

Efficient and robust approximate nearest neighbor search using Hierarchical Navigable Small World graphs

Yu. A. Malkov, D. A. Yashunin

Abstract— We present a new algorithm for the approximate K-nearest neighbor search based on navigable small world graphs with controllable hierarchy (Hierarchical NSW). The proposed approach is fully graph-based, without any need for additional search structures, which are typically used at the coarse search stage of the most proximity graph techniques. Hierarchical NSW incrementally builds multi-layer structure consisting from hierarchical set of proximity graphs (layers) for nested subsets of the stored elements. The maximum layer in which an element is present is selected randomly with an exponentially decaying probability distribution. This allows producing graphs similar to the previously studied Navigable Small World (NSW) structures while additionally having the links separated by their characteristic distance scales. Starting search from the upper layer together with utilizing the scale separation boosts the performance compared to NSW and allows a logarithmic complexity scaling. Additional employment of a heuristic for selecting proximity graph neighbors significantly increases performance at high recall and in case of highly clustered data. Performance evaluation has demonstrated that the proposed general metric space search index is able to strongly outperform many previous state-of-the-art vector-only approaches. Similarity of the algorithm to the skip list structure allows straightforward balanced distributed implementation.

Index Terms—Graph and tree search strategies, Artificial Intelligence, Information Search and Retrieval, Information Storage and Retrieval, Information Technology and Systems, Search process, Graphs and networks, Data Structures, Nearest neighbor search, Big data, Approximate search, Similarity search

1 INTRODUCTION

Constantly growing amount of the available information resources has led to high demand in scalable and efficient similarity search data structures. One of the generally used approaches for information search is the K-Nearest Neighbor Search (K-NNS). The K-NNS assumes you have a defined distance function between the data elements and aims at finding the K elements from the dataset which minimize the distance to a given query. Such algorithms are used in many applications, such as non-parametric machine learning algorithms, image features matching in large scale databases [1] and semantic document retrieval [2]. A naïve approach to K-NNS is to compute the distances between the query and every element in the dataset and select the elements with minimal distance. Unfortunately, the complexity of the naïve approach scales linearly with the number of stored elements making it infeasible for large-scale datasets. This has led to a high interest in development of fast and scalable K-NNS algorithms.

Exact solutions for K-NNS [3-5] may offer a substantial search speedup only in case of relatively low dimensional data due to “curse of dimensionality”. To overcome this problem a concept of Approximate Nearest Neighbors Search (K-ANNS) was proposed, which relaxes the condition of the exact search by allowing a small number of

errors. The quality of an inexact search (the recall) is defined as the ratio between the number of found true nearest neighbors and K . Most popular K-ANNS solutions are based on approximated versions of tree algorithms [6, 7], locality-sensitive hashing (LSH) [8, 9] and product quantization (PQ) [10-17]. Proximity graph K-ANNS algorithms [10, 18-26] have recently gained popularity offering a better performance on high dimensional datasets. However, the power-law scaling of the proximity graph transversal causes extreme performance degradation in case of low dimensional or clustered data making them unusable in those cases.

In this paper we propose the Hierarchical Navigable Small World (Hierarchical NSW, HNSW), a new fully graph based incremental K-ANNS structure, which can offer a much better logarithmic complexity scaling. The main contributions are: explicit selection of the graph’s enter-point node, separation of links by different scales and use of an advanced heuristic to select the neighbors. Alternatively, Hierarchical NSW algorithm can be seen as an extension of the probabilistic skip list structure [27] with proximity graphs instead of the linked lists. Performance evaluation has demonstrated that the proposed general metric space method is able to strongly outperform many previous state-of-the-art approaches suitable only for vector spaces.

• Y. Malkov is with the Federal state budgetary institution of science Institute of Applied Physics of the Russian Academy of Sciences, 46 Ul'yanov Street, 603950 Nizhny Novgorod, Russia. E-mail: yurymalkov@mail.ru.
• D. Yashunin. Address: 31-33 ul. Krasnoyevzdnaya, 603104 Nizhny Novgorod, Russia. E-mail: yashuninda@yandex.ru

2 Related works

2.1 Proximity graph techniques

In the vast majority of studied graph algorithms searching takes a form of greedy routing in k-Nearest Neighbor (k-NN) Graphs [10, 18-26]. For a given proximity graph, we start the search at some enter point (it can be random or supplied by a separate algorithm) and iteratively traverse the graph. At each step of the transversal the algorithm examines the distances to the connections of a current base node and then selects as the next base node the adjacent node that best minimizes the distance, while constantly keeping track of the best discovered neighbors. The search is terminated when some stopping condition is met (e.g. the number of distance calculations).

The main drawbacks of this approach are: 1) the power law scaling of the number of steps with the dataset size during the routing process if starting from a random or a fixed node [28, 29]; 2) a possible loss of global connectivity when using k-NN graphs which leads to poor search results. To overcome these problems many hybrid approaches have been proposed that use auxiliary algorithms applicable only for vector data (such as kd-trees [18, 19] and product quantization [10]) to find better candidates for the initial nodes by doing a coarse search.

In [25, 26, 30] authors proposed a proximity graph K-ANNS algorithm called Navigable Small World (NSW, also known as Metricized Small World, MSW), which utilized *navigable* graphs, i.e. graphs with logarithmic or polylogarithmic scaling of the number of hops during the greedy transversal with the respect of the network size [31, 32]. The NSW graph is constructed via consecutive insertion of elements in random order by bidirectionally connecting them to M closest neighbors from the previously inserted elements. Links to the closest neighbors of the elements inserted in the beginning of the construction later become bridges that keep the overall graph connectivity and allow the greedy hop logarithmic scaling.

The NSW algorithm uses a variant of the greedy search with the overall polylogarithmic time complexity and delivered the state-of-the-art performance on some datasets [33, 34]. However, of the overall polylogarithmic complexity scaling the algorithm still causes severe performance degradation on many of low dimensional datasets, where NSW can lose to tree-based algorithms by orders of magnitude [34].

2.2 Navigable small world models

Networks with logarithmic or polylogarithmic scaling of the greedy graph transversal are known as the navigable small world networks [31, 32]. Such networks are an important topic of complex network theory aiming at understanding of real-life networks formation underlying mechanisms in order to apply them for applications of scalable routing [32, 35, 36] and distributed similarity search [25, 26, 30, 37-40].

The first works to consider spatial models of navigable networks were done by J. Kleinberg [31, 41] as social network models for the famous Milgram experiment [42].

Kleinberg studied a variant of random Watts-Strogatz networks [43], using a regular lattice graph in d -dimensional vector space together with augmentation of long-range links following a specific long link length distribution $r^{-\alpha}$. For $\alpha=d$ the number of hops to get to the target by greedy routing scales polylogarithmically (instead of a power law for any other value of α). This idea has inspired development of many K-NNS and K-ANNS algorithms based on the navigation effect [37-40]. But while Kleinberg's navigability criterion in principle can be extended for more general spaces, in order to build such a navigable network one has to know the data distribution beforehand. In addition, the routing process suffers from a polylogarithmic complexity scalability at best.

Another well-known class of navigable networks are the scale-free models [32, 35, 36], which can reproduce several features of real-life networks and advertised for routing applications [35]. Networks produced by such models, however, have even worse power law complexity scaling of the greedy search [44] and, just like the Kleinberg's model, scale-free models require global knowledge of the data distribution, making them unusable for search applications.

The NSW algorithm uses a simpler, previously unknown model of navigable networks, allowing decentralized graph construction and suitable for data in arbitrary spaces. It was suggested [44] that the NSW network formation mechanism may be responsible for navigability of large-scale biological neural networks (presence of which is disputable): similar models were able to describe growth of small brain networks, while the model predicts several high level features observed in large scale neural networks. However, the NSW model also suffers from the polylogarithmic search complexity of the routing process. It is an open question whether a single layer network can have a logarithmic scalability of greedy routing in principle.

3 Motivation

The ways of improving the NSW search complexity can be identified through the analysis of the routing process, which was studied in detail in [32, 44]. The routing can be divided into two phases: "zoom-out" and "zoom-in" [32]. The algorithm starts in the "zoom-out" phase from a low degree node and traverses the graph simultaneously increasing the node's degree until the characteristic radius of the node links length reaches the scale of the distance to the query. Before the latter happens, the average degree of a node can stay relatively small, which leads to an increased probability of being stuck in a distant false local minimum.

One can avoid the described problem in NSW by starting the search from a node with the maximum degree (good candidates are the first nodes inserted in the NSW structure [44]), directly going to the "zoom-in" phase of the search. Tests show that setting hubs as starting points substantially increases probability of successful routing in the structure and offers significantly better performance at low dimensional data. However, it still has only a polylogarithmic complexity scalability of a single greedy

search at best and performs worse on high dimensional data compared to unmodified NSW.

The reason for the polylogarithmic complexity scaling of a single greedy search in NSW is that the overall number of distance computations is roughly proportional to a product of the average number of greedy algorithm hops by the average degree of the nodes on the greedy path. The average number of hops scales logarithmically [26, 44], while the average degree of the nodes on the greedy path also grows logarithmically due to the facts that: 1) the greedy search tends to go through the same hubs as the networks grows [32, 44]; 2) the number of hub connections is growing logarithmically with an increase of the network size. Thus we get an overall polylogarithmic dependence of the resulting complexity.

The idea of Hierarchical NSW algorithm is to separate the links according to their length scale, producing a multi-layer graph. In this case we can evaluate only a needed portion of the connections for each element independently of the networks size, thus getting a logarithmic scalability at the “zoom-in” phase (see Fig. 1 for illustration). The search starts from the upper layer greedily selecting elements only from the layer until a local minimum is reached. After that, the search switches to the lower layer and restarts from the element which was the local minimum in the previous layer. The average number of connections per element in all layers can be made constant, thus allowing getting a logarithmic complexity scaling.

One way to form such a layered structure is to explicitly set links with different distance scales by artificially introducing layers. For every element we select an integer *level* which defines the maximum layer for which the element belongs to. For all elements that are present in a layer a proximity graph (i.e. graph containing only “short”

links that approximate Delaunay graph) is built incrementally. If we set an exponentially decaying probability of item’s *level* (i.e. following a geometric distribution) we get a logarithmic scaling of the number of layers in the structure. The search procedure is an iterative greedy search starting from the top layer.

In case we merge connections from all layers, the structure becomes similar to the NSW graph (in this case the *level* can be put in correspondence to the node degree in NSW). Note that in contrast to NSW, Hierarchical NSW construction algorithm does not require the elements to be inserted in random order, the randomization is achieved by using random levels.

The Hierarchical NSW idea is also very similar to a well-known 1D probabilistic skip list structure [27] and can be described using its terms. The major difference to skip list is that we generalize the structure by replacing the linked list with proximity graphs. The Hierarchical NSW approach thus can utilize the same methods for making the distributed approximate search/ overlay structures [45].

For selection of the proximity graph connections during the element insertion we utilize a heuristic that takes into account the distances between the candidate elements to create diverse connections (a similar algorithm was utilized in the spatial approximation tree [4] to select the tree children) instead of just selecting the closest neighbors. The heuristic examines the candidates starting from the closest and creates a connection to a candidate only if it is closer to the base element compared to any of the already connected elements (see Section 4 for the details).

When the number of candidates is large enough the heuristic allows getting the exact relative neighborhood graph [46] (an exact superset of which was also used in [18] for proximity graph searching), a minimal sub-

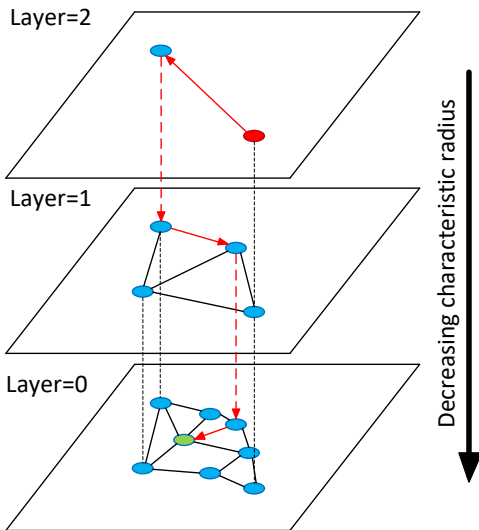


Fig. 1. Illustration of the Hierarchical NSW idea. The search starts from an element from the top layer (shown red). Red arrows show direction of the greedy algorithm from the entry point to the query (shown green).

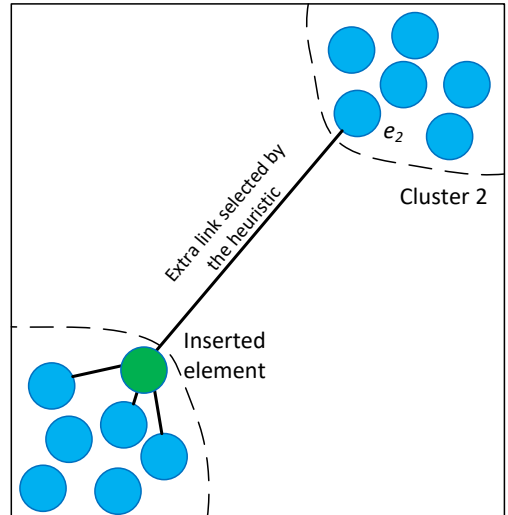


Fig. 2. Illustration of the heuristic used to select the neighbors in the proximity graph. The data in the example consists from two isolated clusters.

A new element is being inserted on the boundary of the first cluster. All of the closest neighbors of the new element are belong to the same (first) cluster thus missing the Delaunay graph links between the clusters. The heuristic, however, selects an element e_2 from second cluster maintaining the global connectivity in case the inserted element is the closest to e_2 compared to any other element from Cluster 1.

graph of the Delaunay graph deducible by using only the distances between the nodes. The relative neighborhood graph allows easily keeping the global connected component, even in case of highly clustered data (see Fig. 2 for illustration). Note that the heuristic creates many extra connections compared to the exact relative neighborhood graph, allowing to control the connections number which is important for search performance. For the case of 1D data the heuristic allows getting the exact Delaunay sub-graph (which in this case coincides with the relative neighborhood graph) by using only information about the distances between the elements, thus making a direct transition from Hierarchical NSW to the 1D probabilistic skip list algorithm.

Similar heuristic was a focus of the FANNG algorithm [47] (published shortly after the first versions of the current manuscript were posted online) with a slightly different interpretation, based on the relative neighborhood graph's property of the exact routing [18].

4 Algorithm description

Network construction algorithm is organized via consecutive insertions of the stored elements into the graph structure. For every inserted element an integer maximum layer *level* is randomly selected with an exponentially decaying probability distribution (normalized by the *levelMult* parameter, see alg. 1).

The first phase of the insertion process starts from the top layer by greedily traversing the graph in order to find the closest neighbor in the layer. After the algorithm finds a local minimum in the layer, it continues the search from the next layer using the found closest neighbors from previous layer as enter points, and the process repeats. Closest neighbors at each layer are found by a variant of the greedy search algorithm described in alg. 2, which is an updated version of the algorithm from [26]. To obtain the approximate *K* nearest neighbors in some layer *level*, a dynamic list of *ef* closest of the found elements (initially filled with enter points) is kept during the search. The list is updated at each step by evaluating the neighborhood of the closest previously non-evaluated element in the list until the neighborhood of every element from the list is evaluated. Such stop condition avoids bloating of search structures by discarding elements that are not fit to the list. As in NSW, the list is emulated via *cQueue* and *wQueue* priority queues for better performance. The distinctions from NSW algorithm (along with some queue optimizations) is that: 1) the enter point is a fixed parameter; 2) instead of changing the number of multi-searches, the quality of the search is controlled by a different parameter *ef* (which was set to *K* in NSW [26]). During the first phase of the search the *ef* parameter is set to 1 (simple greedy search).

When the search reaches the layer that is equal or less than *level*, the second phase of the construction algorithm is initiated. The second phase differs in two points: 1) the *ef* parameter is increased from 1 to *efConstruction* in order to control the recall of the greedy search procedure; 2) the found closest neighbors on each level are also used as candidates for the connections of the inserted element.

Algorithm 1

```

INSERT(hnsw, q, M, efConstruction, levelMult)
1 wQueue = NIL // MIN-PRIORITY-QUEUE
  // key – distance to q
2 visSet = {}
3 epSet = {hnsw.entPoint}
4 efOne = 1
5 level = [-ln(RANDOM(0..1)) • levelMult] // Select a random level
  // with an exponential
  // distribution
6 for l = hnsw.maxLayer downto level+1
7   wQueue = SEARCH-LEVEL(hnsw, q, epSet, efOne, l)
8   epSet = {MIN(wQueue)}
9 for l = min(hnsw.maxLayer, level) downto 0
10  wQueue = SEARCH-LEVEL(hnsw, q, epSet, efConstruction, l)
11  neighborsSet = SELECT-NEIGHBORS(q, wQueue, M, l)
  // alg. 3 or alg. 4
12 bidirectionally connect elements from neighborsSet to q
13 for each e ∈ neighborsSet // shrink lists of connections
14   eConnSet = hnsw.adj(e, l)
15   if eConnSet.size > hnsw.Mmax
16     eConnQueue = MIN-PRIORITY-QUEUE(eConnSet)
17     eNewConnSet = SELECT-NEIGHBORS(e, eConnQueue,
  hnsw.maxM, l) // alg. 3 or alg. 4
18   hnsw.adj(e, l) = eNewConnSet
19 epSet = SET(wQueue)
20 if level > hnsw.maxLayer // update hnsw.entPoint
21   hnsw.maxLayer = level
22   hnsw.entPoint = q

```

Algorithm 2

```

SEARCH-LEVEL(hnsw, q, epSet, ef, l)
1 visSet = epSet
2 cQueue = MIN-PRIORITY-QUEUE(epSet) // key – distance to q
3 wQueue = MAX-PRIORITY-QUEUE(epSet) // key – distance to q
4 while cQueue.size > 0
5   c = EXTRACT-MIN(cQueue)
6   if DIST(c, q) > DIST(MAX(wQueue), q)
7     break // all elements in the list are evaluated
8   for each e ∈ hnsw.adj(c, l) // update cQueue and wQueue
9     if e ∉ visSet
10      visSet = visSet ∪ e
11      if DIST(e, q) < DIST(MAX(wQueue), q) or wQueue.size < ef
12        INSERT(cQueue, e)
13        INSERT(wQueue, e)
14        if wQueue.size > ef
15          EXTRACT-MAX(wQueue)
16 resQueue = MIN-PRIORITY-QUEUE(wQueue) // key – distance to q
17 return resQueue

```

Two methods for the selection of *M* neighbors from the candidates were considered for the algorithm: simple connection to the closest elements (alg. 3) and the heuristic that accounts for the distances between the candidate elements to create connections in diverse directions (alg. 4), described in the Section 3. The heuristic has two additional parameters: *extendCandidates* (set to False by default) which extends the candidate set and useful only for extremely clustered data, and *keepPrunedConnections* which allows getting fixed number of connection per element. The maximum number of connections that an element can have per layer is defined by the parameter M_{\max} for every layer higher than zero (a special parameter $M_{\max 0}$ is used for the ground layer separately). If a node is already full at the moment of making of a new connection, then its extended connection list gets shrunk by the same algorithm that used for the neighbors selection (algs. 3 or 4).

Algorithm 3

```

SELECT-NEIGHBORS-SIMPLE( $cQueue, M$ )
1  $resSet = \{\}$ 
2 for  $i = 0$  to  $M$ 
3    $resSet = resSet \cup \text{EXTRACT-MIN}(cQueue)$ 
4 return  $resSet$ 

```

Algorithm 4

```

SELECT-NEIGHBORS-HEURISTIC( $hmsw, bEl, cQueue, M, l, extendCandidates, keepPrunedConnections$ )
1  $resSet = \{\}$ 
2  $wcQueue = cQueue$  // MIN-PRIORITY-QUEUE,
   // key – distance to  $bEl$ 
3 if  $extendCandidates$ 
4   for each  $e \in cQueue$ 
5     for each  $e1 \in hmsw.adj(e, l)$ 
6       if  $e1 \notin wcQueue$ 
7          $\text{INSERT}(wcQueue, e1)$ 
8    $wSet = \{\}$ 
9   while  $wcQueue.size > 0$ 
10     $e = \text{EXTRACT-MIN}(wcQueue)$ 
11    if  $e$  is closer to  $bEl$  compared to any element from  $resSet$ 
12       $resSet = resSet \cup e$ 
13    else
14       $wSet = wSet \cup e$ 
15    if  $resSet.size > M$ 
16      break
17 if  $keepPrunedConnections$  // add some of the discarded
   // connections
18    $wQueue = \text{MIN-PRIORITY-QUEUE}(wSet)$  // key – distance to  $bEl$ 
19   while  $wQueue.size > 0$ 
20      $resSet = resSet \cup \text{EXTRACT-MIN}(wQueue)$ 
21     if  $resSet.size \geq M$ 
22       break
23 return  $resSet$ 

```

The insertion procedure terminates when the connections of the inserted elements are established on the ground (zero) layer.

The K-ANNS search algorithm used in Hierarchical NSW is presented in alg. 5. It is roughly equivalent to the insertion algorithm for an item with $level=0$. The difference is that the closest neighbors found at ground layer which are used as candidates for the connections are now returned as the search result. The quality of the search is controlled by the ef parameter (corresponding to $efConstruction$ in the construction algorithm).

4.1 Influence of the construction parameters

Algorithm construction parameters $levelMult$ and M_{max0} are responsible for maintaining the small world navigability in the constructed graphs. Setting $levelMult$ to zero (this corresponds to a single layer in graph) and M_{max0} to M leads to production of directed k-NN graphs with a power-law search complexity well studied before [21, 29]

Algorithm 5

```

K-NN-SEARCH( $hmsw, q, K, ef$ )
1  $wQueue = \text{NIL}$ 
2  $epSet = \{hmsw.entPoint\}$ 
3  $efOne = 1$ 
4  $levelZero = 0$ 
5 for  $l = hmsw.maxLayer$  downto 1
6    $wQueue = \text{SEARCH-LEVEL}(hmsw, q, epSet, efOne, l)$ 
7    $epSet = \{\text{MIN}(wQueue)\}$ 
8    $wQueue = \text{SEARCH-LEVEL}(hmsw, q, epSet, ef, levelZero)$ 
9    $resSet = \{\}$ 
10  for  $i = 0$  to  $K-1$ 
11     $resSet = resSet \cup \text{EXTRACT-MIN}(wQueue)$ 
12 return  $resSet$ 

```

(assuming using the alg. 3 for neighbor selection). Setting $levelMult$ to zero and M_{max0} to infinity leads to production of NSW graphs with polylogarithmic complexity [25, 26]. Finally, setting $levelMult$ to some non-zero value leads to emergence of controllable hierarchy graphs with logarithmic search complexity by introduction of layers (see the Section 3).

To achieve the optimum performance advantage of the controllable hierarchy, the overlap between neighbors on different layers (i.e. percent of element neighbors that are also belong to other layers) has to be small. In order to decrease the overlap we need to decrease the $levelMult$. However, at the same time, the decrease of the $levelMult$ leads to an increase of average hop number during a greedy search on each layer, which negatively affects the performance. This leads to existence of the optimal value for the $levelMult$ parameter.

A simple choice for the optimal $levelMult$ is $1/\ln(M)$, this corresponds to the skip list parameter $p=1/M$ with an average single element overlap between the layers. Simulations done on an Intel Core i5 2400 CPU show that the proposed selection of $levelMult$ is a reasonable choice (see Fig. 3 for data on 10M random $d=4$ vectors). In addition, the plot demonstrates a massive speedup on low dimensional data when increasing the $levelMult$ from zero. It is hard to expect the same behavior for high dimensional data since in this case the k-NN graph already has very short greedy algorithm paths [28]. Surprisingly, increasing the $levelMult$ from zero leads to a measurable increase in speed on very high dimensional data (100k dense random $d=1024$ vectors, see plot in Fig. 4), and does not introduce any penalty for the Hierarchical NSW approach. For mid-dimensional data, such as SIFT vectors [1], the performance advantage of increasing the $levelMult$ is moderate (see Fig. 5 for 10-NN search performance on 5 million 128-dimensional SIFT vectors from the learning set of BIGANN [13]).

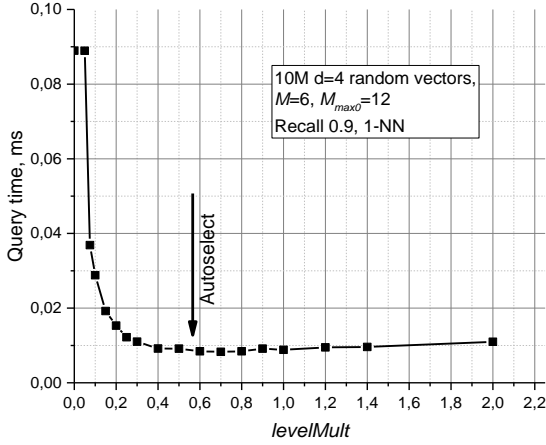


Fig. 3. Plots for query time vs *levelMult* parameter for 10M random vectors with $d=4$. The autoselected value for *levelMult* is shown by an arrow.

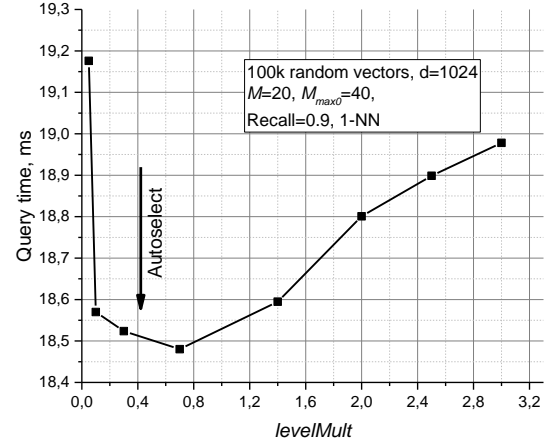


Fig. 4. Plots for query time vs *levelMult* parameter for 100k random vectors with $d=1024$. The autoselected value for *levelMult* is shown by an arrow.

Selection of the M_{max0} (the maximum number of connections that an element can have in the zero layer) also has a strong influence on the search performance, especially in case of high quality (high recall) search. Simulations show that setting M_{max0} to M (this corresponds to k-NN graphs on each layer if the neighbors selection heuristic is not used) leads to a very strong performance penalty at high recall. Simulations also suggest that $2 \cdot M$ is a good choice for M_{max0} : setting the parameter higher leads to performance degradation and excessive memory usage. In Fig. 6 there are presented results of search performance for the 5M SIFT learn dataset depending on the M_{max0} parameter. The suggested value gives performance close to optimal at different recalls.

In all of the considered cases, use of the heuristic for proximity graph neighbors selection (alg. 4) leads to a higher or equal search performance compared to the naive connection to the nearest neighbors (alg. 3). The effect is the most prominent for low dimensional data, at high recall for mid-dimensional data and for the case of highly clustered data (ideologically discontinuity can be regarded as a local low dimensional feature), see the comparison in

Fig. 7. When using the closest neighbors as connections for the proximity graph, the Hierarchical NSW algorithm fails to achieve a high recall for clustered data because the search sticks at the clusters boundaries. Contrary, when the heuristic is used, clustering leads to even higher performance. For uniform and very high dimensional data there is a little difference between the neighbors selecting methods, possibly due to the fact that in this case almost all of the nearest neighbors are selected by the heuristic.

The only meaningful construction parameter left for the user is M . A reasonable range of M is from 5 to 48. Simulations show that smaller M generally produces better results for lower recalls and/or lower dimensional data, while bigger M is better for high recall and/or high dimensional data (see Fig. 8 for illustration). The parameter also defines the memory consumption of the algorithm (which is proportional to M), so it should be selected with care.

Selection of the *efConstruction* parameter is straightforward. As it was suggested in [26] it has to be large enough to produce K-ANNS recall close to unity during the construction process (0.95 is enough for the most use-cases).

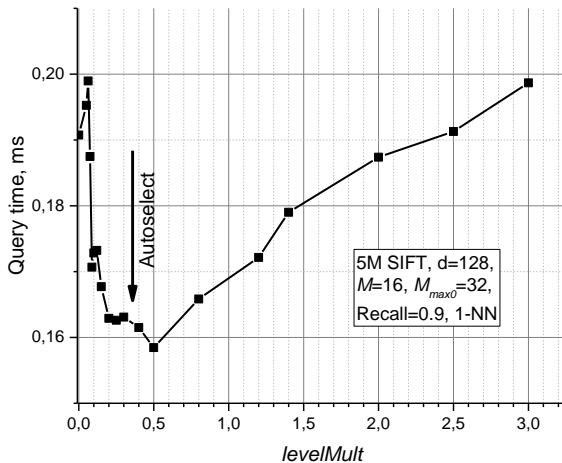


Fig. 5. Plots for query time vs *levelMult* parameter for 5M SIFT learn dataset. The autoselected value for *levelMult* is shown by an arrow.

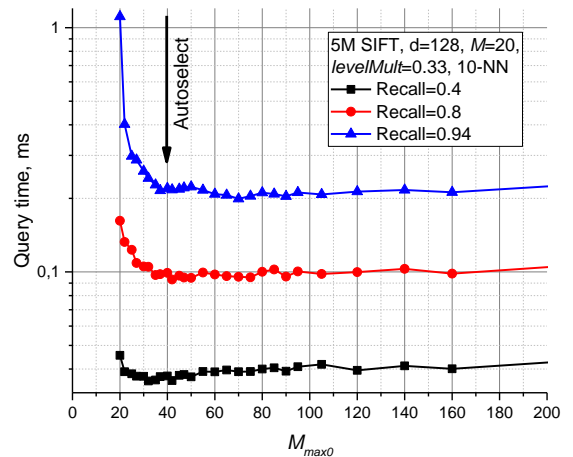


Fig. 6. Plots for query time vs M_{max0} parameter for 5M SIFT learn dataset. The autoselected value for M_{max0} is shown by an arrow.

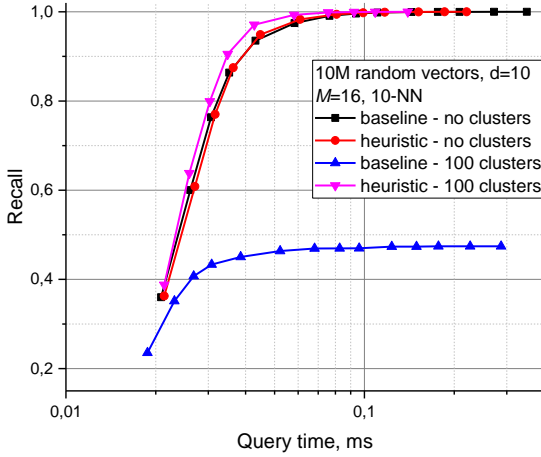


Fig. 7. Effect of the method of neighbor selections (baseline corresponds to alg. 3, heuristic to alg. 4) on clustered (100 random isolated clusters) and non-clustered $d=10$ random vector data.

And just like in [26], this parameter can possibly be auto-configured by using sample data.

The construction process can be easily and efficiently parallelized with only few synchronization points (as demonstrated in Fig. 9) and no measurable effect on index quality. Construction speed/ index quality tradeoff is controlled via *efConstruction* parameter. The tradeoff between the search time and the index construction time is presented in Fig. 10 for a 10M SIFT dataset and shows that a reasonable quality index can be constructed for *efConstruction*=100 on a 4X 2.4 GHz 10-core Xeon E5-4650 v2 CPU server in just 3 minutes. Further increase of the *efConstruction* leads to little extra performance but in exchange of significantly longer construction time.

4.2 Complexity analysis

4.2.1 Search complexity

The complexity scaling of a single search can be analyzed under assumption that we build exact Delaunay graphs instead of the approximate ones. Suppose we have found the closest element on some layer (this is guaranteed by having the Delaunay graph) and then descended to the next level. One can show that the average number of steps before we find the closest element in the layer is

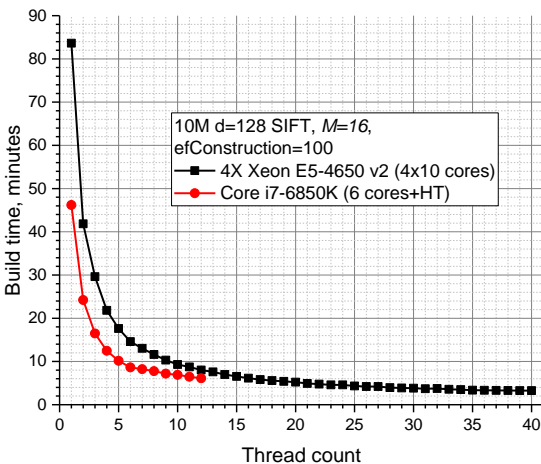


Fig. 9. Construction time for Hierarchical NSW on 10M SIFT dataset for different numbers of threads on two CPUs.

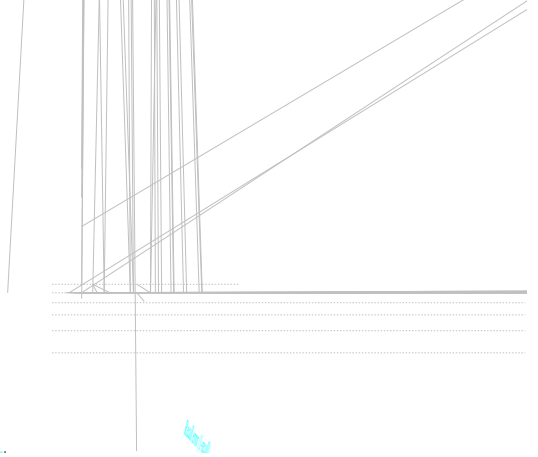


Fig. 8. Plots for query time vs recall for different parameters of M for Hierarchical NSW on 5M SIFT learn dataset.

bounded by a constant. Indeed, the layers are not correlated with the spatial positions of the data elements and thus when we traverse the graph there is a fixed probability ($p=\exp(-levelMult)$) that the next node belongs to the upper layer. But the search on the level always terminates before it reaches the element which belongs to the upper layer (otherwise the search on the upper layer would have stopped on this element), so the probability of not reaching the target on each step is bounded by an exponential function independent of the dataset size. If we assume that the average degree of a node in the Delaunay graph is capped in the limit of the large dataset (this is true at least for random Euclid data [48], but can be in principle violated in exotic spaces), then the overall average number of distance evaluations in the layer is a constant independent of the dataset size. Thus, since the index of the maximum layer scales as $\log(N)$, the overall complexity scaling is $\log(N)$, in agreement with simulations on low dimensional datasets.

4.2.2 Construction complexity

The construction complexity is closely related with the search complexity since the insertion of an element is just a sequence of K-ANN-searches at different layers. For every element we search the base level, while the number

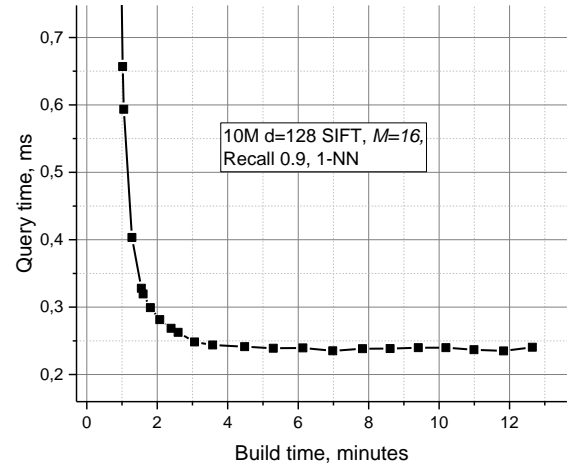


Fig. 10. Plots of the query time vs construction time tradeoff for Hierarchical NSW on 10M SIFT dataset.

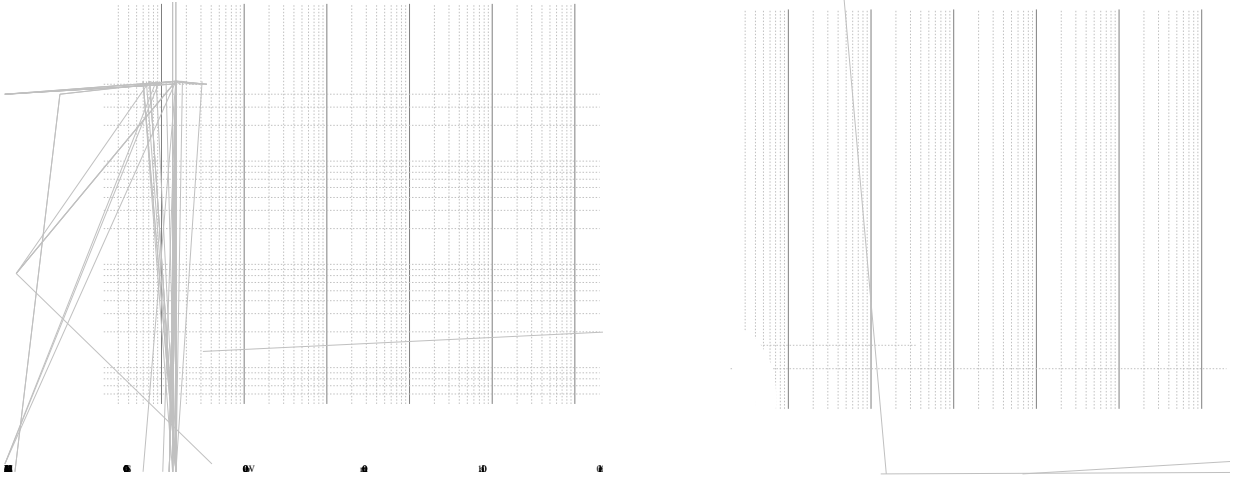


Fig. 11. Performance comparison of NSW and Hierarchical NSW on a 10 million 4 dimensional random vectors dataset.

of additional searches is equal to the element's *level*, which is close to $levelMult+1$ on average. This means that the insertion cost is roughly equal to the search cost. And thus, for relatively low dimensional datasets the construction time can scale as $N \cdot \log(N)$.

4.2.3 Memory cost

The memory cost of the hierarchical structure in most cases can be neglected because of the small number of elements at higher levels, thus the total memory cost for the structure is mainly determined by the number of element connections on the zero layer. Memory cost associated with zero level connections is about $2 \cdot M \cdot \text{number_of_bytes_per_link}$ for each element. If we limit the maximum total number of elements by approximately four billions, we can use four-byte unsigned integers to store the connections. Tests suggest that typical close to optimal M values usually lie in a range between 6 and 48. This means that the typical memory requirements for the index (excluding the size of the data) are about 48-384 bytes per object, which is in a good agreement with the simulations.

5 Performance evaluation

The Hierarchical NSW algorithm was implemented in

C++ on top of the Non Metric Space Library (nmslib) [49]¹, which already had a complete NSW implementation (under name “sw-graph”). Due to several limitations posed by the library, to achieve a better performance, the Hierarchical NSW implementation used its own distance functions implementations together with C-style memory management to avoid unnecessary implicit addressing (which significantly slowed down the NSW implementation in nmslib), which it turn allowed efficient hardware and software prefetching during the graph transversal.

Comparing the performance of K-ANNS algorithms is a nontrivial task since the state-of-the-art is constantly changing as new algorithms and implementations are emerging. In this work we concentrated on comparison with the best algorithms in Euclid spaces that have open source implementations, which is beneficial for the users. An implementation of the Hierarchical NSW algorithm presented in this paper is also distributed as a part of the open source nmslib library¹ together with an external C++ memory-efficient version².

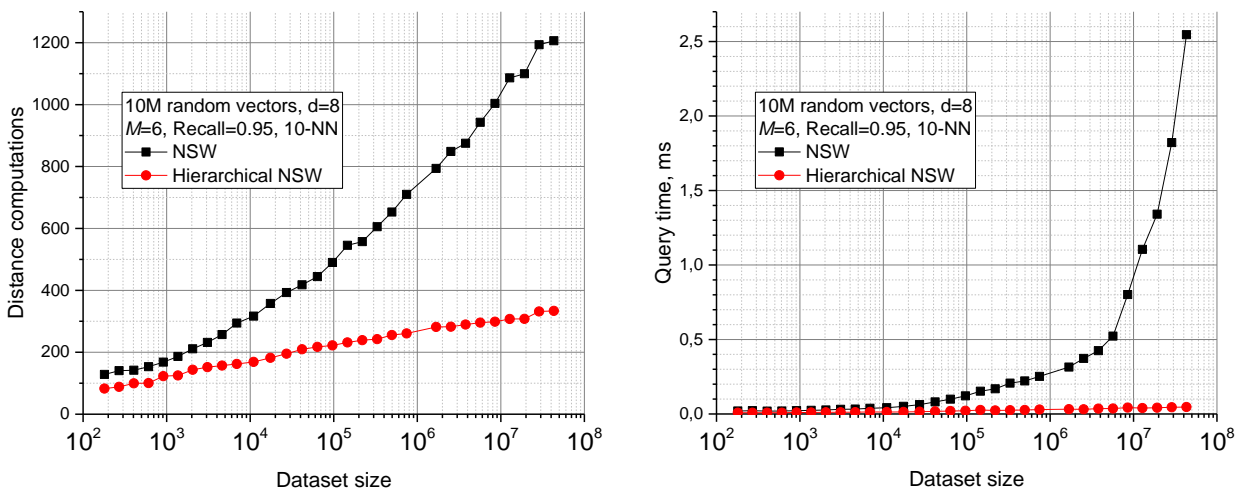


Fig. 12. Comparison between NSW and Hierarchical NSW in terms complexity scaling with the dataset size.

¹ <https://github.com/searchivarius/nmslib>

² <https://github.com/yurymalkov/hnsw>

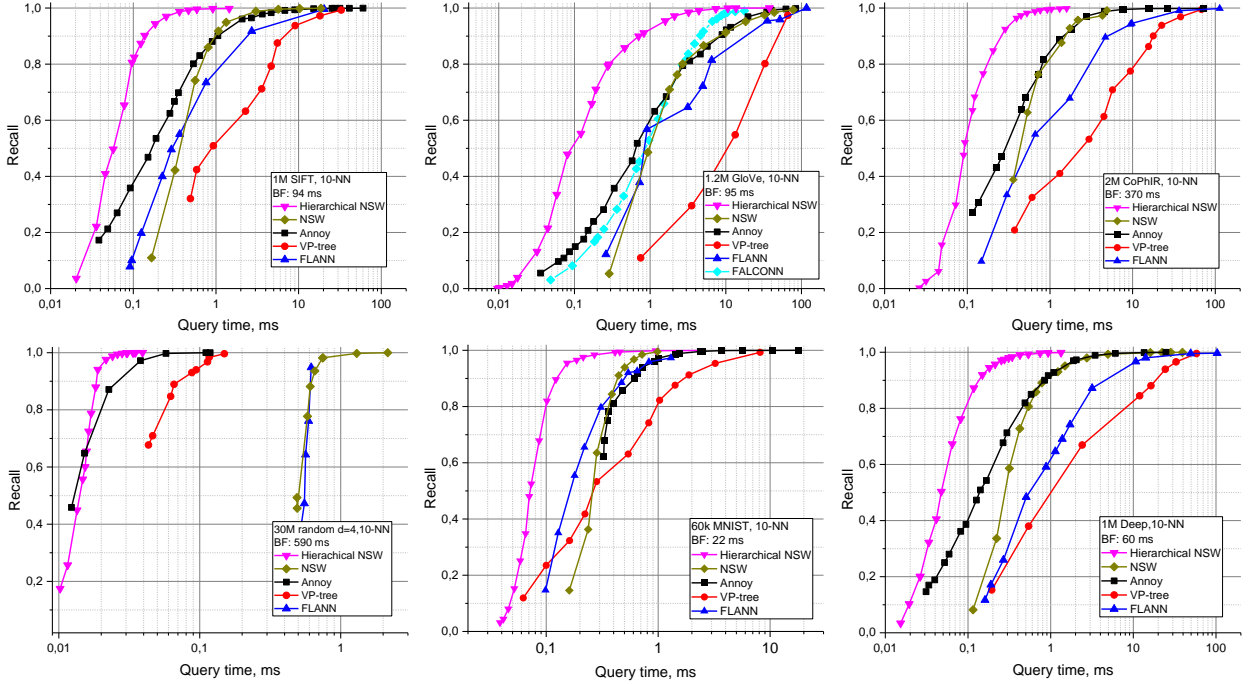


Fig. 13. Results of the comparison of Hierarchical NSW with open source implementations of K-ANNS algorithms on five datasets for 10-NN searches. The time of a brute-force search is denoted as the BF.

The comparison section is constituted of four parts: comparison to the baseline NSW (5.1), comparison to the state-of-the-art algorithms in Euclid spaces (5.2), rerun of the subset of tests [34] in general metric spaces in which NSW failed (5.3) and comparison to state-of-the-art PQ-algorithms on a large 200M SIFT dataset (5.4).

5.1 Comparison with the baseline NSW

For the baseline NSW algorithm implementation, we used the “sw-graph” from nmslib 1.1 (which is slightly faster compared to the implementation tested in [33, 34]) to demonstrate the improvements in speed and algorithmic complexity (measured by the number of distance computations).

Fig. 11 presents a comparison of Hierarchical NSW to the basic NSW algorithm for $d=4$ random hypercube data made on an i5-2400 Intel CPU (10-NN search). Hierarchical NSW uses much less distance computations during a search on the dataset while the advance in actual performance is even higher (more than two orders of magnitude for high recall values) mostly due to better algorithm implementation.

The scalings of the algorithms on a $d=8$ random hypercube dataset for a 10-NN search with a fixed recall of 0.95 are presented in Fig. 12. It clearly follows that Hierarchical NSW has a complexity scaling for this setting not worse than logarithmic and outperforms NSW at any dataset size.

5.2 Comparison in Euclid spaces

The main part of the comparison was carried out on vector datasets with use of the popular K-ANNS benchmark³ as a testbed. The testing system utilized python bindings of the algorithms and consequentially run the K-ANN

search for one thousand queries (randomly extracted from the initial dataset) with preset algorithm parameters producing an output containing recall and average time of a single search. The considered algorithms are:

1. Baseline NSW algorithm from nmslib 1.1 (“sw-graph”).
2. FLANN 1.8.4 [6]. A popular library⁴ containing several algorithms, built-in in OpenCV⁵. We used the available auto-tuning procedure with several reruns to infer the best parameters.
3. Annoy⁶, 02.02.2016 build. A popular algorithm based on random projection tree forest.
4. VP-tree. A general metric space algorithm with metric pruning [50] implemented as a part of nmslib 1.1.
5. FALCONN⁷, version 1.2. A new efficient LSH algorithm for cosine similarity data [51].

The comparison was done on a 4X Xeon E5-4650 v2 Debian OS system with 128 Gb of RAM. For every algorithm we carefully chose the best results at every recall range to evaluate the best possible performance (with initial values from the testbed defaults). All tests were done in a single thread regime. Hierarchical NSW was compiled using the GCC 5.3 with -Ofast optimization flag.

⁴ <https://github.com/mariusmuja/flann>

⁵ <https://github.com/opencv/opencv>

⁶ <https://github.com/spotify/annoy>

⁷ <https://github.com/FALCONN-LIB/FALCONN>

³ <https://github.com/erikbern/ann-benchmarks>

TABLE 1
Parameters of the used datasets on vector spaces benchmark.

Dataset	Description	Size	d	BF time	Space
SIFT	Image feature vectors [13]	1M	128	94 ms	L_2
GloVe	Word embeddings trained on tweets [52]	1.2M	100	95 ms	cosine
CoPhIR	MPEG-7 features extracted from the images [53]	2M	272	370 ms	L_2
Random vectors	Random vectors in hypercube	30M	4	590 ms	L_2
DEEP	One million subset of the billion deep image features dataset [14]	1M	96	60 ms	L_2
MNIST	Handwritten digit images [54]	60k	784	22 ms	L_2

The parameters and description of the used datasets are outlined in Table 1. For all of the datasets except GloVe we used the L_2 distance. For GloVe we used the cosine similarity which is equivalent to L_2 after vector normalization. The brute-force (BF) time is measured by the nmslib library.

Results for the vector data are presented in Fig. 13. For SIFT, GloVe, DEEP and CoPhIR datasets Hierarchical NSW clearly outperforms the rivals by a large margin. For low dimensional data (d=4) Hierarchical NSW is slightly faster at high recall compared to the Annoy while strongly outperforming the other algorithms.

5.3 Comparison in general spaces

A recent comparison of algorithms [34] in general spaces (i.e. non-symmetric or with violation of triangle inequality) showed that the baseline NSW algorithm has severe problems on low dimensional datasets. To test the performance of the Hierarchical NSW algorithm we have repeated a subset of tests from [34] on which NSW performed poorly or suboptimal, for that purpose we used a built-in nmslib testing system which had scripts to run tests from [34]. The evaluated algorithms included the VP-tree, permutation techniques (NAPP and brute force)

TABLE 2.
Used datasets for repetition of the Non-Metric data tests subset.

Dataset	Description	Size	d	BF time	Distance
Wiki-sparse	TF-IDF (term frequency-inverse document frequency) vectors (created via GENSIM [58])	4M	10^5	5.9 s	Sparse cosine
Wiki-8	Topic histograms created from sparse TF-IDF vectors of the wiki-sparse dataset (created via GENSIM [58])	2M	8	-	Jensen-Shannon (JS) divergence
Wiki-128	Topic histograms created from sparse TF-IDF vectors of the wiki-sparse dataset (created via GENSIM [58])	2M	128	1.17 s	Jensen-Shannon (JS) divergence
ImageNet	Signatures extracted from LSVRC-2014 with SQFD (signature quadratic form) distance [59]	1M	272	18.3 s	SQFD
DNA	DNA (deoxyribonucleic acid) dataset sampled from the Human Genome 5 [34].	1M	-	2.4 s	Levenshtein

filtering) [49, 55-57], the basic NSW algorithm and NNDescent-produced proximity graphs [29] (both in pair with the NSW graph search algorithm). As in the original tests, for every dataset the test includes the results of either NSW or NNDescent, depending on which structure performed better. No custom distance functions or special memory management were used in this case for Hierarchical NSW leading to some performance loss.

The datasets are summarized in Table 2. Further details of the datasets, spaces and algorithm parameter selection can be found in the original work [34]. The brute-force (BF) time is measured by the nmslib library.

The results are presented in Fig. 14. Hierarchical NSW significantly improves the performance of NSW and now is a leader for any of the tested datasets. The strongest enhancement over NSW, almost by 3 orders of magnitude is observed for the dataset with the lowest dimensionality, the wiki-8 with JS-divergence. This is the important result that demonstrates the robustness of Hierarchical NSW, as for the original NSW this dataset was a stumbling block.

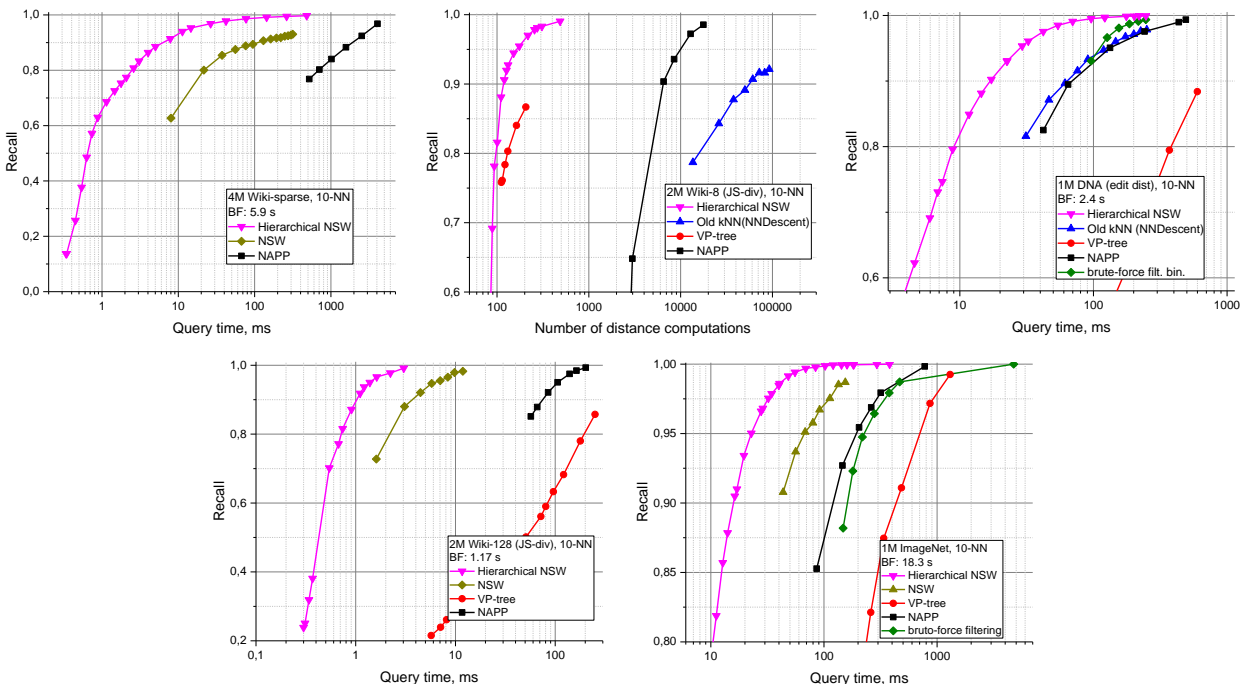


Fig. 14. Results of the comparison of Hierarchical NSW with general space K-ANNS algorithms from the Non Metric Space Library on five datasets for 10-NN searches.

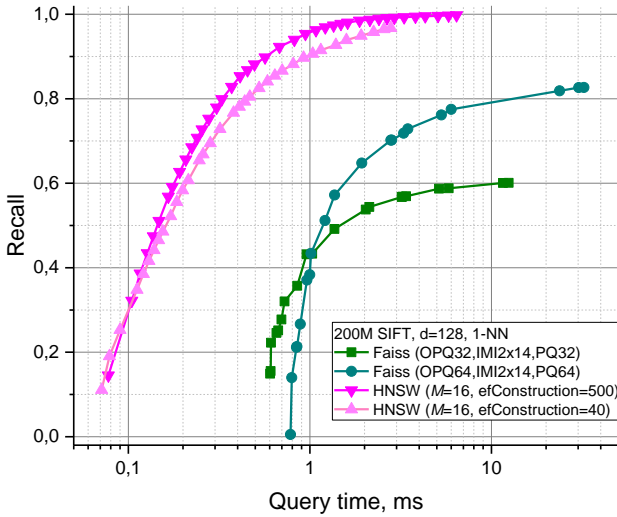


Fig. 15 Results of comparison with Faiss library on the 200M SIFT dataset from [13].

Note that for the wiki-8 to nullify the effect of implementation results are presented for the distance computations number instead of the CPU time.

5.4 Comparison with product quantization based algorithms.

Product quantization K-ANNS algorithms [10-17] are considered as the state-of-the-art on billion scale datasets since they can efficiently compress stored data, allowing modest RAM usage while achieving millisecond search times on modern CPUs.

To compare the performance of Hierarchical NSW against PQ algorithms we used the facebook Faiss library⁸ as the baseline (a new library with state-of-the-art PQ algorithms [12, 15] implementations, released after the current manuscript was submitted) compiled with the OpenBLAS backend. The tests were done for a 200M subset of 1B SIFT dataset [13] on a 4X Xeon E5-4650 v2 server with 128Gb of RAM. The ann benchmark testbed was not feasible for these experiments because of its reliance on 32-bit floating point format (requiring more than 100 Gb just to store the data). To get the results for Faiss PQ algorithms we have utilized built-in scripts with the parameters from Faiss wiki⁹. For the Hierarchical NSW algorithm we used a special build outside of the nmslib with a small memory footprint, simple non-vectorized integer distance functions and support for incremental index construction¹⁰.

The results are presented in Fig. 15 with summarization of the parameters in Table 3. The peak memory consumption was measured by using linux “time -v” tool in separate test runs after index construction for both of the algorithms. While Hierarchical NSW requires significantly more memory, it can achieve much higher accuracy, offers a massive advance in search speed and much faster index construction.

TABLE 3.

Parameters for comparison between Hierarchical NSW and Faiss on a 200M subset of 1B SIFT dataset.

Algorithm	Build time	Peak memory (runtime)	Parameters
Hierarchical NSW	5.6 hours	64 Gb	$M=16$, $efConstruction=500$
Hierarchical NSW	42 minutes	64 Gb	$M=16$, $efConstruction=40$
Faiss	12 hours	30 Gb	OPQ64, IMI2x14, PQ64
Faiss	11 hours	23.5 Gb	OPQ32, IMI2x14, PQ32

6 Discussion

By using structure decomposition of navigable small world graphs together with the smart neighbor selection heuristics the proposed Hierarchical NSW approach overcomes several important problems of the basic NSW structure advancing the state-of-the-art in K-ANN search. Hierarchical NSW offers an excellent performance and is a clear leader on a large variety of the datasets, surpassing the rivals by a large margin in case of high dimensional data. Even for the datasets where the previous algorithm (NSW) has lost by orders of magnitude, Hierarchical NSW was able to come first. Hierarchical NSW supports continuous incremental indexing and can also be used as an efficient method for getting approximate k-NN and relative neighborhood graphs, which are byproducts of the index construction.

Robustness of the approach is a strong feature which makes it very attractive for practical applications. The algorithm is applicable in generalized metric spaces performing the best on any of the datasets tested in this paper, and thus eliminating the need for complicated selection of the best algorithm for a specific problem. We stress the importance of the algorithm’s robustness since the data may have a complex structure with different effective dimensionality across the scales. For instance, a high dimensional dataset can consist of large number of clusters arranged in a line, thus being low dimensional at large distance scale. In order to perform efficient search in such datasets an approximate nearest neighbor algorithm has to work well for both cases of high and low dimensionality.

There are several ways to further increase the efficiency and applicability of the Hierarchical NSW approach. There is still one meaningful parameter left which strongly affects the construction of the index – the number of added connections per layer M . Potentially this parameter can be inferred directly by using different heuristics [4]. It would also be interesting to compare Hierarchical NSW on the full 1B SIFT and 1B DEEP datasets [10-14] and add support for element updates and removal.

One of the apparent shortcomings of the proposed approach compared to the basic NSW is the loss of the possibility of distributed search. The search in the Hierarchical NSW structure always starts from the top layer, thus the structure cannot be made distributed by using the same techniques as described in [26] due to excessive load on the higher layer elements. Simple workarounds can be used to distribute the structure, such as partitioning the data across cluster nodes studied in [6], however in this case, the total parallel throughput of the system does not scale well with the number of computer nodes. Still, there are other possible known ways to make this

⁸ <https://github.com/facebookresearch/faiss>, 2017 May build

⁹ <https://github.com/facebookresearch/faiss/wiki/Indexing-1G-vectors>

¹⁰ <https://github.com/yurymalkov/hnsw>

particular structure distributed. Hierarchical NSW is ideologically very similar to the well-known one-dimensional exact search probabilistic skip list structure, and thus can use the same techniques to make the structure distributed [45]. Potentially this can lead to even better distributed performance compared to the base NSW due to logarithmic scalability and ideally uniform load on the nodes.

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Yury A. Malkov received a Master's degree in physics from Nizhny Novgorod State University in 2009, and a PhD degree in laser physics from the Institute of Applied Physics RAS in 2015. From 2007 to 2013 he was working at the MeraLabs LLC dealing with the problems of distributed similarity search. He is author of 20+ papers on physics and computer science. Yury currently occupies a research position in the Institute of Applied Physics RAS and a leading engineering position at Intelli-Vision Russia. His current research interests include scalable similarity search, complex network theory, biological and artificial neural networks, deep learning.



Dmitry A. Yashunin received a Master's degree in physics from Nizhny Novgorod State University in 2009, and a PhD degree in laser physics from the Institute of Applied Physics RAS in 2015. From 2008 to 2012 he was working at the Mera developing VoIP applications. He is author of 10+ papers on physics. Dmitry currently works at Intelli-Vision Russia in the position of senior software engineer. His current research interests include scalable similarity search, algorithms and data structures, deep learning.