Comparison of nearest-neighbor-search strategies and implementations for efficient shape registration

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Abstract—The iterative closest point (ICP) algorithm is one of the most popular approaches to shape registration currently in use. At the core of ICP is the computationally-intensive determination of nearest neighbors (NN). As of now there has been no comprehensive analysis of competing search strategies for NN. This paper compares several libraries for nearest-neighbor search (NNS) on both simulated and real data with a focus on shape registration. In addition, we present a novel efficient implementation of NNS via k-d trees as well as a novel algorithm for NNS in octrees.

Index Terms—shape registration, nearest neighbor search, k-d tree, octree, data structures

1 INTRODUCTION

Shape registration is the problem of finding the rigid transformation that, given two shapes, transforms one onto the other. The given shapes do not need to be wholly identical. As long as a partial overlap is possible, shape registration seeks the transformation that accomplishes just that overlap. For the extent of this paper we consider a shape to be a set of points in three-dimensional Cartesian space, i.e. a point cloud. The registration problem is most commonly solved using the iterative closest point (ICP) algorithm [1]. In addition to the two shapes, it assumes an estimate of the transformation to be computed. Such an estimate is usually available in contexts where shape matching is of importance. ICP is an iterative algorithm that alternates between determining, based on the current transformation estimate, the nearest neighbors (NN) of every point of one shape, and updating the estimate based on the NN. Updating the estimate is a relatively simple mathematical operation that is linear in the number of neighboring points. Naively implemented, the nearest-neighbor search (NNS) is in \(O(nm)\) where \(n\) and \(m\) are the number of points in the respective point clouds. Exploring every possible pairing of point can be avoided by employing spatial data structures. The average runtime of NNS is then usually in the order of \(O(n \log m)\) but is still by far the most computationally expensive part of shape registration. This paper gives a comprehensive empirical analysis of NNS algorithms in the domain of 3-dimensional shape matching. For this purpose, section 2 gives an overview of spatial data structures and the state of the art on comparison of search algorithms. Section 3 presents the novel search algorithm on octrees and the novel efficient implementation of NNS in k-d trees. We explain our experimental setup in section 4, provide results in section 5 and conclude the paper in section 6.

2 RELATED WORK

Spatial data structures partition space to allow efficient access to the stored elements via positional queries. Most spatial data structures are hierarchical in nature, such as k-d trees [9] and octrees [10]. The grid file [11] is a rare flat non-hierarchical data structure. We explicitly exclude it from consideration here because of its prohibitive memory requirements. A special type of NNS employs the Morton order for arranging the point cloud. A Morton order is a space-filling curve (SFC), i.e. a curve that allows ordering the set of points along one dimension while preserving the locality thereof [12].

In addition to the well known k-d tree and octree we also consider the following hierarchical R-trees [13]. There are other data structures such as the range-tree [14] and vp-tree [15]. Unfortunately, to the authors’ knowledge, there is no publicly available NNS library that employs either the vp- or the range-tree.
An octree [10] is the generalization of quadtrees, which store two dimensional data [16]. Each node in an octree represents the volume formed by a rectangular cuboid, often simplified to an axis-aligned cube. Consequently an octree node has up to eight children, each corresponding to one octant of the overlying cube/node. A node having no children usually implies that the corresponding volume can be uniformly represented, i.e., no further subdivision is necessary to disambiguate. This convention is not completely applicable when storing points, which are dimensionless, i.e., there is no volume associated with them. When storing a point cloud, a stopping rule must be defined for occupied volumes, like a maximal depth or a minimal number of points. Empty volumes will however not be further split up.

The k-d tree [9] is similar to the octree in that each node represents an axis-aligned rectangular cuboid and its children split up the volume to form smaller cuboids. Empty volumes are not subdivided further, and there must be a stopping rule for occupied volumes. However, a k-d tree is a binary tree and the subdivision of the node’s volume must not be regular, i.e. each node also defines an axis-aligned hyperplane that splits the volume in two. Unlike the octree, there is not a unique way of constructing a k-d tree since the splitting plane can be placed at any position in any node. There are several strategies for placing the splitting plane. The standard rule is splitting before the median point along the longest dimension of the node’s volume. Another splitting rule is the so called midpoint rule, which merely splits the current volume in half along its longest dimension.

The R-tree [13] is non-binary and is primarily used for spatial data other than point clouds, i.e. for geographic information systems. Each node represents an axis-aligned bounding box of arbitrary dimension. The represented volumes are allowed to overlap, except for the requirement that a child’s volume must be entirely within the parent’s. There are several variants of the R-tree that differ only in their insertion algorithms. The linear, quadratic and exponential R-tree all insert a new element into the node that requires the least extension, but they use algorithms of different complexities (hence the name) for splitting the node, if necessary. The R*-tree insertion algorithm chooses which node to insert the new element into by a minimum overlap criteria. It also extends the splitting algorithm by the principle of forced reinsertion, i.e. elements that are already stored may be deleted and reinserted into another node [17].

Apart from the data structure, the NNS queries are of interest. There are different types of NNS query that deserve discussion: The first type of query that springs to mind in the context of NNS is the k-NN search. The result of this type of query are the k NN around a specified query point. Another is the fixed radius search, which computes all points within a given radius of the query point. The combination of the two types yields the ranged search, i.e. the retrieval of the k NN with a given maximal distance. The latter query with k = 1 is the type of query needed for shape registration. In the large majority of realistic applications the presence of obstruction leads to only partially-overlapping point clouds. Thus, allowing point correspondences with a too large distance can only infuse the registration process with errors. The range search variant also allows for a large potential for efficient implementation. The maximal radius restricts the search region to only a small subspace of the entire data. This can be efficiently combined with the restriction on the number of points. Even the small subspace does not need to be explored in its entirety if it can be ensured that the k NN points have been located. It is surprising then, that many NNS libraries fail to provide this search variant (cf. Table 1).

To the authors’ knowledge there is little previous work exploring and comparing current NNS libraries in the context of shape registration. Blumenthal et al. [18] give a first evaluation of some available NNS libraries. We compare a wider range of algorithms on a wider range of data, both artificial and real. Pomerleau at al. [19] explore several parameters influencing registration performance, but only one parameter (an early-out approximation factor) is related to the NNS. There have been comparisons of different data structures for NNS, although not specifically for shape registration. Dandamudi et al. [20] compare the binary decision (bd) tree to variants of the k-d tree. Nakamura et al. [21] propose a new data structure, the md-tree and compare it against the k-d tree and the bd-tree. They also find the k-d tree to perform worse than the other data structures in the tested scenarios. Judging from the large number of

### Table 1

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libraries employing the k-d tree it is clear that it is still the favored data structure in general NNS libraries. Greenspan et al. [22], [23] have proposed improved NNS algorithms for shape registration. While these are promising, they have not yet found their way into any of the NN libraries evaluated in this paper.

3 Design and Implementation

In this section we present our highly-optimized implementation of the octree and k-d tree. The octree implementation has specifically been designed for the efficient storage of large point clouds. It is implemented in the 3DTK [2] and supports NNS, point-cloud compression and fast visualization. The fast k-d tree implementation is called libnabo [6] and is not to be confused with the simple k-d tree implementation within 3DTK.

3.1 Octree

Our octree code implements a novel search algorithm as presented in this section. It is written in ISO/IEC C++ 2003 and is integrated into the 3DTK framework as a visualization, shape detection and NNS data structure. It does not rely on other libraries to store its nodes and geometry data as it is optimized for memory efficiency [24]. It is templated to allow for choosing the precision of the point data.

Principally, octrees should allow for extremely efficient implementations of NNS. Due to their regular partitioning of the search space and the high branching factor, coordinate queries are very fast [25]. Yet, most NN libraries are based on k-d trees.

The complication is due to the fact that during NNS, nodes near the query point must be visited. Thus an order of traversal must be found that is both efficient, in that it visits no more nodes than necessary, and easy to compute. The key to an efficient traversal is the order in which children are visited. The number of nodes that need to be visited is best reduced by the closest-child first criteria, i.e. the order of traversal is determined by the distance to the query point. This is trivial to do for the binary k-d tree, but more involved for an octree.

For any node with 8 children there are a total of 96 possible sequences in which to traverse the children. A query point may fall into or be closest to any one of the 8 octants. This is the first child to traverse. For each of those cases there are 12 possibilities in which to traverse further. This is determined by the proximity of the query point to the 3 split planes. The next two children to visit are, in order, the two closest of the three direct neighbors of the first child. The fourth child to visit is either the last remaining direct neighbor or the node that complements the cuboid of visited nodes. The sequence in which to visit the remaining four nodes is entirely dependent on the traversal before and can not change. Thus, there are $8 \cdot 3 \cdot 2 \cdot 2 = 96$ possible traversals in whole.

### Algorithm 1 FindClosest

Input: query point $q$, maximal allowed distance $d$
look up deepest node $N$ containing bounding box of $q$
convert $q$ to octree coordinate $i$
return FindClosestInNode($N$, $q$, $i$, $d$)

### Algorithm 2 FindClosestInNode

Input: query point $q$ and its coordinate $i$
Input: maximal allowed distance $d$ and the current node $N$
1: compute child index $c$ from $i$
2: for $j = 0$ to 7 do
3: get next closest child $C = N$.children[sequence$[c]$[($j$)]]
4: if $C$ is outside of bounding ball then
5: return currently closest point $p$
6: else
7: if $C$ is a leaf then
8: FindClosestInLeaf($C$, $q$, $d$)
9: update currently closest point $p$
10: else
11: FindClosestInNode($C$, $q$, $i$, $d$)
12: update currently closest point $p$
13: end if
14: end if
15: end for
16: return currently closest point $p$

NNS in an octree has to make proximity calculations to 3 split planes, sort the distances and select the appropriate sequence of traversal for every traversed node. Compared to this, the order of traversal in a k-d tree is instantly determined by a single proximity check, thereby avoiding unnecessary computations if nodes need not be visited.

However, the regular subdivisions of an octree can still be leveraged for fast NNS. The biggest benefit is that fast indexing is possible in an octree. This allows us to directly traverse to the deepest octree node, which contains the bounding sphere of the query point. This is done with a constant number of floating-point operations and is considerably faster than the equivalent operation in a k-d tree, which is essentially a lookup of a point already in the tree. However, the speedup gained is clearly dependent on the maximal distance allowed to the query point. The smaller this distance is, the deeper the node enclosing the bounding sphere is on average. The closest child first NNS with backtracking is then performed on this node, i.e. the deeper the node, the fewer the number of steps needed in the NNS.

The number of floating-point operations needed to choose the correct order of traversal out of the 96 possibilities at each node is exceedingly high. By restricting ourselves to 8 possible traversals it is possible to eliminate the need for any floating point operations in the inner nodes. The order of traversal is decided by which octant the query point is closest to. This is done in accordance to Frisken and Perry [25] and requires no floating-point operations. Each of the 8 traversals are identical in nature, first the closest octant is visited, then the three direct neighbors, then the three direct neighbors of those and
finally the most distant node. The approach is summarized in Algorithm 1. The function FindClosestInLeaf is the NNS inside a leaf, a floating-point proximity check of all stored points.

3.2 k-d tree

Our fast k-d tree implementation is called libnabo [6]. Its tree creation and search algorithm is similar to ANN [26], a well-established library [3], but it differs in the implementation details, which significantly improves performance (see Section 5). libnabo is written in ISO/IEC C++ 2003 and provides a nearest-neighbor–search interface, allowing to easily add new search strategies through inheritance. The current version of libnabo provides a brute-force strategy for comparison purpose and the kd-tree strategy. Geometry data are stored in Eigen 3 [27] structures, as this library is quickly becoming a standard for linear algebra in robotics research\(^1\). Other data such as the neighbors heap and the tree nodes are stored in STL containers, such as std::vector.

For creating the tree, libnabo uses the sliding-midpoint rule, that is, when considering a cuboid, it tries to cut it by the middle on its dimension of maximal extent. If this results in a trivial split, that is, if there is one side with no points, libnabo moves the splitting plane such that there is at least one point on each side. The search algorithm is also similar to ANN, doing a recursive descent on the side of the cutting plane the closest to the search point; and exploring alternative branches while going back up until the \(k\) NN are closer than the cutting planes. Algorithm 3 gives an overview of this method. Initially, the minimum distances \(D\) to other points for every dimension and their norm \(r\) are 0. The heap \(H\) of size \(k\) holds the current candidates for the \(k\) NN and allows fast check and insertion. libnabo provides two implementations, a linear- and a tree-based heap. The linear heap is suitable for small \(k\), as it has a complexity of \(O(k)\) with a small constant while the tree heap is in \(O(\log k)\) but with a larger constant. We have experimentally found that up to \(k = 30\), the linear version is faster. Note that \(D\) and \(H\) are passed as mutable references. The other parameters are either passed as constant references or as mutable values.

The difference with ANN lies at the level of data structures. Where ANN employs a tree of objects based on pointers, libnabo uses a compact vector of nodes. To understand why this difference is significant, let us consider floating-point data on a 64-bit architecture and compute the memory footprint. For every split node, ANN holds the cutting dimension (4 bytes), the cutting value (4 bytes), the lower and the upper bounds (8 bytes), and pointers to left and right children (16 bytes). Moreover, the node being a virtual object, it holds at least a pointer to its viable (8 bytes). Therefore, a single node consumes at least 40 bytes of memory. On the contrary, libnabo’s node is a non-virtual class\(^2\) that contains only the cutting dimension and index of right child (first 4-bytes word), and a union of the cutting value or the bucket index (second 4-bytes word). Indeed, if the cutting dimension (the least-significant bits of the first word) is smaller than the number of dimensions, the node is a split node and the second word contains the cutting value. In this case, the left child is the index of this node plus one, and the right child is encoded in the most-significant bits of the first word. On the contrary, if the cutting dimension is equal to the number of dimensions, this node is a leaf node and the second word contains the index of the bucket. This index points to a dense array of point indices, allowing the search algorithm to access the points. Therefore, a node in libnabo is only 8 bytes, a 5-fold spare in memory compared to ANN.

4 EXPERIMENTAL METHODOLOGY

Many factors influence the performance of a NNS query. One factor is the maximal distance parameter, which restricts the search space around the query point. The larger the maximal distance the more of the space the search routine must explore. A second factor is the type of data on which the NN query is being performed. Some data may result in optimally constructed data structures, while others may lead to unfavorable configurations. For this reason we carry out experiments on a

\(^1\) it is being used by ROS and MRPT for instance

\(^2\) Note that the node class is a private inner class in a subclass of the nearest-neighbor–search interface. This interface is implemented as a superclass with virtual members and a static factory function. Thus libnabo is extensible through inheritance.

Algorithm 3 LibnaboFindClosest

**Input:** query point \(q\), node \(N\), heap \(H\), minimum distance \(r\),

**Input:** minimum offsets \(D\), maximal squared allowed distance \(l\)

if \(N\) is a leaf node

- search for closest points to \(q\) in bucket pointed by \(N\)
- update \(H\)

else

- get cut dimension \(c\) and cut value \(v\) from \(N\)
- if \(o_{\text{new}} > 0\) then
  - LibnaboFindClosest\((q, \text{rightChild}(N)), H, r, D, l\)
  - if \(r \leq l\) and \(r < \text{head}(H)\) then
    - \(D[c] = o_{\text{new}}\)
    - LibnaboFindClosest\((q, \text{leftChild}(N)), H, r, D, l\)
    - \(D[c] = o_{\text{old}}\)
  - end if
- else
  - LibnaboFindClosest\((q, \text{leftChild}(N)), H, r, D, l\)
  - if \(r \leq l\) and \(r < \text{head}(H)\) then
    - \(D[c] = o_{\text{new}}\)
    - LibnaboFindClosest\((q, \text{rightChild}(N)), H, r, D, l\)
    - \(D[c] = o_{\text{old}}\)
  - end if
- end if
Fig. 1. Three pairs of real point clouds are used in our experiments. The top data set is a pair of 3D scans that was acquired by an actuated SICK LMS200 laser scanner in an office environment with $\approx 80,000$ points each. The data set in the middle has been acquired by the Microsoft Kinect in an office environment. The clouds contain $\approx 290,000$ points each and are relatively dense. Data courtesy of Jochen Sprickerhof of University of Osnabrück. The data set on the bottom is a high resolution scan taken in the historic city center of Bremen using the Riegl VZ-400 3D scanner. The point clouds contain $\approx 16,000,000$ points each.

multitude of data, both artificial and real. The artificial point clouds are two geometrical primitives each in a hollow and filled variants. It should be noted, that for shape registration the hollow variants are more reminiscent of real data. Shape matching is almost exclusively done on surface data as most devices that capture 3D data like laser scanners and stereo camera acquire only such data. For each data set we have randomly generated 60,000 points in or on the geometrical primitive. We chose this number because it enables us to do a large number of tests while still maintaining experiments that are representative. We choose two shapes, a sphere with a radius of 1 and a cube of side length 2.

In addition to the tests on the artificial data sets, we run experiments under real conditions, i.e. data acquired by 3D range finders with parameters that produce the optimal registration. For this purpose we selected 3 pairs of point clouds that are representative of different types of sensors (see Fig. 1).

For the k-d trees a factor that influences average running time is the splitting strategy. Of the libraries used in this paper, only ANN supports changing the splitting rule. We use the rule suggested by the author’s the sliding midpoint rule [28]. This rule is also used by libnabo. 3DTK’s k-d tree as well as FLANN split the volume of a node along the largest side of
the bounding box of the contained points. CGAL employs the standard median splitting rule along an axis dependent on the level of the tree.

Another notable parameter is the minimal number of points per leaf in the data structure, i.e. the bucket size. The smaller the bucket size is the larger is the overhead of the additional levels in the tree. The larger the bucket size the more points will have to be searched in a linear fashion. An evaluation on the SICK LMS200 data set (cf. Fig. 2), reveals that a bucket size between 5 and 20 is usually optimal. However, these results are not entirely representative and depend on the data sets used. In our experiments on artificial data, where trends are observed rather than absolute comparisons to be made, we use the default bucket size of the respective libraries, with two exceptions. In both FLANN and SpatialIndex we set the bucket size to be 10. This is also the default for most other libraries. In FLANN there is no default bucket size, so a choice had to be made. For SpatialIndex the default is 100 because it is intended that the data structure is cached to disk. However we run SpatialIndex in main memory and a bucket size of 100 gives significantly worse performance. For the experiments under real conditions the absolute running time instead of the trends in the runtime is the most important criteria. To provide clear results we set the bucket sizes to the optimal size as derived from Fig. 2, i.e. 5 for libnabo and 15 for both 3DTK data structures and FLANN. ANN does not allow for the changing of the bucket size.

Approximate search algorithms for the k-d tree, i.e. NNS with no guarantee of finding the exact NN, exist [29] but we opt to only test the exact NNS, since only this is implemented by all libraries. We use two variants of the R-tree for our experiments, the quadratic R-tree and the R*-tree. The exponential R-tree is not implemented in SpatialIndex, and the quadratic variant outperforms the linear one in all our experiments. Three libraries, ANN, FLANN and libnabo support more than a single NN query. Since ANN and FLANN do not support the ranged search, both queries are tested for both libraries. For libnabo, only the ranged search is tested as the k-NN search is implemented as a special case of the ranged search.

We compare a large set of NNS libraries: 3DTK, ANN, CGAL, FLANN, libnabo, SpatialIndex and STANN. Most of these rely on the k-d tree, in fact of these 3DTK is the only library implementing the octree, SpatialIndex the only one to rely on R-trees and STANN is the only one using SFCs. Only very few libraries feature multithreading capabilities, therefore all experiments were performed in single-threaded mode. The results of every library on a handful of chosen testcases has been compared to each other to confirm their correctness.

All libraries were compiled with the gnup compiler collection version 4.4.3 on optimization level 3. The system running all experiments is a 64 Bit Xubuntu Linux (kernel 2.6.32-27) with an Intel(R) Xeon(R) E5520@2.27GHz and 12 GB of memory.

5 Results

The most extensive experiments were done on the aforementioned artificial data sets. For each library we varied the maximal range allowed for the NN from 0 to 1 in steps of 0.02. We repeated the NNS in 100 trials, and plotted the averaged running time.

An interesting combinations of query and model data set is presented in Fig. 3. It is a combination that resembles shape matching most closely, as both the query data set (the cube) and the model data set (the sphere) are surfaces. Clearly, the runtime of the ranged and fixed radius search depend strongly on the maximal distance. The larger the allowed distance, the more query points (near the cube’s corners) have a NN. The more NN that need to be found, and the farther away these are, the longer the search will need to finish. Larger distances affect the fixed radius search algorithms significantly.

![Fig. 2. ICP runtime in seconds on the SICK LMS200 data set.](image)

![Fig. 4. The average times needed for creating different data structures. Note, that due to the large differences in the times the y-axis has been split into a linear and logarithmic scale.](image)
more than the ranged searches. The runtime for the fixed radius search continues to rise polynomially, whereas the ranged searches level off near $\sqrt{3} \approx 0.73$, which is the maximum possible distance in the data set. The runtime of the \textit{k-NN} search is of course not influenced by the maximal distance. Most of them are significantly slower than the ranged searches. Due to the polynomial behavior of the runtime of the fixed radius algorithms all of the \textit{k-NN} are faster for large enough maximal distances. However, only the ANN and FLANN library perform similar or better than the ranged searches for large enough maximal distances. Similar behavior is exhibited in other combinations. For an overview see Fig. 6.

Note, that due to the large differences in running time, the time is on a logarithmic scale. For plots on a linear scale see Fig. 7. There is a large discrepancy in the running time for the search libraries. This discrepancy falls quite neatly along the lines of which type of algorithm is implemented. In almost all cases the best performing \textit{NN} libraries were those implementing the ranged search, i.e. 3DTK and libnabo. The libraries only implementing \textit{k-NN} search, i.e. STANN, CGAL and SpatialIndex can not compete with other algorithms. The remaining libraries, ANN and FLANN are in a few cases faster than some ranged search implementations. For a clearer look into this region, please see Fig. 7. In all non-trivial cases, i.e. when the query data set and the model data set are distinct, libnabo is faster than both FLANN and ANN. There are 2 exceptions to this, where libnabo is equal in runtime to FLANN and ANN. This occurs when the maximal range is at significant fractions of the point clouds size, i.e. $\approx \frac{1}{3}$ to $\frac{1}{2}$. This is also the range at which FLANN and ANN start to beat the other ranged search algorithms. Before this the ranged search implementations are faster than both the \textit{k-NN} search implementations and the fixed radius search implementations.

For shape matching the region of smaller maximal distances are crucial. During the matching process the point clouds move closer towards each other. The average point to point distance is inherently reduced. The effect this has on the runtime of the \textit{NNS} can be tracked on the rightmost column in Fig. 6 and Fig. 7. On the top, the query points (hollow cube) are farthest away from the model data set. The points are closer with the filled cube, even closer with the hollow sphere and finally identical with the filled sphere. The ranged searches as well as the \textit{k-NN} searches speed up due to this progression, whereas the fixed radius search actually slow down.

However, absolute comparisons of the runtime may not be valid based on these results alone when the runtime difference is only several hundreds of milliseconds. Differences may be caused by non-optimal bucket sizes (cf. 4) or by the artificial nature of the data sets. In addition to the artificial data sets, we therefore also compare the runtime of the 5 top performing libraries on real data sets. To ensure bucket sizes play no role in these results, we have chosen the optimal values as per Fig. 2. The results are presented in Fig. 5. The previous trend of the ranged search libraries performing better than FLANN and ANN continues. For the smaller data sets the \textit{k-NN} search performs with similar speeds as the ranged search. For the large data set acquired by professional hardware, the performance is significantly worse. The fixed radius search can compete with the ranged search in the latter case but is significantly worse in the smaller data sets. In contrast to the experiments with artificial data, libnabo tends to perform slightly worse than the 3DTK algorithms on real data sets. This is likely due to the added overhead of converting the query data set into data usable by libnabo, i.e. the 3DTK \textit{NNS} has a home field advantage.

All previous experiments were concerned with the runtime...
of the NNS and excluded the time needed to construct the data sets. Fig. 4 shows the average time for construction for all data structures and every point cloud used in the previous experiments as a model data set. On the whole the libraries perform similarly, except for STANN and SpatialIndex, the latter of which is especially slow. Compared to the time needed for the NNS (Fig. 7) and the ICP (Fig. 5) the construction time is usually negligible, especially considering that the data structure needs to be constructed only once for the entire registration process.

We see that libnabo is always faster than ANN, sometimes by a small amount, often by at least a factor of two, and sometimes much more. As both libraries implement the same algorithm, this discrepancy is solely due to the compactness of libnabo’s data structures, that consume at least 5 times less memory than ANN’s. This is important, because modern computer architectures have multiple levels of cache, and thus memory access is often the bottleneck [30]. The compactness provided by libnabo comes at the price of additional and repeated computations during the exploration of the tree. Yet these work on local variables that are easily contained in cache level 1. This shows that the NNS problem is clearly memory-bound in general and that the choice of compactness is sound.

6 Conclusion

We have made a significant finding regarding the type of search algorithm to use for shape registration. Ranged search queries are ideally suited for shape matching and beat the alternatives in all relevant cases. The reason for this is that shape registration purposefully minimizes the distance to the NN. In the beginning of the registration process the NN range is at its largest. Most ICP iterations are done when the NN range is very small. In fact, the maximal range to begin with is usually only a small fraction of the point clouds’ extent. For our artificial data sets a maximal range of $\approx \frac{1}{2}$ constitutes the largest reasonable range for shape matching.

There is yet another complication for the fastest alternatives to ranged search, i.e. FLANN and ANN in these regions. Choosing between the $k$-NN and the fixed search is non-trivial. This would involve guessing which of the two is more efficient for a given data set and a given maximal range. Since the runtime of the fixed radius search explodes for large ranges, a shape registration library would have to default to $k$-NN search. The performance of $k$-NN search is reasonable on average, but bad in just the region that is important for shape matching.

Since most libraries implement only the k-d tree, it is hard to draw final conclusions as to what data structure is better suited for NNS. The R-tree library SpatialIndex performs about on par to the STANN library. Both were generally slower than the k-d tree implementations. The octree implementation was amongst the best performing algorithms. This effect may not be due to the data structures alone. As Table 1 shows, SpatialIndex was optimized for GIS systems, STANN for multithreaded application while the octree implementation was designed to be used in shape matching.

We have contributed our own novel open-source implementation of NNS and have shown these to perform well on realistic as well as artificial shape registration problems. We have shown that for similar algorithms, the compactness of data structures plays a critical role and carefully-designed structures can double performances.

Supplemental Material

We provide the code as well as the data used to perform all experiments in this paper. Everything is available as a subversion repository under http://slam6d.svn.sourceforge.net/viewvc/slam6d/branches/NNS/. The implemented search algorithms are freely available under http://slam6d.sourceforge.net and https://github.com/ethz-asl/libnabo.

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REFERENCES


[28] S. Maneewongvatana and D. M. Mount, “It’s okay to be skinny, if your friends are fat,” ReCALL, pp. 1–8, October 1999.


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Fig. 6. The results from all algorithms for the artificial data sets on a logarithmic scale. The images on the $x$-axis indicate the data set that was stored in the data structure (model set). The images on the $y$-axis indicate the query point set. The query time in seconds required for the entire data set is plotted on a logarithmic scale for all settings of the maximal allowed distance. The maximal distance was altered between 0 and 1 in steps of 0.02. Construction time for the data structures is not included.
Fig. 7. The results from the best performing algorithms for the artificial data sets on linear scale. Note that the scale has also been changed from 0 to 1 s.