A Comparative Study on Hierarchical Navigable Small World Graphs

Peng-Cheng Lin, Wan-Lei Zhao

Abstract—Hierarchical navigable small world (HNSW) graphs get more and more popular on large-scale nearest neighbor search tasks since the source codes were released two years ago. The attractiveness of this approach lies in its superior performance over most of the nearest neighbor search approaches as well as its genericness to various distance measures. In this paper, several comparative studies have been conducted on this search approach. The role of hierarchical structure in HNSW and the function of HNSW graph itself are investigated. We find that the hierarchical structure in HNSW could not achieve “a much better logarithmic complexity scaling” as it was claimed in the paper, particularly on high dimensional data. Moreover, we find that similar high search speed efficiency as HNSW could be achieved with the support of flat k-NN graph after graph diversification. Finally, we point out the difficulty, faced by most of the graph based search approaches, is directly linked to “curse of dimensionality”. HNSW, like other graph based approaches, is unable to address such difficulty.

Index Terms—nearest neighbor search, graph based approach, NN-Descent, high dimensional.

1 INTRODUCTION

NEAREST neighbor (NN) search is a task that searches for the closest neighbors of a group of given samples with respect to either metric $d(·, ·)$. The closeness between samples is usually predefined by a metric $m(·, ·)$. The complexity of brute-force search is $O(n-d)$, where $n$ is the number of candidates. Although it is linear with respect to either $n$ or $d$. Its computational complexity is very high when both $n$ and $d$ are large. Research on this issue aims to explore approaches whose time complexity is much lower than $O(n-d)$. The early exploration about this issue could be traced back to 1970s [1]. However, it is still a new issue currently in the sense that it becomes more and more imminent given the big data problem arises from various contexts in recent years. This leads to the timely demand in scalable and efficient nearest neighbor search approach on large-scale and high dimensional data. This decades-old issue is therefore shed with new light. However, due to the “curse of dimensionality”, effective solution is still slow to occur.

This issue has been traditionally addressed by a variety of tree partitioning approaches, such as K-D tree [2], R-tree [3] and X-Tree [4], etc. Although they are different in details, they are all designed to partition the space into hierarchical sub-spaces. Such that, the nearest neighbor search only traverses over a few branches of the sub-spaces. However, unlike B-tree in 1D case, the partition scheme does not exclude the possibility that nearest neighbor resides outside of these candidate sub-spaces. Therefore, extensive probing over large number of branches in the tree becomes inevitable. Recent indexing structures FLANN [5] and ANNOY [6] partition the space with hierarchical k-means and multiple K-D trees respectively. Although efficient, sub-optimal results are achieved.

Quantization based search approaches have been widely explored in recent years [7], [8], [9], [10]. In general, the candidate vectors are all compressed via vector (or sub-vector) quantization. This makes it possible to hold the whole large-scale candidate dataset in the memory. The NN search is conducted between the query and the quantized candidate vectors. The distance between query and candidates is approximated by the distance between query and vocabulary words that are used for quantization. Due to the heavy compression on the candidate vectors, high search quality is hardly desirable. Moreover, the quantization is in general only suitable for $l_p$-norm metrics. Hash based approaches [11], [12] face similar issues.

Recently, graph based approaches such as nearest neighbor descent (NN-Descent) [13] or hill-climbing (HC) [14], demonstrate superior performance over other categories of approaches in many large-scale NN search tasks [15], [16], [17]. All the approaches in this category are built upon a k-nearest neighbor (k-NN) graph or an approximate k-NN graph. The search procedure starts from a group of random seeds and traverses iteratively over the graph by the best-first search. Guided by the neighbors of visited vertex’s, the search procedure descents closer to the true nearest neighbor in each round until no better candidates could be found. Approaches in [14], [15], [17], [18], [19] in general follow similar search procedure. The
The major difference between them lies in the structure of k-NN graphs upon which the NN search is undertaken. For most of the graph based approaches, the extra merit is that they are suitable for different distance measures.

Navigable small world graph (NSW) [18] and hierarchical navigable small world graphs (HNSW) [15] are the representative works of this category. The basic idea of NSW is inspired from the small world graph theory [20]. The graph keeps both long range links1 to far neighbors and short range links to close neighbors. The NN-Descent search therefore jumps faster along long range links in early search stage. HNSW reduces unnecessary comparisons further by organizing the links between vertices into an hierarchy. The search is fulfilled from top layer (where long range links are maintained) to the lower (where short range links are maintained). According to the paper [15], such kind of coarse-to-fine search leads to “a much better logarithmic complexity scaling” than NSW. The detailed review on HNSW will be given on Section 2. Since the codes were released on GitHub2, HNSW already receives more than 300 stars in two years. The search approach so far has been integrated with various search systems.

In this paper, several comparative studies are made about HNSW. We are going to show that the hierarchical structure in the HNSW graphs is actually not helpful for the nearest neighbor search when the data dimension goes high. Similar performance could be achieved on flat graph if the NN-Descent procedure is carefully designed. Moreover, we discover that NN search based on an approximate k-NN graph could achieve similar search efficiency as HNSW graphs when the graph is undergone diversification. Furthermore, we point out hierarchical structure in HNSW is unable to address the difficulty faced by other graph based approaches.

2 Review on HNSW Graphs

The hierarchical structure of HNSW is illustrated in Fig. 1. As seen from the figure, the search starts from a random sample on the top layer. The NN search explores the neighbors list of a visited vertex, and descents greedily to a closer neighbor if there exist. The search on one layer stops as no closer neighbor could be found. The discovered closest neighbor on the current layer is treated as the starting point (referred as “enter point” in [15]) of the search on the lower layer. Such kind of top-down greedy search continues until it reaches to the bottom layer. On the bottom layer, the search takes the closest neighbor found from upper layer as the starting point. The standard NN-Descent search [21] is adopted to search for top-k nearest neighbors on this layer. Different from greedy search of upper layers, the NN-Descent search moves towards the query each time by expanding neighbors of vertices in a maintained top-k list. The top-k list is updated as long as any closer top-k neighbor is found.

The recall of the search procedure is controlled by the parameter ef, which is the number of enter points. Larger ef value leads to better search result while it takes more search time. Parameter ef is set to 1 for all non-bottom layer greedy search.

Essentially, NN search on HNSW is undertaken in a coarse-to-fine manner. The early search on top layers traverses along long range links. Compared to NN search on a single flat graph, it moves faster on its early stages. Many short range links between samples far from the query have been skipped. This is the major reason that the author claims that HNSW achieves “a much better logarithmic complexity scaling” in contrast to NN search on single flat graph. From another point of view, the greedy search on non-bottom layers supplies a better/closer starting point for the search on the bottom layer in a more efficient manner than that of NSW.

The search on HNSW requires the support of the hierarchical NSW graphs. The construction of HNSW graphs follows the same procedure as the NN search over it. Each candidate sample is treated as a query to query against the HNSW under construction. Such that HNSW is incrementally built by repetitively inserting candidate samples into the hierarchy. The chance that a query is inserted to a layer is regularized by an exponentially decaying probability distribution. The lower is the layer, the higher of the chance that query is inserted. On the layer that a query sample should be inserted, the discovered M neighbors are kept in the neighbors list of this sample. Accordingly, this query is possibly inserted into the neighbors list of these M neighbors. Parameter M controls the scale of the neighborhood list, the larger M is, the more number of neighbors to be maintained.

Graph diversification (GD) During the the insertion of a sample into the graph of each layer, the insertion

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1. The terms “link”, “connection” and “edge” are inter-changeable across this paper.
2. https://github.com/nmslib/hnswlib
operation is verified by a heuristic pruning strategy to enhance the diversity of a vertex’s neighborhood. This pruning strategy is shown in Fig. 2. As seen in the figure, the neighborhood of sample \( a \) is already inserted with samples \( b \) and \( c \). For an incoming sample \( e \), we check whether it should be inserted into the \( k \)-NN list of \( a \). According to the strategy, sample \( e \) is allowed to join the neighborhood iff \( m(e, a) < m(e, b) \) and \( m(e, a) < m(e, c) \). Similarly given \( e \) is inserted, if another sample \( f \) is going to join the graph, its distance to \( a \) should be greater than the distances of all joined samples (samples \( b, c \) and \( e \)) to sample \( a \). It is imaginable that HNSW graph of each layer has been diversified by this strategy.

The motivation behind this strategy is to avoid comparing query to close neighbors. If samples are close to each other, it is redundant to visit them all since they offer similar amount of guiding information for a query. From now on, this strategy is called as graph diversification (GD). This strategy is also adopted in [22] for graph diversification. We find such kind of strategy is feasible for \( k \)-NN graph or approximate \( k \)-NN graph. In the experiment section, we are going to show the search performance when such kind of strategy is applied on flat approximate \( k \)-NN graph.

### 3 Overview of Comparative Study

In our study, we aim to investigate three major issues. Firstly, we investigate the role of hierarchical structure in the search. As claimed in the paper [15], since the search jumps along the long range links on top layers, it is able to skip many far neighbors in the early search. The search goes down to more fine-grained layer when no closer sample could be found. It therefore skips far neighbors as much as possible. The hierarchy seemingly achieves “logarithmic complexity scaling” as B-tree does on one dimensional data. In our study, the search performance of HNSW is compared to the one based on flat graph, which is exactly the bottom layer of HNSW graphs. The standard NN-Descent search is adopted as the search procedure. The search starts from \( ef \) random samples.

In the second experiment, we investigate whether it is necessary to adopt HNSW graphs in order to achieve superior performance. Namely, HNSW graphs is replaced by a graph that is derived from an approximated \( k \)-NN graph for the NN search. The graph is produced in three steps. Firstly, approximate \( k \)-NN graph \( G \) is built for candidate data by package KGraph [13], [21]. Graph \( G \) is further diversified by the pruning strategy introduced in HNSW (illustrated in Fig. 2). For a graph with \( L \) approximate neighbors, \( L/2 \) neighbors at most are selected. For diversified graph \( G^* \), the reverse neighbors of each sample in \( G^* \) are appended to the diversified neighborhood. Since overlapping happens between the neighbors and reverse neighbors, we actually take the union of diversified neighbors and reverse neighbors.

As one will see, based on the above two experiments, the claimed “much better logarithmic complexity scaling” [15] is not observable for HNSW on high dimensional data. Another tentative experiment is conducted to figure out the reason why HNSW and other graph based approaches fail on high dimensional case.

### 4 Experiments

#### 4.1 Experiment Setup

The experiments are conducted on eight datasets. Namely, there are three real-world datasets, SIFT1M, GIST1M and GloVe1M, which are popularly adopted in NN search evaluation [8], [16], [17]. Meanwhile, five synthetic datasets are adopted. The data dimension ranges from 4 to 100. For the synthetic data, each data dimension is randomly sampled from the range \([-1, 1]\). Datasets RAND1M, GIST1M and GloVe1M are marked as challenging datasets in [16]. The search performance is measured by Recall@1 across all our experiments. The performance is reported as the recall curve against the speed-up achieved over exhaustive search. The brief information about all eight datasets (both queries and candidate set) are summarized in Tab. 1. In addition, the time costs for exhaustive NN search on each dataset are attached. \( l_2 \)-norm is adopted for all synthetic datasets, SIFT1M and GIST1M. Cosine distance is adopted for GloVe1M.

Usually the real data dimension is lower than dimension \( d \) since data are embedded in a sub-space of \( d \)-dimensional space [16], [23]. The local intrinsic dimension (LID) is proposed to estimate the dimension of such sub-space [23]. In Tab. 1, LID of each dataset estimated by [23] is shown in the 6th column. As shown in the table, LIDs of synthetic data are roughly 1.5~2.0 times lower than their data dimension \( d \). In contrast, LIDs of three real-world datasets are much lower than their data dimension. As revealed in [16], high speed-up is achieved for graph based approaches on dataset whose the ratio between \( d \) and LID is high. In another words, the NN search becomes challenging when both dimension \( d \) and LID are high. To this end, we see the advantage of using synthetic datasets in the evaluation. By this way, the performance trend becomes more observable with respect to the variation of real data dimension.

All the approaches considered here are implemented in C++ and compiled with GCC 5.4. All the experiments...
are conducted on workstation with CPU E5-2620 2.4GHz Xeon and 110G memory setup. All the multi-threads, SIMD and pre-fetching instructions are disabled in the codes for all the approaches. There are two parameters (namely M and ef) in HNSW construction. They are all optimized according to the suggestions from project hnswlib.

4.2 Hierarchical vs. Flat Search

In the first experiment, we are going to investigate the performance difference between NN search on HNSW graphs and NN search on flat graph. The flat graph is exactly the bottom layer of HNSW graphs. In the hierarchical search (given as HNSW), the search procedure from “hnswlib” package is adopted, which is the same as [15]. In the NN search on flat graph (given as flat-HNSW), NN-Descent procedure from KGraph package\(^3\) is adopted. For fair comparison, the NN-Descent procedure is extracted from KGraph package [21] and integrated with “hnswlib” package. The NN-Descent procedure used in the bottom layer of HNSW is actually the same as the one used on flat-HNSW. The only difference lies in the selection of starting points. For HNSW, the starting points are supplied from non-bottom layer search. While for flat-HNSW, the starting points are random seeds.

The performance evaluation is presented in Fig. 3. Fig. 3(a)-(e) show the performance of two approaches on synthetic random datasets. While the results on three million level datasets from real-world are presented on Fig. 3(f)-(h).

As shown in the figure, HNSW is around two times faster than flat-HNSW on 4-dimensional data. While the efficiency of HNSW over flat-HNSW drops significantly as the data dimension reaches to 8. When the data dimension goes as high as 32, there is no considerable difference between these two approaches. A clear trend is observable that the superiority of HNSW fades away as the dimension goes higher. Specifically, the hierarchical search is no longer helpful when the data is beyond medium dimension (e.g., 32).

On the real-world datasets, the performance of HNSW and flat-HNSW is similar on all the cases. It is interesting to see the speed-ups on GloVe1M and RAND1M are different while they are on the same dimensionality and the same scale. The speed-up on GloVe1M is considerably higher than that of on RAND1M. This is mainly

3. https://github.com/aaalgo/kgraph
due to the difference in local intrinsic dimension. LID of GloVe1M is estimated as 39.5 as shown in Tab. 1. Although this estimation is imprecise, it indicates the search on GloVe1M is undertaken on a much lower sub-space. As explained in [16] and [17], the approximate k-NN graph is able to capture the structure of data distribution in each neighborhood of the candidate samples. When the data distributed in the embedded sub-space, such kind of sub-space can be presented as inter-chained k-NN lists in the graph. NN-Descent therefore moves along the sub-spaces instead of exploring the whole space exhaustively, which leads to significantly higher efficiency. This is actually the advantage of graph based approaches over other categories of NN search [15], [16], [17]. As observed from results on real-world datasets, both HNSW and flat-HNSW are able to take advantage of the latent data distribution. The hierarchical structure in HNSW brings no extra bonus.

4.3 HNSW Graphs vs. approximate k-NN Graph

On one hand, it is clear to see hierarchical structure is not helpful for high dimensional data. On the other hand, tens to hundreds times speed-up are observed when the search is based on HNSW graphs (either hierarchical or flat). In this experiment, we further study the role of HNSW graphs in the fast NN search. In the experiment, NN search based on HNSW graphs is treated as comparison baseline. Its performance is compared to NN search based on approximate k-NN graph built by KGraph package [13], [21]. We want to see whether high speed-up is only achievable with HNSW graphs. Two different configurations are considered for the approximate k-NN graph produced by [21]. For the first configuration, the produced k-NN graph by [21] is directly adopted for search. It is given as “KGraph” in the experiment. For the second configuration, the k-NN graph is undertaken on a much lower sub-space. As shown in Tab. 1, although this estimation is imprecise, it indicates the search on GloVe1M is undertaken on a much lower sub-space. When the local intrinsic dimension gets higher, its performance becomes even slightly better than that of HNSW. Similar trend is also observed on real-world datasets. The major difference between KGraph+GD and KGraph lies in the incorporation of graph diversification. As seen from the figures, graph diversification, which reduces the redundancy, is helpful for high dimensional data.
dant comparison during the search, boosts the performance of KGraph considerably. It is therefore safe to say the superiority of HNSW over KGraph largely owes to the graph diversification operation instead of hierarchical structure.

To this end, it is clear to see similar or even better performance over HNSW is achievable with approximate \(k\)-NN graph produced in other way around. The advantage of HNSW is only observable when the data dimension is low. Moreover, the speed efficiency achieved in such case is around two times better than the one based on flat graphs. Compared to HNSW, flat \(k\)-NN is more attractive in the sense it takes less memory to hold the structure and less time for construction.

5 Curse of Dimensionality in NN-Descent

Based on the above experiments, we learn that the hierarchical structure in HNSW helps to skip far away neighbors on the low dimensional case. However the advantage of such kind of long range jump fades away as the dimensionality goes higher. In order to figure out the reason, a close investigation is carried out about HNSW as the search is conducted on RAND1M, on which most of the approaches fail to show descent performance [16], [17]. According to our observation, the average distance from random starting points to the query is around 15.2 at the beginning, after three layers of greedy search, the distance from the found closest neighbor on non-bottom layer to the query is reduced to around 11.8. It takes only around 1,800~2,200 comparisons for the greedy search. However, it takes more than 8,000 comparisons on the bottom layer to reach to the expected closest neighbor, which is around 10.6 from the query. Another investigation is carried out about flat-HNSW on RAND1M. This time NN-Descent takes around 11,000 comparisons to reach to the closest neighbor, which is nearly on the same par as HNSW. Surprisingly, it takes only slightly more comparisons than greedy search for NN-Descent to reach to the samples, which are around 11.8 from the query. On both cases, it takes around 8,000 comparisons to move from 11.8 to 10.6. In contrast, it only takes around 2,000 comparisons to move from 15.2 to 11.8. The pace of NN-Descent is much slower when the search reaches to “close neighborhood” on both cases.

On one hand, the long range jump still works (although insignificant) as it does on low dimensional case. On the other hand, the high search efficiency in “far neighborhood” is dwarfed by the low search efficiency in “close neighborhood”. This phenomenon is illustrated in Fig. 5. Noticed that the close neighborhood is usually an non-convex region. As the search reaches to the “close neighborhood”, it could be trapped in a local optima when the maintained top-\(k\) list is short. Alternatively, it could search around the “close neighborhood” exhaustively when top-\(k\) list is sufficiently long. As a result, it leads to either high efficiency while with low recall or high recall while with low efficiency. In the low dimensional case, this will not be a big problem as samples in this neighborhood reside in the inter-chained NN lists. NN-Descent therefore converges quickly. In this case, the number of comparisons in “far neighborhood” takes a large portion. As a result, the time cost saved by the hierarchical search becomes significant. In the high dimensional case, samples in this neighborhood may reside in the NN lists that are isolated from each other. They may be relatively close to each other while hardly overlap on their NN lists. It is therefore hard to guide NN-Descent to jump from one local optima to another. As the data dimension goes higher, this problem becomes more apparent. As a consequence, when both the data dimension and real data dimension are high, HNSW, as other graph based approaches, is unable to address such difficulty.

6 Conclusion

We have presented our comparative studies over HNSW. Three major issues are investigated. Firstly, we find that the hierarchical structure of HNSW only shows superior performance over flat graph on low dimensional data. The speed-efficiency over approaches without hierarchy support is around two times to its best. The advantage that the hierarchical structure brings fades away as the dimension goes as high as around 32. Moreover, it is possible to achieve similar speed efficiency as HNSW with the support of approximate \(k\)-NN graph, after it has been undergone graph diversification. Furthermore, we find that most of the graph based approaches face the same difficulty when both data dimension and the intrinsic data dimension are high. This difficulty is directly linked to “curse of dimensionality”. HNSW, like other approaches, is unable to address this issue.

Acknowledgment

This work is supported by National Natural Science Foundation of China under grants 61572408.
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Peng-Cheng Lin received his Bachelor degree of Engineering from Fujian Normal University, China in 2017. He is currently a graduate student at Department of Computer Science, Xiamen University. His research interest is large-scale nearest neighbor search.

Wan-Lei Zhao received his Ph.D degree from City University of Hong Kong in 2010. He received M.Eng. and B.Eng. degrees in Department of Computer Science and Engineering from Yunnan University in 2006 and 2002 respectively. He currently works with Xiamen University as an associate professor, China. Before joining Xiamen University, he was a Postdoctoral Scholar in INRIA, France. His research interests include multimedia information retrieval and video processing.