains very well the increased performance.

Comparing brute force against the fully optimised implementation of exact KNN computations with k-d trees, we achieve an incredible speed-up, particularly for datasets of roughly size 4 million. with D=2 and K=12, the speed-up is 78.7, and for D=8 we achieve a speed-up of 17.6. See table 3.

The report is structured as follows. Section 2 elaborates the background of computing KNN with k-d trees. Section 3 goes into the implementation details of brute force, the tree construction, the tree traversal and the application as a whole. Section 4 demonstrates the performances gained by the solutions described in section 3, and section 5 concludes the whole project.

The code can be found at `https://github.com/smhyatt/kdann`.

1.1 Acknowledgements

Acknowledgements go to Cosmin Oancea for his contribution with some of the following key ideas used in this project.

- Constructing the tree with padding, allowing regular nested parallelism.
- Optimising the tree traversal, such that the stack is represented as one integer.
- Optimising the tree traversal to check all dimensions, rather than one, resulting in fewer traversals due to the increased accuracy.

Additional acknowledgements go to Fabian Gieseke for providing a full Python implementation of approximate nearest-neighbours computations using propagation-assisted k-d trees, on two images.

2 Background

KNN is used find the K nearest neighbours in some dimensionality D, and it is widely applied due to its simplicity and excellent empirical performance, it has no training phase and it works well handling multi-dimensional datasets.

We look at a D dimensional space, where we have a set of reference points of size n, and a set of queries of size m, and we aim to compute the nearest neighbours according to a measured distance for each query.

The naive approach is using brute force, in which each reference point is compared with each query, meaning the complexity of the search will be $O(m \times n)$. The brute force approach is explained further in section 3.1. Although brute force is a simple solution, there exists several alternative techniques for computing KNN. One commonly applied method is using a generalisation of the binary tree, known as the k-d tree.

The k-d tree consists of a root, internal nodes and leaves. The reference points are fully partitioned, such that all the internal nodes on each level represent all reference points. Two nodes on the same level do not intersect in terms of the reference points they represent. The leaves do not necessarily contain one reference point each, they may contain several reference points, and in our approach we apply brute force on the leaves.

Using a k-d tree improves search performance, where in principal the average work complexity is $O(m \ \log \ n)$ (Friedman, Bentley, & Finkel, 1977).

The goal is to implement the solution using Futhark since Futhark is a pure functional data-parallel array language, that works efficiently on the GPU. It is a great advantage to write fully parallel code in a high-level functional language. However, since Futhark utilises regular parallelism it does not support recursion. With this in mind, the pseudo-code, demonstrated next, will need to be rewritten without divide-and-conquer recursion, which is demonstrated in the sections 3.2 and 3.3.

2.1 Pseudo-code for the Computing KNN using k-d Trees

Algorithms 1, 2 and 3 below represent an implementation of the k-d tree construction and the tree traversal as high-level pseudo-code. Both Algorithms 2 and 3 use divide and conquer recursion. Algorithm 1 is the `main` function in which a k-d tree is created of the reference points, and iterations through the queries call `TRAVERSE` to find the best neighbours for query.

Algorithm 1 Main

```
1: procedure MAIN(k, queries, refs)
2:     $tree \leftarrow$ BUILDTREE($refs, refs.idxs, 0, 0,$ NONE)
3:     $neighbours \leftarrow$ NONE
4: foreach query in queries do:
5:     $neighbours \leftarrow$ TRAVERSE($tree,\ query,\ 0,\ neighbours,\ k$)
6: return neighbours
```

2.2 Construction the Tree

Algorithm 2 represents the construction of the k-d tree. The tree construction is divided into two stages; one that processes the internal nodes (lines 3-18) and another the handles the leaves (lines 19-20). The condition is implemented by comparing the current level with the tree height, and if the two are equal, it means that we have reached the leaves.

For a given node, at any given node level the reference points are partitioned by finding the dimension with the widest spread across the points represented by that node, and choosing the median value of that dimension. The left child of that node will represent the first half of the reference points in sorted order, and the right child of that node will represent the rest. The nodes, therefore, contain a dimension and a median value. Line 4 uses the function GetSplitDimension to find the dimension of widest spread, lines 5-6 sort the indices and patches w.r.t the chosen dimension and lines 8-9 pick out the median index and value. Once done, the median and the dimension are ready to be stored, which essentially creates that particular node of the tree. Lines 12-18 compute the indices of the left and right children of the current node for the next iteration, and recursively call the BuildTree function again, in order to complete the creation of nodes in the tree.

Last, lines 20-21 sorts the leaves w.r.t the indices that were sorted and partitioned throughout the recursive node creation.

Algorithm 2 Building the Tree

```
1: procedure BuildTree(refs, indices, depth, index, tree)
2:
3:     if IsLeaf(depth) then
4:         $dim \leftarrow$ GetSplitDimension($refs$)
5:         $indices \leftarrow$ SortByDim($indices, dim$)
6:         $points \leftarrow refs[indices]$
7:
8:         $medianIdx \leftarrow$ Length($indices$)$/2$
9:         $median \leftarrow points[medianIdx]$
10:
11:        $tree[index] \leftarrow (median, dim)$
12:        $depth \leftarrow depth + 1$
13:
14:        $leftIdx \leftarrow$ GetLeftChild($index$)
15:        $rightIdx \leftarrow$ GetRightChild($index$)
16:
17:        BuildTree($points[: medianIdx], indices[: medianIdx], depth, leftIdx, tree$)
18:        BuildTree($points[medianIdx :], indices[medianIdx :], depth, rightIdx, tree$)
19:    else
20:        $leaves[index].refs \leftarrow refs$
21:        $leaves[index].idxs \leftarrow indices$
```

2.3 Tree Traversal

The traversal is presented in Algorithm 3 below. Each query is going to traverse the k-d tree, and at each internal node in the tree, it is going to decide whether it has to visit a certain child by making a conservative test to whether the KNN can possibly be improved in the regions that that node represents. If a leaf is reached, a brute force is performed w.r.t the query and all the reference points represented in that leaf, this is shown in line 2-4. The rest of the code corresponds to the recursive traversal, lines 6-21.

Algorithm 3 The Tree Traversal

```
 1: procedure TRAVERSE(tree, query, nodeIndex, neighbours, k)
 2:     if IsLeaf($nodeIndex$) then
 3:         $neighbours \leftarrow$ BRUTEFORCE($tree, query, nodeIndex, neighbours, k$)
 4:         return neighbours
 5:
 6:     $dimens \leftarrow tree[nodeIndex].dims$
 7:     $median \leftarrow tree[nodeIndex].meds$
 8:     $queryV \leftarrow query[dimens]$
 9:
10:     if queryV <= median then
11:         $first \leftarrow$ GOLEFT($nodeIndex$)
12:         $second \leftarrow$ GORIGHT($nodeIndex$)
13:     else
14:         $first \leftarrow$ GORIGHT($nodeIndex$)
15:         $second \leftarrow$ GOLEFT($nodeIndex$)
16:
17:     $neighbours \leftarrow$ TRAVERSE($tree$, $query$, $first$, $neighbours$, $k$)
18:     $worstNeighbour \leftarrow$ LAST OF $neighbours$
19:
20:     if (median - queryV) < worstNeighbour then
21:         $neighbours \leftarrow$ TRAVERSE($tree$, $query$, $second$, $neighbours$, $k$)
22:   return neighbours
```

The code denotes by first, the child of the current node that is on the same side as median w.r.t the query, similarly second denotes the child of the current node that is on the opposite side of the median. This can be observed between the computations on lines 10-15. If the query value of the current dimension is less than the median of the current node, then first is the left child, and right otherwise.

If we reach this node, then since the query is on the same side as the current median, as the node denoted first, one recursive call is always going to be made, because it means that we can always reach a leaf that potentially has a neighbour better than the worst one found so far.

The recursive call that follows the second node is not necessarily made, since it is guarded by a conservative condition that tests whether the distance from the query to the current median is better than the worst found neighbour so far. If this condition does not hold, it is safe not to visit the left child, because it is ensured that no better neighbours can be found, which is visible in lines 20-21.

2.4 Related Work

2.4.1 PatchMatch

PatchMatch uses a randomised algorithm for quickly finding approximate nearest neighbour fields (ANNF) between image patches.

While previous solutions use KD-Trees with dimensionality reduction, PatchMatch instead searches through a 2D space of possible patch offset. The initial step is choosing random patches followed by 4-5 iterations containing two processes: (1) propagation applying a statistic that can be used to examine the relation between two signals or data sets, known as coherence, (2) random search in the concentric neighbourhood to seek better matches by multiple scales of random offsets. The argument is that one random choice when assigning a patch is non-optimal, however applying a large field of random assignments is likely a good choice because it populates a larger domain.

The gains are particularly performance enabling interactive image editing and sparse memory usage, resulting in runtime O(mM log M) and memory usage O(M), where m is the number of pixels and M the number of patches. The downside is that PatchMatch depends on similar images because it searches in nearby regions in few iterations, which in turn also affects its accuracy.

2.4.2 Coherency Sensitive Hashing

Coherency Sensitive Hashing (CSH) is inspired by the techniques of Locality Sensitive Hashing (LSH) and PatchMatch. CSH uses a likewise hashing scheme of LSH and is built on two overall stages, indexing and searching.

The indexing stage applies 2D Walsh-Hadamard kernels in which the projections of each patch in image A and B are initially computed onto the WH kernels. Subsequently the hash tables are created by the following. First, it takes a random line defined by a patch and divides it into bins of a constant width while shifting the division by a random offset. Second, the patch is projected onto the most significant 2D Walsh-Hadamard kernels. Last, a hash value is assigned, being the index of the bin it falls into.

Applying hash tables has the benefit that similar patches are likely to be hashed into the same entry.

The searching stage starts by initialising an arbitrary candidate map of ANNF. This is followed by iterations through each patch in image A where: (1) the nearest neighbour candidates of image B are found using the current ANNF and the current hash table, (2) the current ANNF mapping is updated with approximate distances.

Selecting candidates follows the appearance-based techniques of LSH and as well as the coherence-based techniques of PatchMatch. Choosing among the candidates is done in an approximate manner where the WH kernels rejection scheme for pattern matching is applied beneficially.

CSH has '46%' better performance than PatchMatch and a higher level of accuracy with error rates that are '22%' lower in comparison

3 Implementation

3.1 Brute Force

The pseudo-code for the brute force implementation is found in Listing 1. It is constructed with an outer parallel map on line 2, in which the body of the map is sequential, consisting of a loop nest on lines 4 and 9.

The first for-loop iterates through the reference points, while computing the distance between the query and each reference point, in line 6. Lines 8-18 choose the KNN for each reference point by iterating through a list of size K, which contains the current nearest neighbours. If a better candidate is found, it will be interchanged to its correct position in the list, and the rest of the list will be forwarded.

The advantages of implementing the body of the map sequentially, is that the number of queries is large enough to saturate all hardware threads on the GPU, see more in section 4 for a specialisation of the hardware used. Meaning that the Futhark compiler will spawn all active threads, such that each thread will compute the KNN for a query given to that thread. Figure 18 in section 4 shows the performance of brute force with various size of dimensions D and Ks.

```
1  entry nnk [m][n][d] (qs:[m][d]real) (refs:[n][d]real) : [m][k](int,real) =
2      map (\q ->
3          let  nn = replicate k (-1i32, real_inf)
4          in loop nn for j < n do
5              let ref = refs[j]
6              let dist = seq_euclidean q ref
7              let r_idx = j in
8              let (_, _, nn') =
9                  loop (dist, r_idx, nn) for i < k do
10                     let cur_nn = nn[i].1  in
11                     if dist <= cur_nn then
12                         let tmp_ind = nn[i].0
13                         let nn[i] = (r_idx, dist)
14                         let r_idx = tmp_ind
15                         let dist  = cur_nn
16                         in  (dist, r_idx, nn)
17                     else    (dist, r_idx, nn)
18             in  nn'
19     ) qs
```

Listing 1: Futhark implementation of the Brute Force.

While this pseudo-code shows the full brute force of all queries and reference points, it is conceptually similar to the brute force performed on each leaf-level in the k-d tree implementation. Thus, it will not be discussed further.

3.1.1 Difficulties and Shortcomings

The distance computed on line 6 in Listing 1 was initially implemented as a map-reduce composition, while still called inside the first loop on line 4. The result of this was poor performance because the Futhark compiler would see that there was some inner parallelism, which it would exploit, even though it is inefficient. It was, therefore, more efficient to compute the distance sequentially, as described previously.

3.2 k-d Tree Construction

Listing 2 represents Futhark-like pseudo-code to demonstrate the overall steps and parallel constructs that are applied in constructing the k-d tree. Note that the structure is not equivalent to the final code, due to some shortcoming of Futhark that are discussed in subsection 3.2.1.

Recall the tree construction Algorithm 2 from section 2 using divide-and-conquer recursion, which is not supported by Futhark. The way we account for the divide-and-conquer recursion in Listing 2, is by iterating through a sequential loop from level 0 to $h+1$, in line 8, and computing for each level the number of nodes per level and number of points per node per level, lines 9-10, in order to unflatten the arrays containing the reference point data into sections that fit the current number of nodes for each level. This is illustrated in figure 1. Once the reference points are sorted within the bounds of each node, the arrays with reference data will be re-flattened, ready for the next iteration of the for-loop.

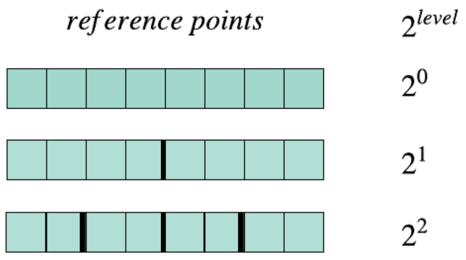


Fig. 1: A demonstration of dividing the reference points at each node level.

The completed tree will consist of the reorganised array of reference points, the original indices of the reference points and two arrays containing the dimensions with the widest spread and the median values, that together represent the splitting values of each node. In our optimised solution, the tree also consists of two 2D arrays containing the upper and lower bounds for each dimension at each current node. This idea is elaborated further in section 3.3.

The dimension with the widest spread is computed on lines 16-20, and subsequently, the values in that dimension are sorted, and the reference points and indices are gathered accordingly, on lines 21-24. The median value is picked out on line 25, and both the median and dimension are scattered into the tree arrays containing all medians and dimensions in lines 34-35. Since the upper and lower bounds are computed when finding the dimension with the widest spread, they too are scattered into the tree arrays containing all upper and lower bounds, in lines 36-37.

```
 1 entry buildTree [m][d] (points : [m][d]f32) (h: i32) =
 2     let num_pads =     (...)   -- computing the padding needed
 3     let padding  = map (...)   -- creating the padding array
 4     let reference = points ++ padding
 5 
 6     let (ref_idxs, reference, median_vals, median_dims, lower_bounds, upper_bounds) =
 7             (...) -- initalising the loop variables
 8         for level < (h+1) do
 9             let num_nodes_pr_lvl = 1 << level
10             let num_points_pr_node_pr_lvl = m // num_nodes_pr_lvl
11             let reference = unflatten num_nodes_pr_lvl num_points_pr_node_pr_lvl reference
12             let ref_inds  = unflatten num_nodes_pr_lvl num_points_pr_node_pr_lvl ref_idxs
13 
14             let (indices', reference', node_info', lower, upper) = unzip5 <|
15                 map3 (\i node_arr inds ->
16                         let dim_arrs = transpose node_arr   |> intrinsics.opaque
17                         let smallest = map o reduce         |> intrinsics.opaque
18                         let largest  = map o reduce         -- max numbers for each dim
19                         let differences = map        (...) -- computing differences
20                         let (dim,_)     = reduce_comm (...) -- dimension w/ widest spread
21                         let extract_dim = map        (...) -- extract dimension values
22                         let d_sort_idxs = extract_dim |> sort |> map (.0)
23                         let indices     = gather d_sort_idxs inds
24                         let node_arrp   = gather2D d_sort_idxs node_arr
25                         let median      = node_arrp[num_points_per_node_per_lvl // 2, dim]
26                         let node_info   = (median, dim)
27                         in (indices, node_arrp, node_info, smallest, largest)
28                     ) (iota num_nodes_per_lvl) reference ref_inds
29 
30             let (medians, dims) = unzip node_info'
31             let inds = map (...)   -- computing indices for scatter
32             in (flatten ref_idxs',
33                 flatten reference',
34                 scatter median_vals inds medians,
35                 scatter median_dims inds dims,
36                 scatter2D lower_bounds inds lower,
37                 scatter2D upper_bounds inds upper)
38 
39     in (ref_idxs, reference, median_vals, median_dims, lower_bounds, upper_bounds)
```

Listing 2: Futhark implementation of the tree creation.

One essential optimisation of the k-d tree construction is the use of padding. Since the datasets might be of sizes that are not dividable with the number of leaves, then padding the dataset to match the number of leaves would mean the parallel dimension will have the same size overall the elements of the map, allowing regular parallelism and flattening, which is much more efficient.

Arguably, the proposed solution uses at most one padded element per leaf, accounting to less than 1% overhead. Assuming that we choose a height that fits that dataset size, such that the number of points per leaf is in the hundreds.

The upper bound of the number of pads should not exceed the number of leaves, thus, we want to see how many pads that amount per leaf. In Equation 1 and 2 we denote n to be the total number of reference points, 2^{h+1} computes the total number of leaves, where h is the height of the tree excluding the leaves. Thus, $\left\lceil \frac{n}{2^{h+1}} \right\rceil$ denotes the number of points per leaf. In Equation 1 we multiply the number of leaves with the number of points per leaf, we get the number of elements that are dividable with the total number of leaves, and by subtracting n, we will have the number of pads needed. In Equation 2 we divide with the number of leaves on each side, resulting in less than or equal to 1 pad per leaf.

$$\left\lceil \frac{n}{2^{h+1}} \right\rceil \times 2^{h+1} - n \leq 2^{h+1} \tag{1}$$

$$\left\lceil \frac{n}{2^{h+1}} \right\rceil - \frac{n}{2^{h+1}} \leq 1 \tag{2}$$

3.2.1 Difficulties and Shortcomings

In the construct above in Listing 2, the original solution was to use a merge sort on line 19. However, although it was safe for Futhark to perform a loop distribution and loop interchange between the outer map inside both for loops, it did not realise, in which case the interchange was not performed. Thus, causing poor performance for the tree construction. The solution was to (1) use batched merge sort, which operates on 2D arrays rather than 1D arrays, (2) distribute the map from line 12, across the body of the map function, such that the sorting is outside the map.

Another shortcoming shows by the use of `intrinsics.opaque` at lines 14-15 in Listing 2, where the purpose is to prevent the Futhark compiler from fusing the two map-reduce compositions on lines 15-16. The reasoning behind this is that both map-reduce compositions call on the same size array, namely m.

Since the Futhark compiler uses moderate flattening, a map-reduce composition will execute in parallel. However, in a map-reduce composition inside a map, as we have in lines 13 and 15-16, the inner map-reduce composition will be sequentialised, and thus resulting in inefficient code. By adding `intrinsics.opaque` and preventing the fusion, the compiler will create two reduce inside a map, which in return will exploit all parallelism.

3.3 Tree Traversal

In section 2 the tree traversal Algorithm 2, is created using recursion, and as in section 3.2 we must re-write the traversal without recursion. The proposed solution uses a stack, and the stack is represented as an integer, since the height of the tree never exceeds 32.

The traversal has two overall stages: (1) the first traversal finding the unique leaf in which the query naturally belongs, (2) traverse backwards in the tree to find additional or better KNNs.

3.3.1 The First Traversal

As described in section 2, first denotes the child of the current node that is on the same side as median w.r.t the query, similarly second denotes the child of the current node that is on the opposite side of the median. Figure 2 demonstrates how the tree is traversed to the leaf in which the query belongs, note that the leaf marked with red is denoted first and its sibling leaf is denoted second.

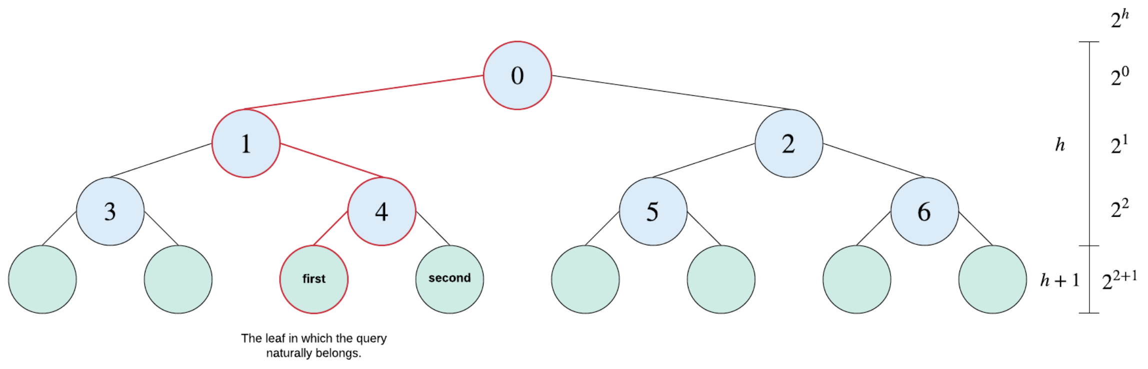


Fig. 2: The first traversal finding the leaf in which the query naturally belongs.

3.3.2 The Traversal for Additional Leaves

In this demonstration, we look at a fictive traversal in which we always check the second node. The validation technique as to whether to check the second node or not, is elaborated in section 3.3.3. The traversal looks at three overall elements (1) the current node index, which is initialised as the last visited leaf, (2) a stack and a stack pointer, (3) the second child of the parent node, if it is to be visited.

Figure 3 is a continuation of figure 2, in which the initial leaf is reached. Thus, the node index is set to the parent of the initial leaf, namely 4, and the stack is popped to see if the second node has been visited or not. Since it had not been visited and we pretend the condition to visit always holds, the traversal also visits the second node.

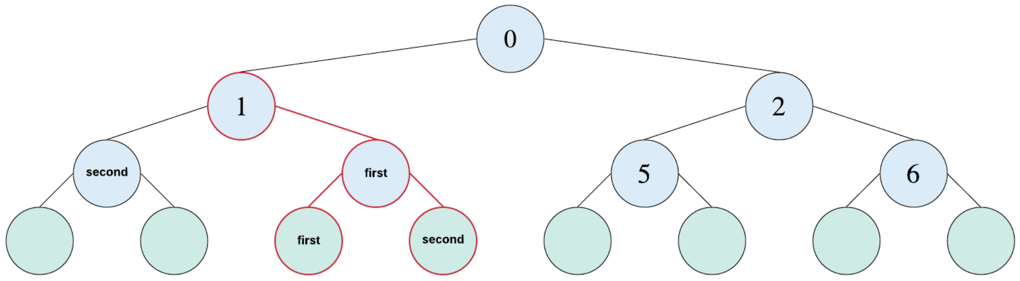


Fig. 3: Visiting the second node of the initial leaf.

In figure 4 the traversal looks to the parents second child, and since that has not yet been visited, it traverses to the first leaf of the parents second child.

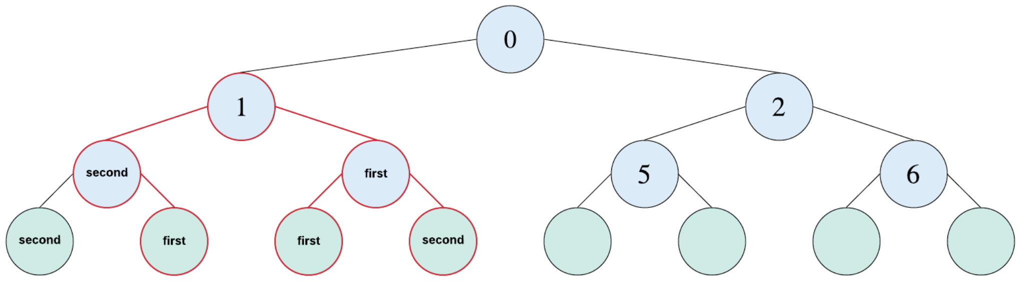


Fig. 4: Visiting first node of the parents second child.

Pretending that we still have not found the KNN, the traversal will continue into the second leaf of the parents second child, as in figure 5. If the KNN is still not found, the traversal will continue to the second child of the root until the whole tree has been traversed, or the KNN is found. When the query is done, it returns -1

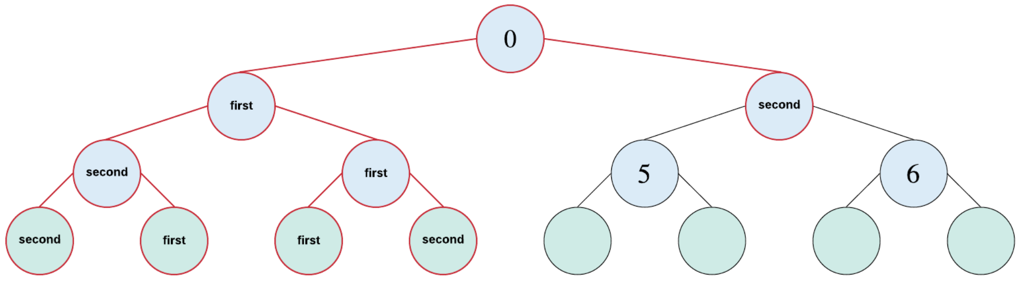


Fig. 5

3.3.3 Validating Whether to Look at the `second`

We propose an optimised solution for checking whether to visit the second node or not. $wknn$ denotes the worst found neighbour so far, R denotes our reference points, Q denotes our queries, lb and ub denote the arrays containing the upper and lower bounds and M denotes the array containing the median values for each node.

$$\forall i.[lb_i, ub_i].\ \forall q \in Q_m.\ \forall p \in R_n.\ \forall m \in M_{nn}.$$

The original solution determines whether to visit the second node by checking if the distance from the query to the current median is smaller than the worst found neighbour, as in Equation 3. However, the solution looks only at one dimension when checking whether to visit or not, meaning it is likely that another dimensionality could contain information that would otherwise have prevented the second visit. Especially, if the number of dimensions is high, because then a lot of values will be overlooked.

$$\mid q_i - m_i \mid > \ wknn \tag{3}$$

The naive approach would be to compute all distances, as in Equation 4. Although this has a higher level of accuracy compared to the original solution, it also inefficient.

$$\sqrt{\sum_i (p_i - q_i)^2} \;\geq\; wknn \tag{4}$$

Instead, we propose a solution that achieves a higher level of accuracy compared to the original solution, while still running efficiently. The idea is that the upper and lower bounds for each dimension is saved, for each node, and then used to compute the distance between the query to the upper and lower bounds, respectively. Thus, instead of checking one dimension, we check all dimensions, but only against the upper and lower bounds. This is formulated in Equation 5 and it corresponds to lines 11-26 in Listing 3.

$$\sqrt{\sum_i (p_i - q_i)^2} \;\geq\; \sqrt{\sum_i \begin{smallmatrix} (q_i - lb_i)^2 \text{ , if } & q_i \leq lb_i \\ (q_i - ub_i)^2 \text{, if } & q_i \geq ub_i \\ 0 \quad , & \text{otherwise} \end{smallmatrix}} \;\geq\; wknn \tag{5}$$

Section 4.2 demonstrates the increased performance by using this solution. On a dataset of size roughly 4 mio., with dimensionality D=12 and K=5, we obtain a speed-up of 5.6. The reason for this is elaborated further in Section 4.2.1, which demonstrates how checking all the upper and lower bound on all dimensions reduces the number of visits to additional node, due to its increased accuracy. Thus, reducing the steps made in the traversal and improving the performance.

```
let (parent_rec, stack, count, rec_node) =
    loop (node_index, stack, count, rec_node) =
         (last_leaf, stack, height, -1)
          while (node_index != 0) && (rec_node < 0) do
              let parent = getParent node_index
              let second = node_index + addToSecond node_index in

              if isVisited stack count
              then (parent, stack, count-1, -1)
              else
                let ack = loop ack = 0.0f32
                    for i < d do
                        let cur_q = query[i]
                        let lower = lower_bounds[second,i]
                        let upper = upper_bounds[second,i] in

                        if cur_q <= lower then
                            let res = (cur_q-lower)*(cur_q-lower)
                            in (ack + res)
                        else if cur_q >= upper then
                            let res = (cur_q-upper)*(cur_q-upper)
                            in (ack + res)
                        else (ack + 0.0)

                let to_visit = (f32.sqrt ack) < wknn in
                if !to_visit
                then (parent, stack, count-1, -1)
                else
                  let second = node_index + addToSecond node_index
                  let stack  = setVisited stack count in
                  (parent, stack, count, second)
```

Listing 3: A part of the tree traversal demonstrating checking upper and lower bound to determine visits.

3.4 The Full Implementation

Listing 4 shows, in pseudo-code, the overall structure of the main function that puts all parts together. We experiment with two solutions for splitting the queries that have found their KNN, with the ones that need to continue traversing the tree. The first solution is using the two-way partition, elaborated further in section 3.4.1. The second solution is to sort the queries by the leaves, and this is elaborated further in section 3.4.2.

The structure of Listing 4 is as follows. The first step is building the tree of the reference points, on line 3. The second step is to perform the first traversal for each query to the leaves in which the queries naturally belong, on line 4. The third step is a sequential outer while-loop, on lines 12-37, which continues to iterate until all queries have found their KNN.

Inside this loop, we have a parallel map which performs two main tasks, (1) performing brute force on each ongoing query with its current leaf, in line 19, and (2) traversing the tree to find new leaves for the ongoing queries, on line 21.

On lines 25-29, we either sort or partition the completed queries, from the non-completed queries. Since both partition and sorting reorganise the contents of the arrays, they do not change the sizes of them. Thus, in lines 31-37 the arrays are cut for the next iteration of the loop.

```
entry main [n][m][d] (k: i32) (h: i32) (qs : [m][d]f32) (refs : [n][d]f32) =

  let (ref_idxs, leaves, meds, dims, lower, upper, ppl) = buildTree refs h
  let init_leaves = map (\qi -> firstTraverse h dims qs[qi] meds) (iota m)

  -- For sorting, the queries af sorted by the initial leaves.

  let ongoing_knn   = replicate a (replicate k (-1i32, f32.inf))
  let completed_knn = copy ongoing_knn
  let stacks  = replicate a 0i32

  let (_, _, _, completed_knn, _, _, _) =
      loop (not_comp_qs, init_leaves, stacks, completed_knn, ongoing_knn, on_knn_idxs, trues) =
        (...) -- loop initialisation

          while (length not_comp_qs) > 0 do
            let (ongoing_knns, new_leaves, new_stacks) = unzip3 <|
                map4 (\q lidx st klst ->
                        let neighbours = bruteForce q leaves[lidx] ref_idxs[lidx] klst
                        let wknn = neighbours[k-1].1
                        let (new_l, new_s) = traverse h dims meds wknn q st lli lower upper
                        in (neighbours, new_l, new_s)
                     ) not_comp_qs init_leaves stacks ongoing_knn

            -- Sorting the queries by the leaves and getting the number of finished elements,
            -- or Partitioning the finished elements from the rest, returning the number of
            -- not finised queries.

            -- Gathering after sorting.

            in (not_comp_qs'[finished:],
                ongoing_leaf_idxs[finished:],
                stacks'[finished:],
                scatter2D completed_knn (...), -- scatter completed into collective array
                ongoing_knns'[finished:],
                on_knn_idxs'[finished:],
                trues')
  in completed_knn
```

Listing 4: The overall structure of the main function putting everything together.

3.4.1 Using Partition to Extract the Finished Queries

In the missing parts on lines 25-27 in Listing 4, we may insert Listing 5 below, as this performs the call to partition.

```
    while (length not_comp_qs) > 0 do
      (...)

      let (trues, ongoing_leaf_is, not_comp_qs', on_knn_idxs', ongoing_knns', stacks') =
          partition2 sortFinishedQueries new_leaves not_comp_qs
          ongoing_knn_idxs new_stacks ongoing_knns

      (...)
```

Listing 5: The missing piece of Listing 4 in the partition solution.

Listing 6 shows the implementation of the two-way partition applied to reorganise the order of the queries, leaf indices, stacks and KNNs. The first parameter is a boolean function that checks whether the leaf indices are equal to -1, it uses this to organise all leaf indices that show completion to the right of the array and all the continuing leaf indices to the left, which results in a list of new indices, on lines 6-17. The KNNs, completed queries, leaf indices and stacks are then scattered into new arrays in the reorganised order.

```
 1  let partition2 [n][k] (expr: (i32 -> bool)) (leaf_idxs:         [n]i32)
 2                        (completed:   [n]i32) (knn_inds:          [n]i32)
 3                        (stack:       [n]i32) (knn_dsts: [n][k](i32,f32))
 4                        : (i32, [n]i32, [n]i32, [n]i32, [n][k](i32,f32), [n]i32) =
 5
 6      let tflgs = map (\e -> if expr e then 1 else 0) leaf_idxs
 7      let fflgs = map (\b -> 1 - b) tflgs
 8
 9      let indsT = scan (+) 0 tflgs
10      let tmp   = scan (+) 0 fflgs
11      let trues = if n > 0 then indsT[n-1] else -1
12      let indsF = map (+trues) tmp
13
14      let inds  = map3 (\leaf indT indF -> if expr leaf
15                                           then indT-1
16                                           else indF-1
17                       ) leaf_idxs indsT indsF
18
19      let leaf_idxsp = scatter (replicate n 0i32) inds leaf_idxs
20      let completedp = scatter (replicate n 0i32) inds completed
21      let knn_inds'  = scatter (replicate n 0i32) inds knn_inds
22      let knn_dsts'  = scatter2D (replicate n (replicate k (0i32, 0.0f32))) inds knn_dsts
23      let stackp     = scatter (replicate n 0i32) inds stack
24      in  (trues, leaf_idxsp, completedp, knn_inds', knn_dsts', stackp)
```

Listing 6: Implementation of the two-way partition.

3.4.2 Using Sorting to Extract the Finished Queries

In the missing parts on line 6 and lines 25-29 in Listing 4, we may insert Listing 6 below, as this performs sorting of the queries by the leaves. Line 3-4 sort the initial leaves after the first traversal, and uses gather to reorganise the non-completed queries. Line 8 in the loop represents the call to brute force and traverse from the full implementation, once these operations are performed, lines 10-13 sort the queries by the leaves and extracts the number of completed queries as well as the ongoing ones. Thus, lines 15-18 uses the order to gather the rest of the needed arrays.

```
(...)

let (sorted_idxs_fst, init_leaves) = init_leaves |> sort
let not_completed_queries = gather2D sorted_idxs_fst qs

(...)
        while (length not_comp_qs) > 0 do
          (...)

          let (ongoing_leaf_idxs, sorted_idxs) = sortQueriesByLeaves new_leaves
          let finished = map (\ll -> if ll == -1 then 1 else 0) ongoing_leaf_idxs
                      |> reduce (+) 0
          let trues' = trues - finished

          let not_completed_queries' = gather2D sorted_idxs not_comp_qs
          let on_knn_idxs'  = gather sorted_idxs on_knn_idxs
          let ongoing_knns' = gather2Dtuples sorted_idxs new_ongoing_knns
          let stacks' = gather sorted_idxs new_stacks

          (...)
```

Listing 7: The missing pieces of Listing 4 in the sorting solution.

3.4.3 Why Sorting over Partition

While partition is efficient, due to its use of map, scan and scatter, it still lacks to optimise temporal locality since all the queries are accessing the leaves in random order. By sorting the queries by the leaves before performing brute force, we can optimise temporal locality, since the leaves are then accessed in the same order.

However, the experiments in section 4.1 show that sorting is only faster when working on datasets that are approximately 500000 or larger, meaning the overhead of sorting has a higher impact compared to optimising temporal locality, for datasets smaller than 500000.

For datasets smaller than 500000, we see that partition performs slightly better with a speed-up of nearly 1, on the other hand, for dataset between 500k-2000k, we see that sorting performs better with a speed-up between 1.5-5.

4 Experimental Evaluation

This section describes and demonstrates the performance of each optimisation described in sections 3.2 and 3.3, as well as the overall performance gains achieved of the k-d tree solution compared to the brute force from section 3.1.

Each solution has been validated against the result of the brute force solution, using Futhark benching. All tests have been performed on GPU04 RTX2080TI, having 4352 CUDA cores and 11 GB RAM, that requires at least 70000 hardware threads to fully utilise the machine.

4.1 Optimisation using Sorting over Partition

The following subsection demonstrates the results for solutions using partition and sorting, respectively, described in section 3.2.

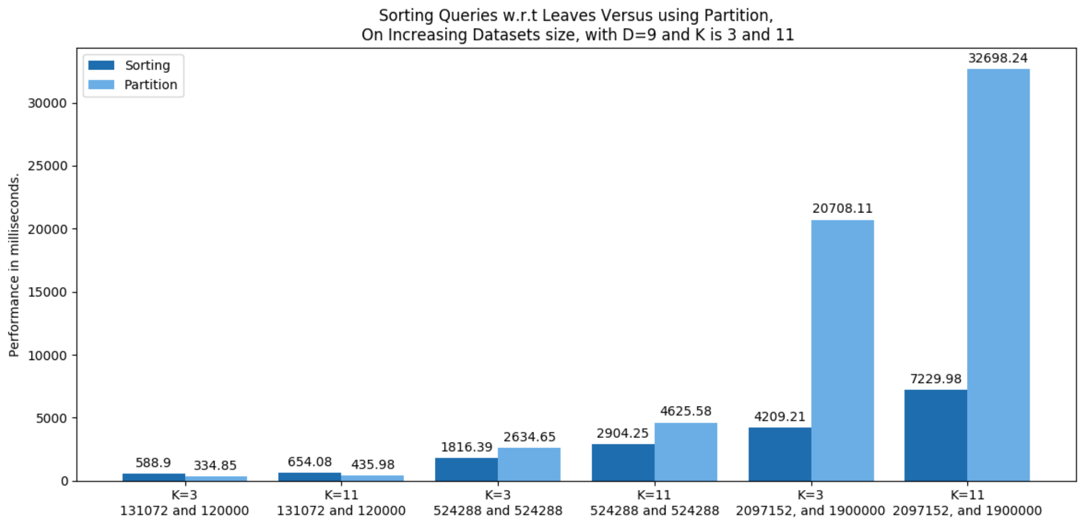


Fig. 6: Testing for D=9 with datasets of sizes, 2097152 and 1900000, 524288 and 524288, and 131072 and 120000.

In figures 6 and 7, we compare the performances between sorting and partition. It shows that sorting works faster for datasets larger than 524288, with higher dimensionality such as D=9, or lower dimensionality such as D=4 with a high K, such as K=11.

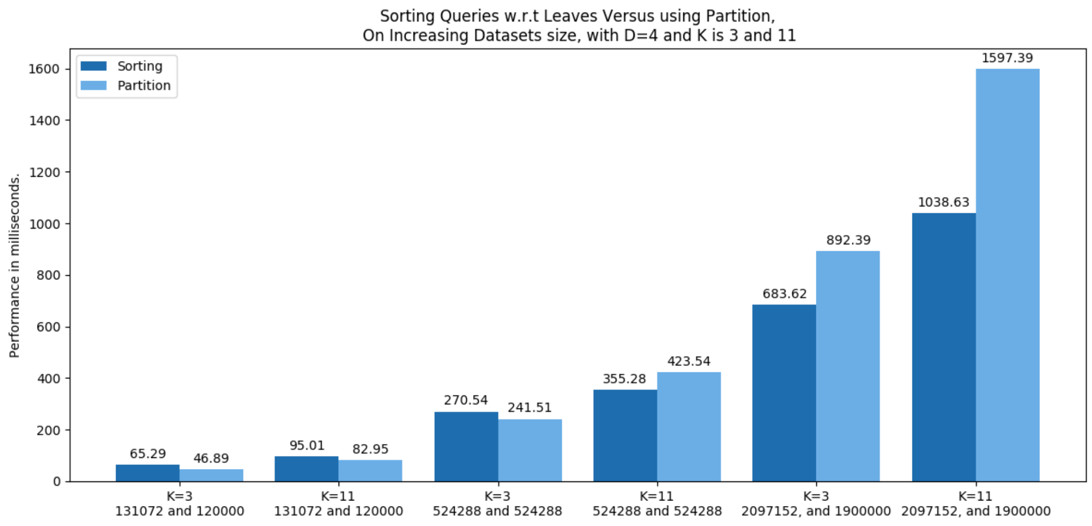


Fig. 7: Testing for D=4 with datasets of sizes, 2097152 and 1900000, 524288 and 524288, and 131072 and 120000.

However, by looking at the speed-ups presented in table 1, we see that K does not have any remarkable effect, since the speed-up is higher for K=3 on the dataset of size 524288, and the speed-up is higher for K=11 on the dataset of size 2097152. We also see that increasing D has a positive effect on the speed-ups. The datasets of sizes 2097152 and 1900000 have a speed-ups that are 3.61 and 3.99 times higher when using a dimension of size 9 over 4.

	131072, 120000		524288, 524288		2097152, 1900000	
D	*K=3*	*K=11*	*K=3*	*K=11*	*K=3*	*K=11*
4	0.71	0.87	0.89	1.19	1.3	1.53
9	0.56	0.66	1.45	1.59	4.91	4.52

Table 1: Speed-ups gained by increasing the dataset sizes, for sorting against partition.

In conclusion, we see that sorting works incrementally better for increasing sizes in D and datasets.

4.2 Optimising Tree Traversal with Full Dimensionality Checking

The following demonstrates the results for the optimisation described in section 3.3.

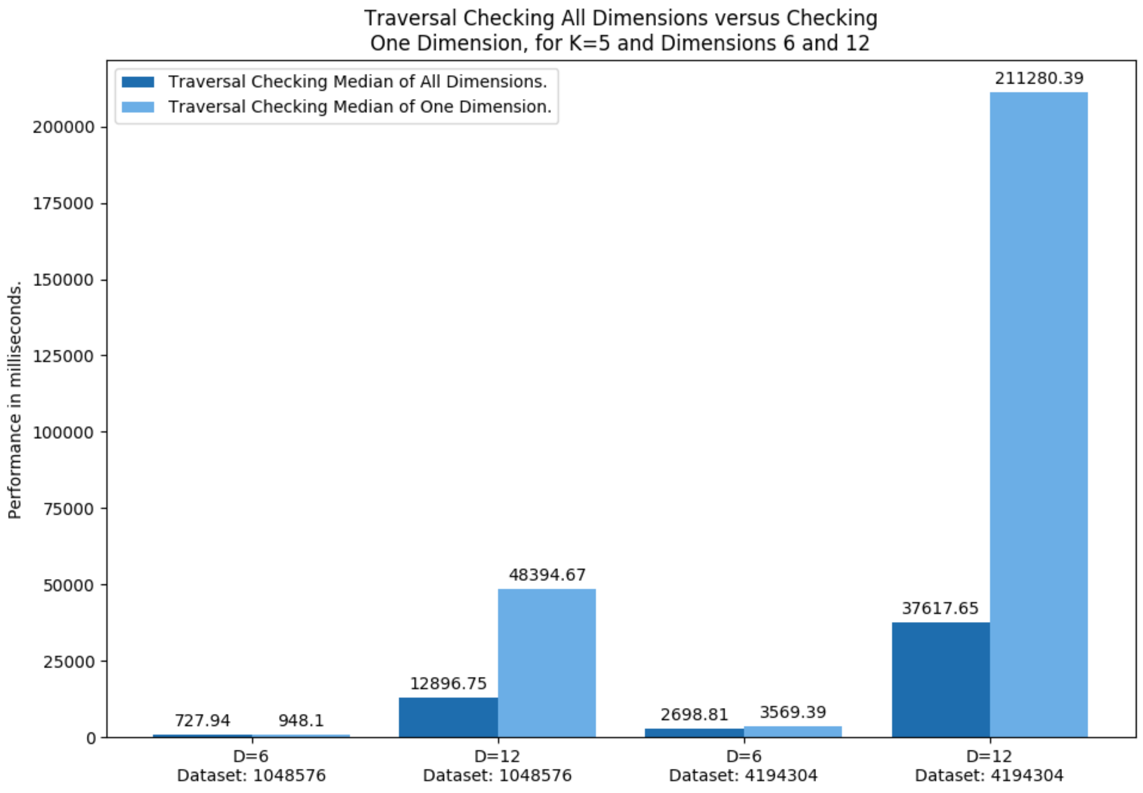


Fig. 8: Traversal comparing results w.r.t varying sizes for D on a smaller and larger dataset.

Figure 8 shows that increasing the size of D as well as the dataset sizes will give a better performance for the optimised solution that checks at all dimensions. The test uses a static size K=5 and tests on D=6 and D=12 for both small and large datasets, where the light blue is the traversal checking one dimension and the dark blue is the traversal checking all dimensions. In comparison, the speed-ups for D=12 is 2.45 and 4.3 times faster than D=6, respectively.

Datasize	*K=1*	*K=5*	*K=17*
1048576	2.47	4.47	4.3
4194304	3.14	3.37	2.65

Table 2: Speed-ups gained by increasing the size of K for both small and large datasets.

In the next illustration, figure 9, we experiment to see whether increasing and decreasing K amounts to a speed-up. Testing with D=12 for both small and large datasets the speed-ups, visible in table 2, show that the performance in both cases are best with a K=5, however, it shows no correlation between a small or large K amounting to a speed-up.

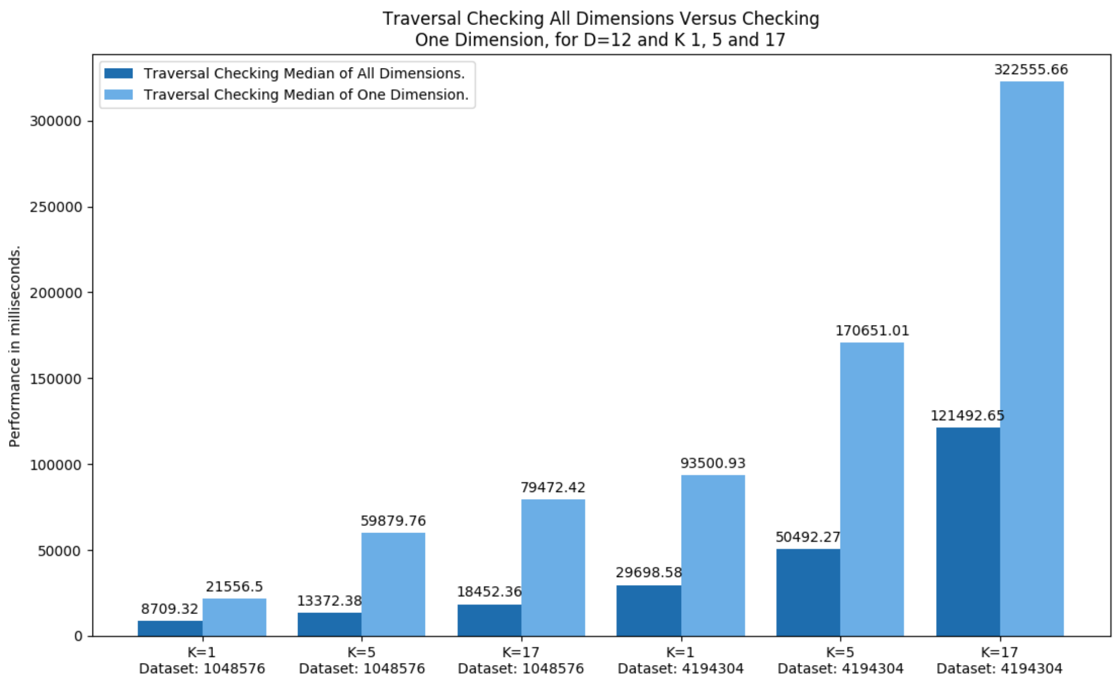


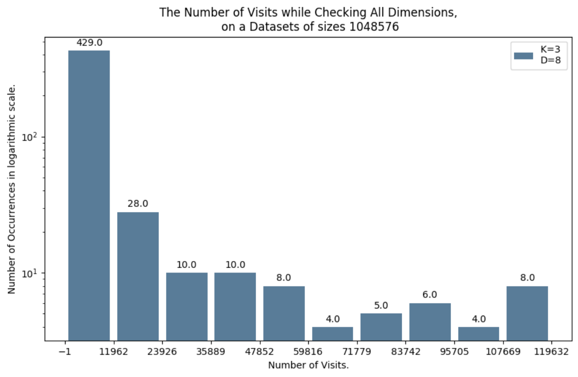
Fig. 9: Traversal comparing results w.r.t varying sizes for K on a smaller and larger dataset.

4.2.1 Demonstrating a Comparison of the Number of Leaf Visits

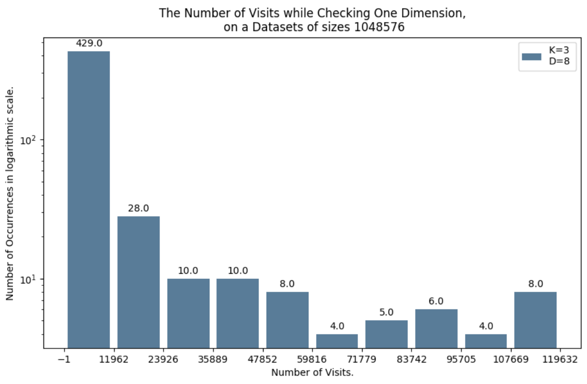
The following histograms demonstrate the number of visits to leaves performed when searching for the exact KNN. The size of the visits-array is initialised to the total number of leaves, after which each search iteration will store the number of new visits in the array. The small example below shows that the program would finish finding the exact KNN after six iterations of searches through leaves. The three -1's indicating that no further leaves are visited.

$$[100, 99, 85, 62, 33, 18, -1, -1, -1]$$

Thus, in the histograms below, a large number of -1's to the left will indicate a few visits, resulting in better performance, while a large number to the right will indicate many visits and poor performance.



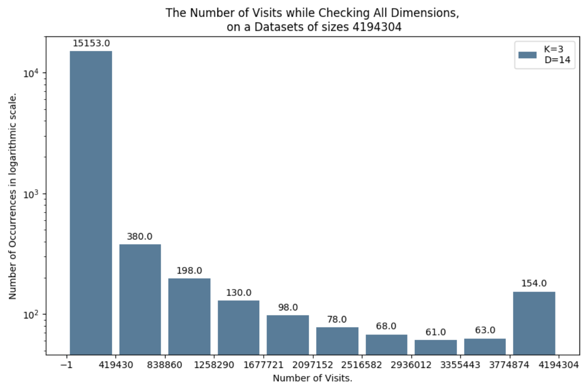
(a) Checking all dimensions.



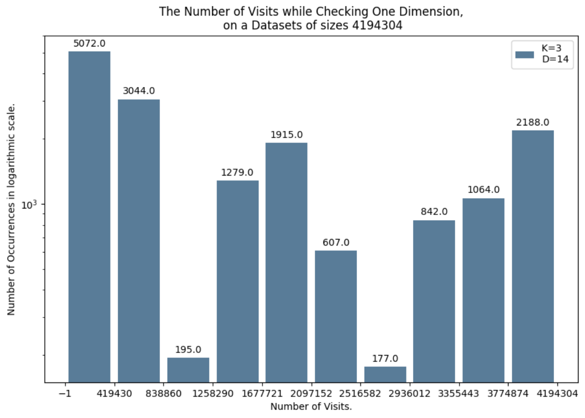
(b) Checking one dimension.

Fig. 10: Figure a and b show the same result for K=3 and D=8 on both traversal solutions, on datasets of sizes 1048576.

As figures, 10a and 10b demonstrate, for a small K of size 3 and a relatively small D of size 8, we see that the number of visits to leaves in both solutions is equal. However, figures 11a and 11b show increasing D to 16 drastically changes the outcome, such that the method of checking all dimensions excels.



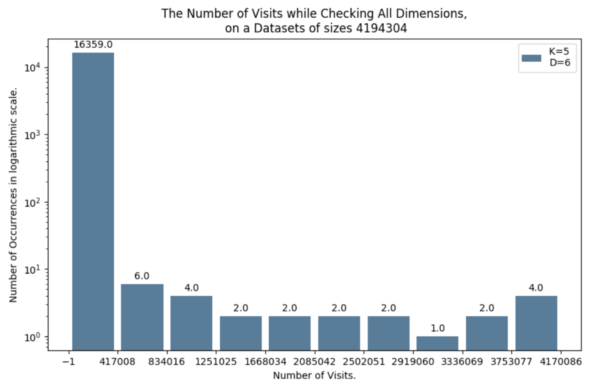
(a) Checking all dimensions.



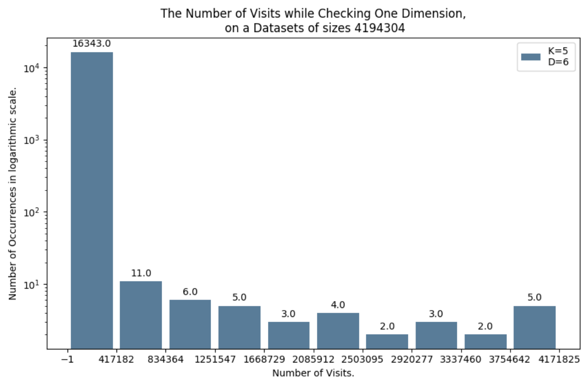
(b) Checking one dimension.

Fig. 11: Figure a and b show the same result for K=3 and D=14 on both traversal solutions, on datasets of sizes 4194304.

If we experiment further by increasing K to 5 while testing against both a small and large size D, namely 6 and 14, we see in figure 12 that even for a small D there is a slight decrease in the number of visits when checking all dimensions in 12a compared to checking one dimension in 12b. The figures in 13 show that for a K=5 and a D=14, the difference is incredibly in favour of the solution checking all dimensions. Thus, all histograms show increasing sizes for K and D will likewise have increasingly better performance on the solution checking all dimensions compared to checking one dimension.

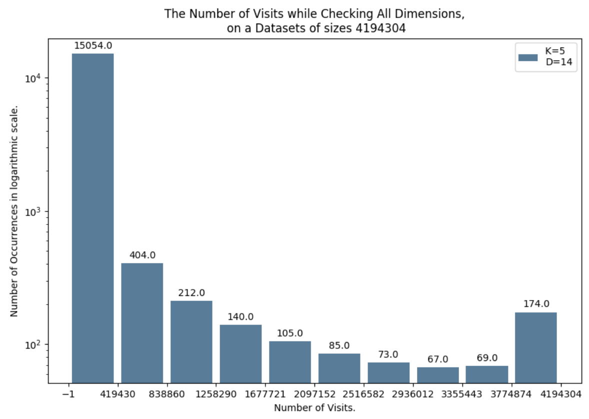


(a) Checking all dimensions.

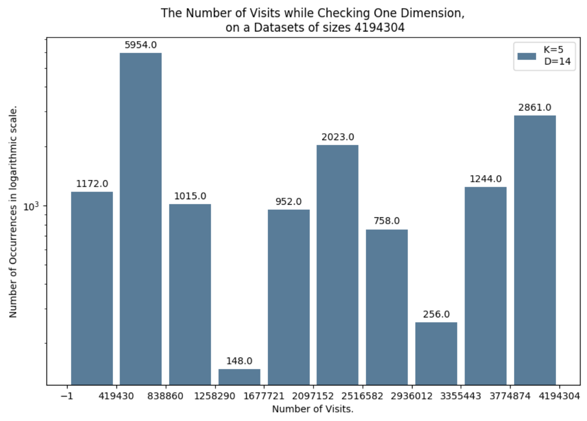


(b) Checking one dimension.

Fig. 12: Figure a and b show the same result for K=5 and D=6 on both traversal solutions, on datasets of sizes 4194304.



(a) Checking all dimensions.



(b) Checking one dimension.

Fig. 13: Figure a and b show the same result for K=5 and D=14 on both traversal solutions, on datasets of sizes 4194304.

4.3 Brute Force versus k-d Trees for Computing KNN

Table 3 summarises the speed-ups for testing the fully optimised k-d tree implementation against the brute force implementation, where we look at D sizes ranging from 2-14 and K sizes 2, 6 and 12. Figures showing the performance for K=2 and K=6, referenced in the table, can be found in the Appendix 6 figures 15, 16 and 17.

K	*D=2*	*D=4*	*D=6*	*D=8*	*D=10*	*D=12*
12	78.7	58.57	40.04	17.6	8.26	4.77
6	65.49	53.96	38.16	14.41	6.0	3.08
2	34.64	33.42	27.47	13.17	5.72	2.81

Table 3: Speed-ups achieved by the k-d tree solution compared to the brute force solution, based on datasets of sizes 1048576.

The results show that any given size of K and D results in a speed-up in favour of the k-d tree solution. This increased performance applies particularly for small dimensions and large K, for instance, K=12 and D=2 result in a speed-up of almost 79. Figure 14 below illustrates the performance for a static K=12.

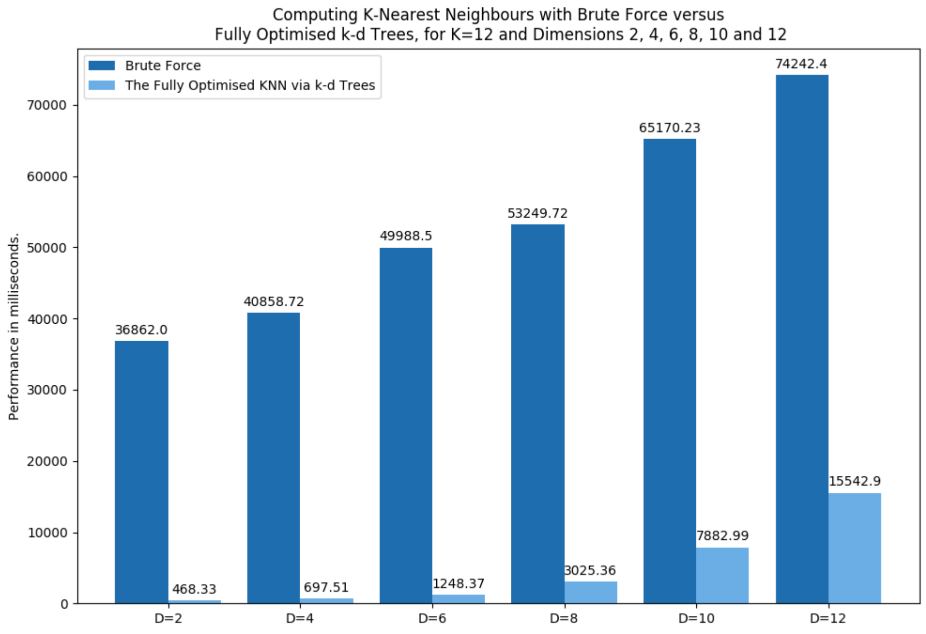


Fig. 14: Performance comparison of k-d tree versus brute force, with a static K=12 on datasets of sizes 1048576.

5 Conclusion

In conclusion the implementation was successfully made, and successful optimisations w.r.t tree traversal, and sorting of queries by leaves proved to improve the performance.

Given more time, it would be interesting to experiment whether the ratio between the height of the tree and the size of the datasets have an impact on the performance.

6 Appendix

6.1 Additional Graphs for Performance of Brute Force versus k-d Trees

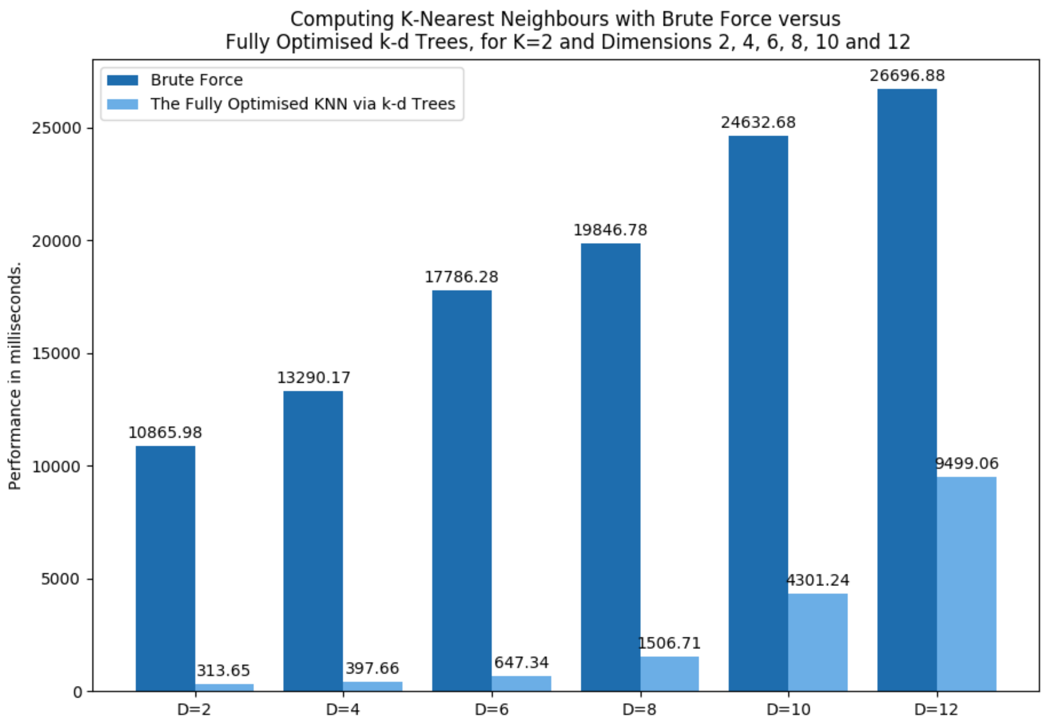


Fig. 15: Performance comparison of k-d tree versus brute force, with a static K=2 on datasets of sizes 1048576.

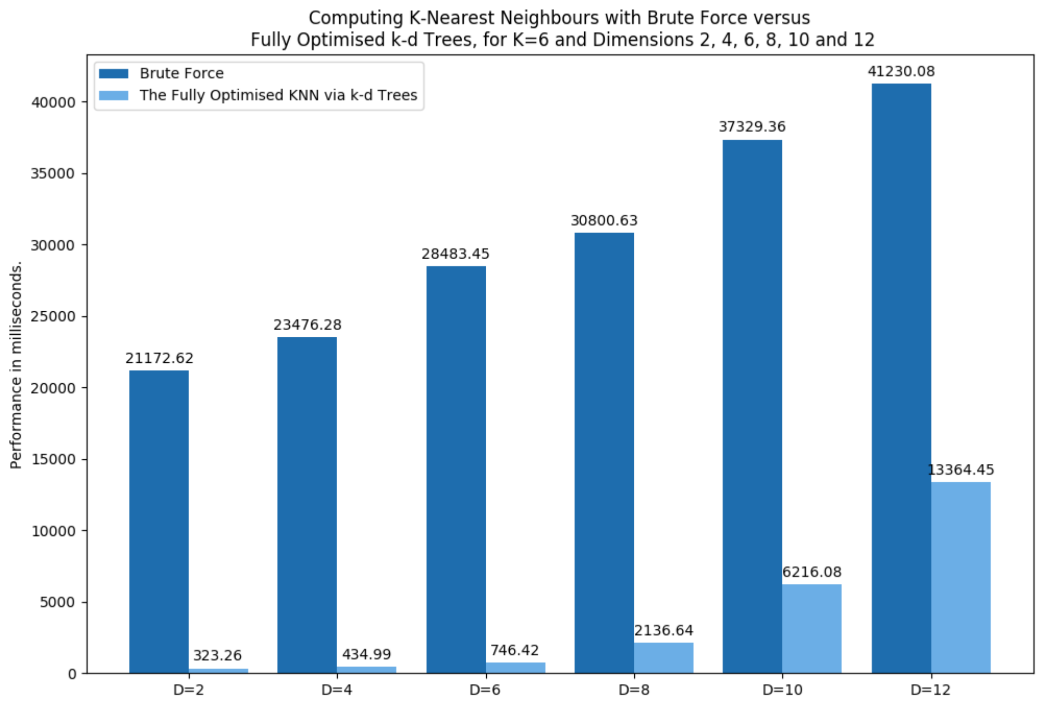


Fig. 16: Performance comparison of k-d tree versus brute force, with a static K=6 on datasets of sizes 1048576.

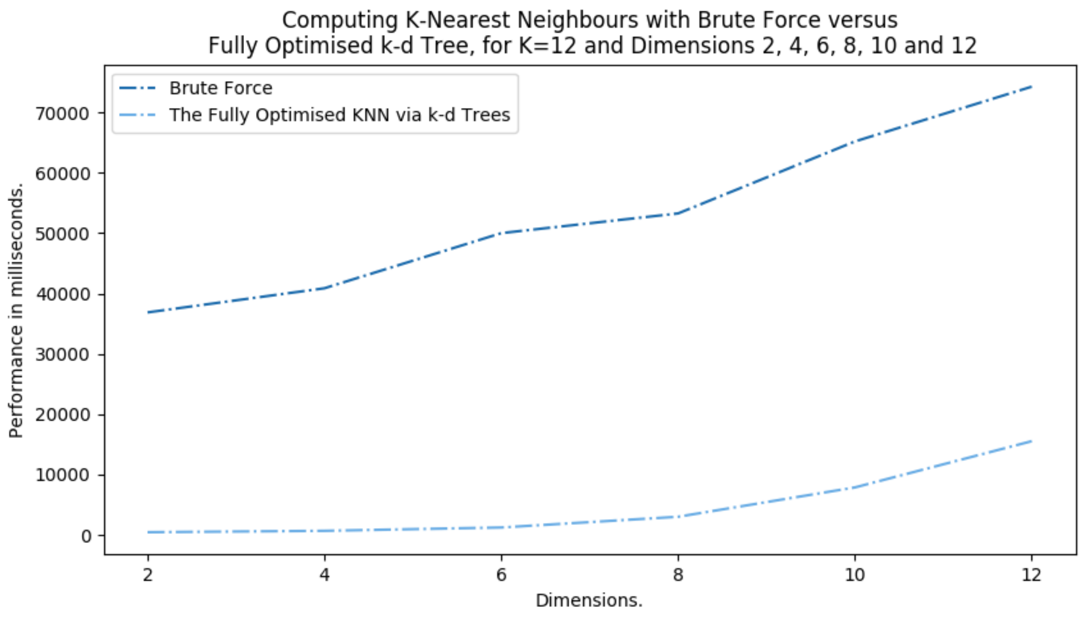


Fig. 17: Performance comparison of k-d tree versus brute force, with a static K=12 on datasets of sizes 1048576.

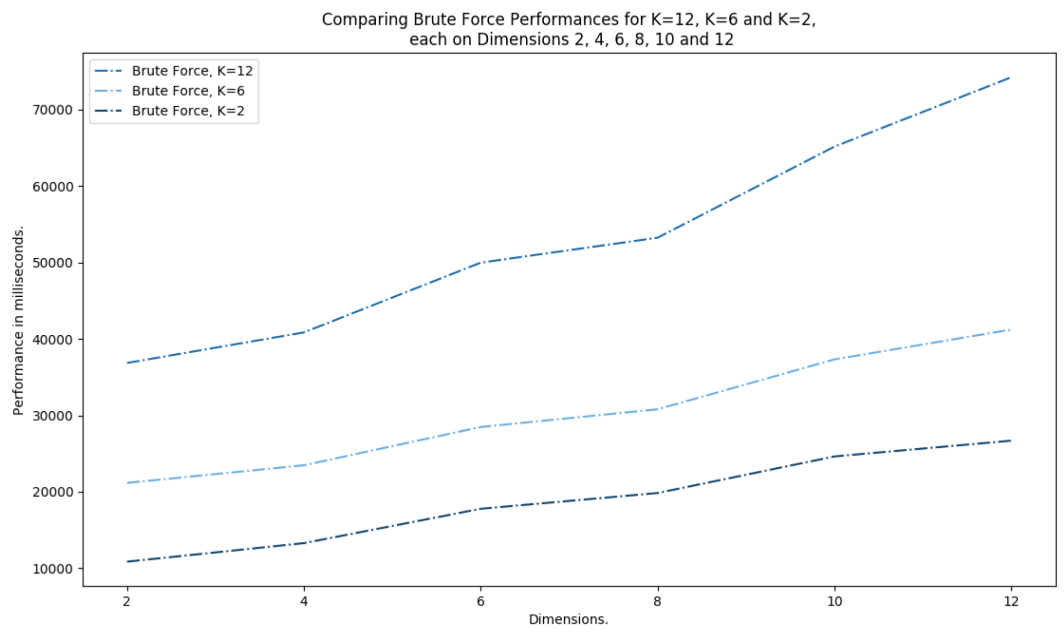


Fig. 18: Performance comparison of brute force, with K=12, K=6 and K=2, on datasets of sizes 1048576.

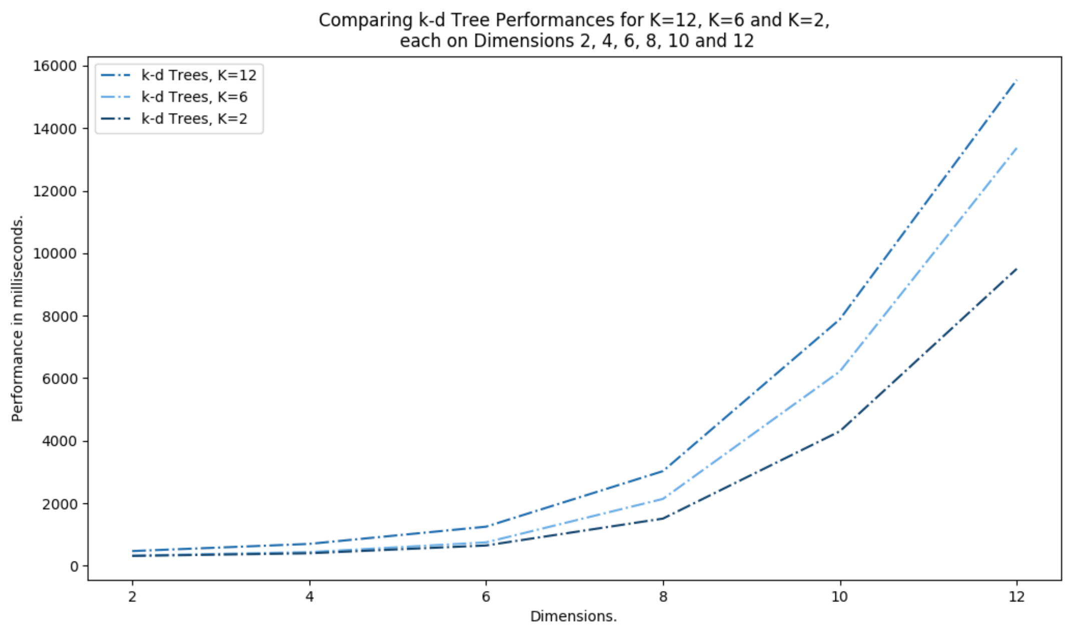


Fig. 19: Performance comparison of k-d tree, with K=12, K=6 and K=2, on datasets of sizes 1048576.

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