

\textbf{k-NN Graph Construction:} \\
\textbf{a Generic Online Approach}

\textbf{Wan-Lei Zhao}

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\textit{Abstract—}Nearest neighbor search and \textit{k}-nearest neighbor graph construction are two fundamental issues arise from many disciplines such as information retrieval, data-mining, machine learning and computer vision. Despite continuous efforts have been taken in the last several decades, these two issues remain challenging. They become more and more imminent given the big data emerges in various fields and has been expanded significantly over the years. In this paper, a simple but effective solution both for \textit{k}-nearest neighbor search and \textit{k}-nearest neighbor graph construction is presented. Namely, these two issues are addressed jointly. On one hand, the \textit{k}-nearest neighbor graph construction is treated as a nearest neighbor search task. Each data sample along with its \textit{k}-nearest neighbors are joined into the \textit{k}-nearest neighbor graph by sequentially performing the nearest neighbor search on the graph under construction. On the other hand, the built \textit{k}-nearest neighbor graph is used to support \textit{k}-nearest neighbor search. Since the graph is built online, dynamic updating of the graph, which is not desirable from most of the existing solutions, is supported. Moreover, this solution is feasible for various distance measures. Its effectiveness both as a \textit{k}-nearest neighbor construction and \textit{k}-nearest neighbor search approach is verified across various datasets in different scales, various dimensions and under different metrics.

\textit{Index Terms—}\textit{k}-nearest neighbor graph, nearest neighbor search, high-dimensional, hill-climbing

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\textbf{I. INTRODUCTION}

Given a dataset \( S \), \textit{k}-NN graph refers to the structure that keeps top-\( k \)-nearest neighbors for each sample in the dataset. It is the key data structure in the manifold learning [1], [2], computer vision, machine learning and information retrieval, etc [3]. Due to the fundamental role it plays, it has been studied for several decades. Basically, given a metric, the construction of \textit{k}-NN graph is to find the top-\( k \) nearest neighbors for each data sample. When it is built in brute-force way, the time complexity is \( O(dn^2) \), where \( d \) is the dimension and \( n \) is the size of dataset. Due to the eminence of big data issue in various contexts, both \( d \) and \( n \) could be very large. As a result, it is computationally prohibitive to build an exact \textit{k}-NN graph in an exhaustive manner. For this reason, works in the literature [3]–[6] only aim to search for an approximate but efficient solution.

Despite numerous progress has been made in recent years, the major issues latent in \textit{k}-NN graph construction still remain challenging. First of all, many existing approaches only perform well on low-dimensional data. And the scale of data they are assumed to cope with is usually less than one million. Moreover, most of approaches are designed under specific metric i.e., \( L_2 \)-norm. Only recent few works [3], [7], [8] aim to address this issue in the generic metric spaces. Thanks to the introduction of NN-Descent in [3], the construction complexity has been reduced from \( O(n^{1.94}) \) [7] to \( O(n^{1.14}) \) for data with medium dimensions (e.g., 24) [3]. However, the performance of NN-Descent turns out to be unstable for data with high intrinsic dimension.

Besides the major issues aforementioned, many existing approaches still face another potential issue. In practice, it is possible that the dataset changes from time to time. This is especially the case for large-scale Internet applications. For instance, the photos and videos in Flickr grows on a daily basis. In visual object tracking [9], the new object templates are joined into the candidate set, and the obsolete templates should be swapped out, as the tracking continues. In these scenarios, one would expect the \textit{k}-NN graph that works behind should be updated from time to time. Unfortunately, for most of the existing approaches, the dataset is assumed to be fixed. Any update on the dataset invokes a complete reconstruction on the \textit{k}-NN graph. As a consequence, the aggregated cost is high even the dataset is in small-scale. It is more convenient if it is allowed to simply insert/remove the samples into/from the existing \textit{k}-NN graph. Nevertheless, it is complicated to update the \textit{k}-NN graph with the support of conventional indexing structure such as locality sensitive hashing [10], R-Tree [11] or k-d tree [12].

Recent study [13] shows that it is possible to build \textit{k}-NN graph incrementally by invoking \textit{k}-nearest neighbor search directly on an existing \textit{k}-NN graph. Unfortunately, limited speed-up (10 to 20 times) is observed in [13]. In order to support fast indexing, \textit{k}-medoids is called in the approach to partition the samples that are in \textit{k}-NN graph, which becomes very slow when both \( d \) and \( n \) are large. Moreover, since it is built upon \textit{k}-medoids, it only works in certain metric spaces.

Another problem that is closely related to \textit{k}-NN graph construction is \textit{k}-nearest neighbor search (\textit{k}-NN search), which, like \textit{k}-NN graph construction, arises from a wide range of applications. The nearest neighbor search problem is defined as follows. Given a query vector (\( q \in R^d \)), and \( n \) candidates in \( S \) that are under the same dimensionality. It is required to return sample(s) for the query that are closest to it according to a given metric.

Traditionally, this issue has been addressed by various space partitioning strategies. However, these methods are hardly scalable to high dimensional (e.g., \( d > 20 \)), large-scale and dense vector space. In such case, most of the traditional approaches such as \textit{k}-d tree [12], R-tree [11] and locality sensitive hashing (LSH) [10] are unable to return decent results.

Recently, there are two major trends in the literature that
aim to address this issue. In one direction, $k$-NN search is undertaken based upon vector quantization [14]–[16]. The primary goal of this way is to compress the reference set by vector quantization. Such that it is possible to load the whole reference set (after compression) into the memory in the case that the reference set is extremely large. The distance between query and the reference set is measured in the compressed space, which is more efficient than it is undertaken in the original space. Due to the quantization loss, high accuracy is undesirable from this type of approaches. Alternatively, another more promising way is to conduct the $k$-NN search based on an approximate $k$-NN graph [4], [17], [18] or the like [19], [20] with hill-climbing strategy [21].

In this paper, a generic $k$-NN graph construction approach is presented. The $k$-NN graph construction is treated as a $k$-NN search task. The $k$-NN graph is incrementally built by invoking each sample to query against the $k$-NN graph under construction. After one round of $k$-NN search, the query sample is joined into the graph with the resulting top-$k$ nearest neighbors. The $k$-NN lists of samples (already in the graph) that are visited during the search are accordingly updated. The $k$-NN search basically follows the hill-climbing strategy [21]. In order to achieve high performance in terms of both efficiency and quality, three major innovations are proposed.

- The hill-climbing procedure is undertaken on both $k$-NN graph and its reverse $k$-NN graph. In order to avoid the high cost of converting the intermediate $k$-NN graph to its reverse $k$-NN graph each time, the data structure “orthogonal list” is adopted, in which $k$-NN graph and reverse $k$-NN graph are maintained as a whole.
- To further boost the performance, a lazy graph diversification (LGD) scheme is proposed. It helps to avoid unnecessary distance computations during the hill-climbing while involving no additional computations.
- Moreover, recursive neighborhood propagation (RNP) is proposed to introduce the new sample to its most likely neighbors, which enhances the quality of $k$-NN graph considerably.

The advantages of this approach are several folds. Firstly, the online construction avoids repetitive distance computations that most of the current $k$-NN graph construction approaches suffer from. Secondly, online construction is particularly suitable for the scenario that dataset is dynamically changing. Moreover, our approach has no specification on the distance measure, it is therefore a generic solution, which is confirmed in our experiments. Thanks to aforementioned two innovations, the $k$-NN search turns out to be very cost-effective. When turning off the graph update operations, it is also an effective $k$-NN search algorithm. Namely, the problems of $k$-NN graph construction and $k$-NN search have been jointly addressed in our solution.

The remaining of this paper is organized as follows. In Section II, a brief review about the research works on $k$-NN graph construction and approximate $k$-NN search is presented. Section III presents an enhanced hill-climbing algorithm upon which the $k$-NN graph construction approach is built. Section IV presents two online $k$-NN graph construction approaches, which are $NN$ search approach as well when turning off the graph update operations. The experimental studies over the $k$-NN graph construction and $k$-NN search are presented in Section V. Section VI concludes the paper.

II. RELATED WORKS

A. $k$-NN Search

The early study about the $k$-NN search issue could be traced back to 1970s, when the need of NN search on the file system arises. In those days, the data to be processed are in very low dimension, typically 1D. This problem is well-addressed by B-Tree [22] and its variant $B^{+}$-tree [22], based on which the NN search complexity could be as low as $O(\log(n))$. B-tree is not naturally extensible to more than 1D case. More sophisticated indexing structures were designed to handle NN search in multi-dimensional data. Representative structures are $k$-d-tree [12], R-tree [11] and $R^{*}$-tree [23]. For $k$-d tree, pivot vector is selected each time to split the dataset evenly into two. By applying this bisecting repeatedly, the hyper-space is partitioned into embedded hierarchical subspaces. The NN search is performed by traversing over one or several branches to probe the nearest neighbors. 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 the large number of branches in the tree becomes inevitable. For this reason, $NN$ search with $k$-d tree and the like could be very slow. Recent indexing structure FLANN [24], [25] partitions the space with hierarchical $k$-means and multiple k-d trees. Although efficient, sub-optimal results are achieved.

For all the aforementioned tree partitioning methods, another major disadvantage lies in their heavy demand in memory. On one hand, in order to support fast comparison, all the candidate vectors are loaded into the memory. On the other hand, the tree nodes that are used for indexing also take up considerable amount of extra memory. Overall, the memory consumption is usually several times bigger than the size of reference set.

Aiming to reduce the memory consumption, quantization based approaches [14], [16], [26]–[28] compress the reference vectors by quantization [29]. For all the quantization based methods, they share two things in common. Firstly, the candidate vectors are all compressed via vector (or sub-vector) quantization. This makes it easier than previous methods to hold the whole dataset in the memory. Secondly, $NN$ search is conducted between the query and the compressed 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 reference vectors, high search quality is hardly desirable. Furthermore, this type of approaches are only suitable for metric spaces of $l_p$-norm.

Apart from above approaches, several attempts have been made to apply LSH [10], [30] on NN search. In general, there are two steps involved in the search stage. Namely, step 1. collects the candidates that share the same or similar hash...
keys as the query; step 2. performs exhaustive comparison between the query and all these selected candidates to find out the nearest neighbor. Similar as FLANN, computational cost remains high if one expects high search quality. Additionally, the design of hash functions that are feasible for various metrics is non-trivial.

Recently, the hill-climbing (HC) strategy that performs NN search based on k-NN graph has been also explored [4], [8], [17], [19], [21]. The hill-climbing starts from a group of random seeds (random locations in the vector space). The search traverses iteratively over an approximate k-NN graph (built in advance) by best-first search. Guided by the k-search traverses iteratively over an approximate random seeds (random locations in the vector space). The major difference lies in the strategies that are used to build the graph. According to recent study [31], these graph based approaches demonstrate superior performance over other types of approaches across variety types of data.

B. k-NN Graph Construction

The approaches for k-NN graph construction can be roughly grouped into two categories. Approaches such as [6], [32] basically follow the divide-and-conquer strategy. On the first step, samples are partitioned into a number of small sub-sets, exhaustive comparisons are carried out within each sub-set. The closeness relations (viz. edges in the k-NN graph) between any two samples in one sub-set are established. In the second step, these closeness relations are collected to build the k-NN graph. To enhance the performance, the first step is repeated for several times with different partitions. The produced closeness relations are used to update the k-NN graph. Since it is hard to design partition scheme that is feasible for various generic spaces, they are generally only effective in l2-space.

Another category of k-NN Graph Construction, typically NN-descent [3] avoids such disadvantage. The graph construction in NN-descent starts from a random k-NN graph. Based on the principle “neighbor’s neighbor is likely to be the neighbor”, the k-NN graph evolves by invoking comparisons between samples in each sample’s neighborhood. Better closeness relations that are produced in the comparisons are used to update the neighborhood of one sample. This approach turns out to be generic and efficient. Essentially, it can be viewed as performing hill-climbing [21] batchfully. Recently, the mixture scheme derived from the above approaches is also seen in the literature [4].

It is worth noting that approaches proposed in [8], [19], [20], [31] are not k-NN graph construction algorithms. The graphs are built primarily for k-nearest neighbor search. In these approaches, the samples which should be in the k-NN list of one sample are deliberately omitted for comparison efficiency. While the links to remote neighbors are maintained [19], [20]. As a consequence, graphs constructed by these approaches are not k-NN graph in the real sense. Such kind of graphs are hardly supportive to tasks beyond k-NN search.

In most of the approaches aforementioned, one potential issue is that the construction procedure has to keep records on the comparisons that have been made between sample pairs to avoid repetitive comparisons. However, its space complexity could be as high as $O(n^2)$. Otherwise the repetitive comparisons are inevitable even by adopting specific sampling schemes [3]. In this paper, the k-NN graph construction and k-NN search are addressed jointly. The k-NN graph construction is undertaken by invoking each sample as a query to query against the k-NN graph that is under construction. Since the query is new to the graph under construction each time, the issue of repetitive comparisons is overcome. More interestingly, we discover that the k-NN graph construction and k-NN search are beneficial to each other. Namely, high quality k-NN search leads to the high quality of intermediate k-NN graphs. In turn, the efficiency and quality of k-NN search are guaranteed with the support of high quality of intermediate k-NN graphs.

III. Baseline Search Algorithm

Since our k-NN graph construction approach is based on k-NN search. Before we introduce the construction approach, the baseline k-NN search algorithm that is based on a pre-built k-NN graph is presented. It essentially follows hill-climbing strategy [21], while considerable modifications have been made.

**Algorithm 1:** Enhanced Hill-Climbing NN search (EHC)

**Input:** q: query, G: k-NN Graph, $\overline{G}$: reverse k-NN Graph, $S_{n \times d}$: reference set

**Output:** Q: k-NN list of q

1: Q ← 0; Flag[1 · · · n] ← 0; 
2: while _updated_ do 
3: R[1 · · · p] ← p random seeds in [0, n) 
4: for each r ∈ R do 
5: insertQ(r, m(q, r), Q); 
6: end for
Accordingly, a more efficient scheme for minor performance fluctuation is observed across different graphs because overlappings between \( k \)-NN graphs are seen in Fig. 1. With the support of \( k \)-NN graph and its reverse graph \( G \), the baseline search algorithm is presented in Alg. 1.

As shown in Alg. 1, the hill-climbing starts from \( p \) random seeds, the compared samples are kept in \( Q \), which is sorted in ascending order\(^1\) all the way. The neighbors and reverse neighbors of sample \( r \), which are not visited and ranked closest to the query, are compared sequentially (Line 5–19). Notice that \( Q \) is updated as soon as a closer sample is found. The distance function \( m(\cdot) \) could be any distance metric defined on the input dataset. This search algorithm is generic in the sense that there is no specification or assumption related to the distance metric. This is also true for the \( k \)-NN construction algorithm that will be presented afterwards. The iteration (Line 4–21) continues until no closer sample \( r \) is identified. Although this algorithm starts from random location, only minor performance fluctuation is observed across different runs. In order to avoid repetitive comparisons, variable \( \text{Flag} \) keeps the status whether a sample has been expanded.

The major difference between Alg. 1 and original hill-climbing [21] lies in the use of both \( k \)-NN graph and its reverse \( k \)-NN graph. Thanks to the introduction of reverse \( k \)-NN graph, its performance is already very competitive in comparison to the state-of-the-art approaches [19], [20], [31].

IV. ONLINE \( k \)-NN GRAPH CONSTRUCTION

The prerequisite for \( k \)-NN search algorithm in Alg. 1 are the \( k \)-NN graph \( G \) and its reverse \( k \)-NN graph \( \overline{G} \). In this section, we are going to show how a \( k \)-NN Graph and its reverse Graph are built based on \( k \)-NN search algorithm itself. Additionally, a more efficient scheme for \( k \)-NN Graph and in turn for \( k \)-NN graph construction is presented. Moreover, a strategy called recursive neighborhood propagation is proposed to further enhance the quality of \( k \)-NN graph.

\(^1\)Without the loss of generality, it is assumed that the smaller of the distance the closer of two samples across the paper for description convenience.
Fig. 2: An illustration of orthogonal list $G$ for Fig. 1(a), which is the union of $G$ and $\overline{G}$. As shown in the figure, two links are kept for each vertex, they point to the $k$-NN list and reverse $k$-NN list of a vertex respectively. In our implementation, the samples in $k$-NN list are kept in ascending order according to their distances to the vertex. While the samples in the reverse $k$-NN list are kept in the order of being inserted.

In order to support efficient search and the $k$-NN graph construction, an orthogonal list $G$ (as shown in Fig. 2) is adopted to keep the both $G$ and $\overline{G}$ (Line 8) in the implementation. As shown in Fig. 2, two linked lists are kept for one sample, one is $k$-NN list and another is reverse $k$-NN list. While for clarity, graph $G$ and $\overline{G}$ are still referred in our description.

In Alg. 2, the procedure of $k$-NN graph construction is basically a repetitive call of the search algorithm in Alg. 1 (Line 10–26). The major difference is that function $insertG(a, b, m(a, b), G)$ is called after the query is compared to a sample in the graph. Function $insertG(\cdot)$ is responsible for inserting an edge into $k$-NN list of $a$ in graphs $G$ and $\overline{G}$. The major operations inside $insertG(\cdot)$ involve updating the $k$-NN list of $a$ and the reverse $k$-NN list of $b$. Sample in the rear of $k$-NN list is deleted if a closer sample is joined in. Distance $m(a, b)$ is kept in $k$-NN list of $a$, which allows the list to be sorted all the time. In the end of each loop, $insertG(\cdot)$ is called again to join the $k$-NN list of query $q$ into $G$.

Although the size of input dataset is fixed in Alg. 2, it is apparently feasible for an open set, where new samples are allowed to join in from time to time. As will be revealed in the experiments (Section V), Alg. 2 already performs pretty well. In the following, two novel schemes are presented to further boost its performance.

B. Lazy Graph Diversification

In Alg. 1, when expanding sample $r$ in the rank list $Q$, all the samples in the neighborhood of $r$ will be compared with the query. According to recent studies [8], [20], [31], when samples in the neighborhood of $r$ are so close to each other that the distances between them are smaller than their distances to $r$, it is no need to compare to all of them during the expansion. The expansion on these close samples later will likely lead the climbing process to the same local region. The phenomenon that samples in the $k$-NN list are closer to each other than they are to $r$ is called as “occlusion” [8]. An illustration of occlusion is shown in Fig. 3. In the illustration, samples $b$ and $e$ are occluded by sample $a$. It is easy to see one sample can only be occluded by samples which are closer to $r$ than that of it. According to [8], [20], [31], the hill-climbing will be more efficient when samples like $b$ and $e$ are not considered when expanding $r$.

In order to know whether samples in a $k$-NN list are occluded one by another, the pair-wise comparisons between samples in the $k$-NN list are required, which is the practice in [8], [20], [31]. This is unfeasible for an online construction procedure (i.e., Alg. 2). First of all, $k$-NN list is dynamically changing, pair-wise distances cannot be simply computed and kept once for all. Secondly, it is still too costly to update the pair-wise occlusion relations as long as a new sample is joined, which involves a complete comparison between the new neighbor and the rest. Moreover, the occluded samples cannot be simply removed from a $k$-NN list since our primary goal is to build the $k$-NN graph.

In this paper, a novel scheme called lazy graph diversification is proposed to identify the occlusions between samples during the online graph construction. To achieve that, an occlusion factor $\lambda$ is introduced as the attribute attached to each sample in a $k$-NN list. $\lambda$s of all the samples in the list are initialized to 0, when the $k$-NN list of a new query is joined into the graph. Factor $\lambda$ will be updated when another new sample is joined into the $k$-NN list in the later stage. Given a new sample $q$ to be inserted into sample $r$'s $k$-NN list, we should know the distances of all the neighbors to $r$ and the distances between $q$ and other neighbors in the list. The distances to $r$ are known as they are kept for sorting. While the distances between this new sample and the rest are unknown. Instead of performing a costly thorough comparison between $q$ and the rest neighbors, we make use of distances that are computed during the hill-climbing. To do that, another variable $D$ is introduced to keep the distances between sample $q$ and the samples that have been compared during the hill-climbing. It is possible that not all the samples in $k$-NN list of $r$ are joined in the comparisons during hill-climbing. However, according to the principle “neighbor of a neighbor is likely to be a neighbor”, the “old” samples in the $k$-NN list of $r$ are likely being encountered by $q$. With the support of $D$,
occlusion factor $\lambda$ of all the samples in the $k$-NN list is updated with following three rules.

- **Rule 1**: $\lambda$ is kept unchanged for samples ranked before $q$;
- **Rule 2**: $\lambda$ of sample $q$ is incremented by 1 if a sample ranked before $q$ is closer to $q$ than $q$ is to $r$;
- **Rule 3**: $\lambda$ of a sample ranked after $q$ is incremented by 1 if its distance to $q$ is smaller than $q$ is to $r$.

The default distance of each sample to $q$ is set to $\infty$. As a result, the $\lambda$s of not-being-visited neighbors will not be updated according to Rule 1 and Rule 3. This is reasonable because the not-being-visited neighbors should be sufficiently far away from $q$, otherwise they are already being visited according to the principle “a neighbor of a neighbor is also likely to be a neighbor”. Since we have all the possible distances (between $q$ and samples in the graph) only after the hill-climbing converges, the operations of inserting $q$ into $k$-NN list of $r$ and updating factor $\lambda$ in the list are postponed to the end of hill-climbing search. Fig. 4 illustrates a search trail that is formed by the hill-climbing. In the $k$-neighborhood of $r$, the LGD operations are applied.

Once the occlusion factor is available, the search algorithm (Alg. 1) and the construction algorithm (Alg. 2) are accordingly modified. When the query is compared to the neighbors in one $k$-NN list, we only consider the samples whose $\lambda$ is no greater than the average occlusion factor $\bar{\lambda}$ of this list. Notice that this is different from the way proposed in [8], [20], in which the occluded samples ($\lambda > 0$) are simply omitted. We find such kind of rule is too restrictive in our case. In our case, only samples that are occluded by many other neighbors are ignored. The operation of skipping samples with high factor $\lambda$ could be interpreted as performing diversification in the graph [31]. Different from [31], the diversification is undertaken in a lazy way in the sense no exhaustive comparison is involved within the $k$-NN list. This scheme is therefore called as lazy graph diversification (LGD). The three rules used to calculate occlusion factor are called as LGD rules. The $k$-NN graph construction algorithm with LGD is accordingly named as LGD, which is summarized in Alg. 3.

**Algorithm 3**: Online $k$-NN Graph Constr. with LGD (LGD)

1. **Input**: $S_{n \times d}$: dataset; $k$: size of NN list; $p$: num. of seeds
2. **Output**: $G$: $k$-NN Graph
3. $Q \leftarrow \emptyset$; $D[1 \cdots n] \leftarrow \infty$; $E[1 \cdots n] \leftarrow 0$
4. Extract a small subset $I$ from $S$;
5. Initialize $G$ and $\overline{G}$ with $I$;
6. $G = G \cup \overline{G}$;
7. for each $q \in S - I$ do
8. while _isUpdated_ do
9. $R[1 \cdots p] \leftarrow p$ random seeds in $[0, n)$
10. for each $r \in R$ do
11. InsertQ($r$, $m(q, r)$, $Q$);
12. end for
13. for $r \leftarrow top(Q)$ do
14. if $E[r] = 0$ then
15. for $n_i \in G[r] \& \& \lambda(n_i) \leq \bar{\lambda}(r)$ do
16. insertQ($n_i$, $d(q, n_i)$, $Q$);
17. $D[n_i] = m(q, n_i)$;
18. end for
19. for $n_i \in \overline{G}[r] \& \& \lambda(n_i) \leq \bar{\lambda}(r)$ do
20. insertQ($n_i$, $m(q, n_i)$, $Q$);
21. $D[n_i] = m(q, n_i)$;
22. end for
23. end if
24. $E[r] = 1$;
25. end for
26. end while
27. for each visited $n_i$ do
28. updateG($n_i$, $q$, $D$, $\overline{G}$);
29. end for
30. for each $r \in Q$ do
31. insertG($q$, $r$, $d(q, r)$, $\overline{G}$);
32. end for
33. $Q \leftarrow \emptyset$; $D[1 \cdots n] \leftarrow \infty$; $E[1 \cdots n] \leftarrow 0$;
34. end for

Compared to Alg. 2, Alg. 3 is different in three major aspects. In Alg. 3, query sample is compared to samples whose occlusion factor is no greater than average factor $\bar{\lambda}$ in both $k$-NN list and reverse $k$-NN list (see line 15 and Line 19). After $q$ is compared to a sample $n_i$ in the $k$-NN list, $k$-NN list of $n_i$ is not updated immediately. Instead, the distance from $q$ to sample $n_i$ is collected into $D$ (Line 17, Line 21) for later use. The update of $k$-NN lists for all the samples so far encountered are postponed to the end of $k$-NN search (Line 27–30). Function updateG($\cdot$) is basically similar as insertG($\cdot$). The additional operation inside updateG($\cdot$) is to update $\lambda$ of all the neighbors according to LGD rules. It is easy to see Alg. 3 becomes a fast $k$-NN search algorithm when the updateG and insertG operations are turned off.

In the experiment section, we are going to show Alg. 3 turns out to be more cost-effective than Alg. 2 in both $k$-NN construction and $k$-NN search approach when turning off their updateG($\cdot$) and insertG($\cdot$) operations.

C. Recursive Neighborhood Propagation

In the last steps of both Alg. 2 and Alg. 3, the query sample $q$ is inserted to the neighborhood of $rs’$ as long as $q$ is in their $k$-NN range. Noticed that only a few $rs$ that are sufficiently close to $q$ will be considered. In the neighborhood of such $rs’$, it is possible that there are some samples are not compared to $q$ during the hill-climbing search (as is shown in the dashed circle of Fig. 4). Based on the principle that “neighbor’s neighbor is likely to be the neighbor”, these unvisited samples are likely to be close neighbors of sample $q$. It is therefore reasonable to insert $q$ and these unvisited samples to the neighborhoods of each other, in terms of $k$-NN range and reverse $k$-NN range as well. After this insertion, it is possible that $q$ is introduced to meet with more unvisited neighbors. As a result, such kind of insertion could be undertaken recursively until no new
unvisited neighbors are encountered. This operation is called as recursive neighborhood propagation (RNP). We found this operation further boosts the quality of k-NN graph from 2-15%, while only inducing minor computational overhead. The LGD graph construction method with the support of RNP is given as \( \text{LGD}^+ \).

D. Sample Removal from the Graph

In practice, we should allow samples to be dropped out from the k-NN graph. A good case is to maintain a k-NN graph for product photos for an e-shopping website, where old-fashioned products should be withdrew from sale. The removal of samples from the k-NN graph dynamically is supported in our approach. If the graph is built by Alg. 2, the removal operation is as easy as deleting the sample from k-NN lists of its reverse neighbors and releasing its own k-NN list. If the graph is built by Alg. 3, before the sample is deleted, the occlusion factors of the samples living in the same k-NN list have to be updated. Fortunately not all the samples in the list should be considered. According to LGD Rule 3, only samples ranked after current sample should be considered. The update operations involves \( k^2 / 2 \) times distance computations in average. Given \( k \) is a small constant, the time cost is much lower than fulfilling a query. Notice that such kind of dynamic updating operation is not necessarily supported by other online algorithms [13], [20], in which the deleting operation may lead to collapse of the indexing structure.

Discussions Two k-NN graph construction approaches namely OLG (Alg. 2) and LGD (Alg. 3) in general follow the same framework. In both processes, the construction starts from a small-scale k-NN graph of 100% quality. The search process appends a k-NN list of a new sample to the graph each time. At the same time, the k-NN lists of the already inserted samples will be possibly updated when the new sample happen to be in their neighborhoods. It is therefore a win-win situation for both graph construction and NN search. Effective search procedure returns high quality k-NN list. While k-NN graph with high quality gives a good guidance for the hill-climbing process.

Besides the size of NN list \( k \), there is another parameter involved in OLG and LGD. Namely, the number of seeds \( p \). Usually, the size of NN list \( k \) should be no less than the intrinsic data dimension \( d^\ast \), which is less than or equal to the data dimension \( d \). The number of seeds is usually set to be no bigger than \( k \). When \( d \) is very high (i.e., several hundreds to thousands) and \( d^\ast \) is close to \( d \), the construction process could be slow when \( k \) is set to be close to \( d \). In such situation, a good trade-off is hardly achieved between the quality of k-NN graph and the efficiency of the construction.

V. EXPERIMENTS

In this section, the performance of the proposed algorithms is studied both as a k-NN graph construction and an approximate nearest neighbor search approach. In the evaluation, the performance is reported on both synthetic random data and data from real world. It is believed that the intrinsic dimension of synthetic data is roughly equal to the data dimension [3], [8]. While for the datasets from real-world, the intrinsic dimension is usually smaller than the data dimension [8]. The brief information about the datasets that are adopted in the evaluation are summarized in Table I.

In the nearest neighbor search task, the performance of the proposed search approaches is studied in comparison to the representative approaches of different categories. Namely they are graph based approaches such as DPG [31], HNSW [20]. The typical locality sensitive hash approaches [10], [33], namely SRS [34] is considered. For quantization based approach, product quantizer (PQ) [14] is incorporated in the comparison. FLANN [24] and Annoy [35] are selected as the representative tree partitioning approaches, both of which are popular NN search libraries in the literature.

A. Evaluation Protocol

For k-NN graph construction, five synthetic random datasets sized of 100K are used in the evaluation. Their dimension ranges from 2 to 100. Data in each dimension are independently drawn from the range \([0, 1]\) under uniform distribution. It guarantees the intrinsic dimension of the synthetic data largely equals to the data dimension. The top-1 (recall@1) and top-10 (recall@10) recalls on each dataset are studied under \( l_1 \) and \( l_2 \) metrics respectively. Given function \( R(i, k) \) returns the
number of truth-positive neighbors at top-k NN list of sample \( i \), the recall at top-k on the whole set is given as

\[
\text{recall}@k = \frac{\sum_{i=1}^{n} R(i, k)}{n \times k}.
\]

Besides \( k \)-NN graph quality, the construction cost is also studied by measuring the scanning rate [3] of each approach. Given \( C \) is the total number of distance computations in the construction, the scanning rate is defined as

\[
c = \frac{C}{n \times (n - 1)/2}.
\]

In addition, another seven datasets are adopted to evaluate the performance of both nearest neighbor search and \( k \)-NN graph construction. Among them, six datasets are derived from real world images or text data. In particular, all four datasets (namely GIST1M, Glove1M, NUSW and Rand1M) that are marked as most challenging datasets in [31] are adopted in the evaluation. For each of the dataset, another 1,000 or 10,000 queries of the same data type are prepared. Different metrics such as \( l_2 \), Cosine and \( \kappa^2 \) are adopted in accordance with the data type of each set. The search quality is measured by the top-1 recall for the first nearest neighbor. In order to make our study comparable under different hardware settings, the search quality is reported along with the speed-up one among different approaches considered in this study are compiled by g++ 5.4. In order to make our study to be fair, we disable all the multithreads, SIMD and pre-fetching instructions in the codes. All the experiments are pulled out on a PC with 3.6GHz CPU and 32G memory setup.

### B. Performance of Baseline NN-Search

In the first experiment, the focus is to verify the effectiveness of the baseline search algorithm upon which our \( k \)-NN graph construction is built. Four different configurations are tested. Firstly, the NN search is supplied with prebuilt \( k \)-NN graph from NN-Descent [3] and the true \( k \)-NN graph. In the experiment, \( k \) is fixed to 40. The experiment is pulled out on SIFT1M and GIST1M datasets. The quality of 40-NN graph from NN-Descent is above 0.90 in terms of its top-1 and top-10 recall for both datasets. These \( k \)-NN graphs are supplied to hill-climbing (HC) [7] and enhanced hill-climbing (EHC, Alg. 1). EHC differs from HC mainly in the use of reverse \( k \)-NN graph during the search. The search performance in terms of recall@1 is shown in Fig. 5. The performance is compared to the state-of-the-art approach HNSW [20].

As seen from the figure, there is a significant performance gap between EHC and HC. The NN list of each sample in EHC is usually longer than that of HC due to the incorporation of reverse nearest neighbors. On one hand, EHC has to visit more samples during the expansion, and therefore should be slower. On the other hand, the reverse nearest neighbors also provide short-cuts to the remote neighbors for the hill-climbing, which is similar as the mechanism offered by small-world graph [19], [20]. As a result, EHC turns out to be more efficient. Another interesting discovery is that, the NN search performance based on approximate \( k \)-NN graph is very close to that of being based on true \( k \)-NN graph. This indicates minor difference in \( k \)-NN graph quality does not lead to any big difference in the search performance. Above observations apply to other datasets that are considered in this paper.

With the support of the effective search procedure, it becomes possible to build the \( k \)-NN graph with the search results. In the following, we are going to show the quality of \( k \)-NN Graph that is built based on this search algorithm.

### C. \( k \)-NN Graph Construction

In the second experiment, the performance about \( k \)-NN graph construction is studied when the enhanced hill-climbing is employed as a graph construction approach. In the evaluation, the performance of OLG (Alg. 2), LGD (Alg. 3) and LGD+ (LGD with recursive neighborhood propagation) is compared to NN-Descent [3], which is still recognized as the most effective \( k \)-NN graph construction approach that works in the generic metric spaces. In order to be in line with the experiments in [3], synthetic data in the same series of dimensions are used. In the test, the shared parameter \( k \) among different approaches are tuned to be close to the data dimension and no higher than 50. Meanwhile, we ensure the scanning rate of different approaches to be on the same level. Usually, the higher is the scanning rate the better is the \( k \)-NN graph quality. The scanning rate of all four approaches are reported in Table II. While the top-1 and top-10 recall of all

---

**TABLE I: Summary on Datasets used for Evaluation**

| Name     | \( n \)       | \( d \)       | # Qry | \( m(\cdot) \) | Type       |
|----------|--------------|--------------|--------|----------------|------------|
| Rand100K| \( 1 \times 10^5 \) | \( 3 \sim 100 \) | -      | \( l_2 \)       | synthetic  |
| Rand100K| \( 1 \times 10^5 \) | \( 3 \sim 100 \) | -      | \( l_3 \)       | synthetic  |
| SIFT1M  | \( 1 \times 10^6 \) | \( 128 \times 10^4 \) | \( l_2 \) | SIFT [36]      |            |
| SIFT1M  | \( 1 \times 10^6 \) | \( 128 \times 10^4 \) | \( l_2 \) | SIFT          |            |
| GIST1M  | \( 1 \times 10^6 \) | \( 960 \times 10^4 \)  | \( l_2 \) | GIST [37]     |            |
| GloVe1M | \( 1 \times 10^6 \) | \( 100 \times 10^4 \)  | \( \text{Center} \) | Test        |            |
| NUSW [39]| 22, 660      | 500 \( 3 \times 10^3 \)  | \( l_2 \) | BoVW [40]      |            |
| NUSW [39]| 22, 660      | 500 \( 3 \times 10^3 \)  | \( \kappa^2 \) | BoVW         |            |
| YFCC1M  | \( 1 \times 10^6 \) | \( 128 \times 10^4 \)  | \( l_2 \) | Deep Feat.    |            |
| Rand1M  | \( 1 \times 10^6 \) | \( 100 \times 10^4 \)  | \( l_2 \) | synthetic     |            |
the approaches under $l_1$ and $l_2$ distance measures are shown in Fig. 6.

As seen from the figure, in most of the cases, the quality of $k$-NN graph from OLG, LGD and LGD$^+$ is considerably better than NN-Descent when the their scanning rates are similar to each other. This is particularly true under $l_1$-norm. The scanning rates of all the approaches increase steadily as the dimension of data goes higher. Meanwhile, the recall that one approach could reach drops. As shown in the figure, when $d$ reaches to 100, the scanning rates of all the approaches are above 10%, which is too high for them to be practically useful. In general, NN-Descent, OLG, LGD and LGD$^+$ are effective in the similar range of data dimensions, namely [2, 50]. Within this dimensional range, LGD$^+$ achieves the best trade-off between scanning cost and the graph quality. Due to the superior performance LGD$^+$ over LGD, only the performance of LGD$^+$ is reported in the following experiments for clarity. While OLG is treated as the comparison baseline.

### TABLE II: Scanning rate $c$ of OLG, LGD and LGD$^+$ in comparison to NN-Descent [3] under $l_1$-norm and $l_2$-norm

| $m$ | $d$ | NN-Descent | OLG | LGD | LGD$^+$ |
|-----|-----|------------|-----|-----|--------|
| $l_1$ | 1 | 0.0040 | 0.0036 | 0.0060 | 0.0217 | 0.1133 | 0.135 |
|     | 5 | 0.0039 | 0.0035 | 0.0060 | 0.0209 | 0.1034 | 0.136 |
|     | 10 | 0.0039 | 0.0037 | 0.0067 | 0.0205 | 0.1016 | 0.135 |
|     | 20 | 0.0034 | 0.0034 | 0.0060 | 0.0194 | 0.1081 | 0.138 |
|     | 50 | 0.0037 | 0.0035 | 0.0053 | 0.0194 | 0.0984 | 0.135 |
|     | 100 | 0.0037 | 0.0035 | 0.0053 | 0.0194 | 0.0984 | 0.135 |

![Fig. 6: Top-1 and Top-10 recall for five 100K synthetic datasets under $l_1$-norm and $l_2$-norm.](image)

Fig. 7: Top-1 and Top-10 recall of $k$-NN graphs produced by NN-Descent, OLG and LGD$^+$ on eight datasets.

### D. Nearest Neighbor Search

In our third experiment, the performance of NN search with the support of $k$-NN graph built by OLG and LGD$^+$ is evaluated. Six datasets derived from real world data are adopted. Among them, NUS-k is tested under both $l_2$ and $\kappa^2$ distance measures. In addition, another 100-dimensional random dataset sized of one million is adopted. The brief information about all the datasets are summarized in Table I. When we use OLG (Alg. 2) and LGD$^+$ (LGD with recursive neighborhood propagation) to build the approximate $k$-NN graph for search, the parameter $k$ and $p$ are fixed to 40 for all the datasets. Once $k$-NN graphs are built, algorithms OLG and LGD (Alg. 3) are used as NN search procedures as we turn off their update and insertion operations. For convenience, the NN search approaches based on the graph constructed by OLG and LGD$^+$ are given as OLG and LGD$^+$ respectively.

In the evaluation, the NN search performance is compared to three representative graph based approaches. Namely, they are NN-Descent [3], DPG [31] and HNSW [20], all of which work in generic metric spaces. Additionally, all the approaches use the similar hill-climbing search procedure. The major difference lies in the graph upon which the search procedure is undertaken. DPG graph is basically built upon NN-Descent. In DPG, the $k$-NN graph built by NN-Descent is diversified by an off-line post-process. Additionally, the diversified NN list of each sample has been appended with its reverse NN list. In the experiment, NN-Descent shares the same $k$-NN graph with DPG for each dataset. Parameter $k$ in NN-Descent is fixed to 40 for all the datasets$^2$. LGD$^+$ searches over graph which is a merge of $k$-NN graph and its reverse $k$-NN graph that are produced by LGD$^+$, NN search in LGD$^+$ is on a $k$-NN graph merged with its reverse $k$-NN graph that have been diversified online by LGD rules. While for HNSW, the search is undertaken on a approximate small world graph. The graph maintains links between close neighbors as well as long range links to the remote neighbors, which are kept in a hierarchy. The parameter $M$ in HNSW is fixed to 20. The edges kept for each sample in the bottom-layer is 40. Its size of NN list is therefore on the same level as NN-Descent, DPG, OLG and LGD$^+$.

$^2$This is to be in line with the experiments in [31]
TABLE III: Scanning rate $c$ of OLG and LGD$^+$ on eight datasets in comparison to NN-Descent [3]. The shared parameter $k$ in all the approaches is fixed to 40.

| Dataset  | NN-Descent | OLG  | LGD$^+$ | $\text{mt}^{-1}$ |
|----------|------------|------|---------|-----------------|
| SIFT1M   | 0.01085    | 0.00597 | 0.00547 | $l_2$           |
| SIFT10M  | 0.00131    | 0.00075 | 0.00068 | $l_2$           |
| GIST1M   | 0.01665    | 0.02140 | 0.0161  | $l_2$           |
| GloVe1M  | 0.01393    | 0.00826 | 0.00679 | Cosine          |
| NUSW-$l_2$ | 0.05750  | 0.09686 | 0.07475 | $l_2$           |
| NUSW-$\kappa^2$ | 0.06167 | 0.09410 | 0.07547 | $\kappa^2$    |
| YFCC1M   | 0.01113    | 0.00651 | 0.00569 | $l_2$           |
| Rand1M   | 0.0161     | 0.0312  | 0.02856 | $l_2$           |

TABLE IV: Time cost (s) in total (of all the queries) by exhaustive search on eight datasets.

| Dataset  | SIFT1M   | SIFT10M  | GIST1M  | GloVe1M  |
|----------|----------|----------|---------|----------|
| # Qry    | $1 \times 10^4$ | $1 \times 10^4$ | $1 \times 10^4$ | $1 \times 10^4$ |
| Time     | 892.4    | 8923.6   | 748.5   | 79.6     |

| Dataset  | NUSW-$l_2$ | NUSW-$\kappa^2$ | YFCC1M  | Rand1M  |
|----------|------------|----------------|---------|---------|
| # Qry    | $1 \times 10^4$ | $1 \times 10^4$ | $1 \times 10^4$ | $1 \times 10^4$ |
| Time     | 100.8     | 805.8       | 870.0   | 72.4    |

Since the search is conducted based on a $k$-NN graph for NN-Descent, DPG, OLG and LGD$^+$, the recall@1 and recall@10 of corresponding $k$-NN graph from NN-Descent and our approaches are shown in Fig. 7. Accordingly, their scanning rate $c$ on each dataset is reported in Table III. As shown in the table, the scanning rates of LGD$^+$ on five out of eight datasets from real world are at least 20% lower than that of NN-Descent and OLG. While as is shown in Fig. 7, the recall of $k$-NN graph from LGD is the best on all the datasets. The graph quality that achieved by different approaches is generally similar, while one exception comes from NN-Descent. It shows considerably poor performance on GloVe1M, whose intrinsic dimension is believed to be high [31].

The search performance on eight datasets is shown in Fig. 9. In order to make the search results comparable to the results that are pulled out under different hardware setups, the performance is reported as the recall curve against the speed-up achieved over exhaustive search. The time costs of exhaustive search on each dataset are reported separately on Table IV. It is therefore also convenient for the readers who want to see the efficiency that our approach achieves with current setup.

As shown in the figure, the performance from NN-Descent and HNSW are unstable across different datasets. LGD$^+$ performs marginally better than OLG on most of the datasets. While LGD$^+$ shows close performance as DPG on two datasets (SIFT1M and YFCC1M) and outperforms it on the other six datasets, most of which are marked as “most challenging” in [31]. As the relative better performance is observed from DPG, OLG and LGD$^+$, it is clear to see the performance boost mainly owes to the use of reserve $k$-NN and the introduction of graph diversification. The best performance is observed from LGD$^+$ in most of the cases. On one hand, this indicates the search procedure is closely related to the quality of $k$-NN graph. On the other hand, it also shows the search gets more cost-effective when skipping occluded samples.

Comparing the result presented in Fig. 9(a) to the one presented in Fig. 9(b), the high scalability is achieved by the proposed approaches. As seen in the figure, the size of reference set has been increased by 10 times, while the time cost only increases from 0.207ms (per query) to 0.307ms (per query), when the search quality is maintained on 0.9 level. Similar high scalability is observed on deep features i.e., YFCC1M (Fig. 9(d)). This is good news given the deep features have been widely adopted in different applications nowadays. In contrast, such kind of high speed-up is not achievable on NUSW, GloVe1M and Rand1M, although the dimensionality of GloVe1M and Rand1M is lower than that of SIFT1M and YFCC1M. We found that the speed-up that graph-based approaches could achieve is partly related to the intrinsic data dimension [3], [8]. When the intrinsic data dimension is low, with the guidance of a $k$-NN graph, the hill-climbing search is actually undertaken on the sub-spaces where most of the data samples lying in. Due to the low dimensionality of these sub-spaces, the search complexity is lower than it seemingly is. Fig. 8 illustrates this phenomenon. This is one of the major reasons that the graph based approaches exhibit superior performance over other type of approaches.

E. Comparison to state-of-the-art $k$-NN Search

Fig. 10 further compares our approach with the most representative approaches of different categories in the literature. Besides aforementioned HNSW, NN-Descent and DPG, approaches considered in the comparison include tree partitioning approaches Annoy [35] and FLANN [24], locality sensitive hashing approach SRS [34], and vector quantization approach product quantizer (PQ) [14]. In the figures, the speed-ups that each approach achieves are reported when recall@1 is set to 0.8 and 0.9 levels. For PQ, it is impossible to achieve top-1 recall above 0.5 due to its heavy quantization loss. As an exception, its recall is measured at top-16 for SIFT1M and NUSW, and measured at top-128 for GIST1M and Rand1M respectively.
As shown in the figure, the best results come from graph based approaches. LGD+ performs the best in most of the cases. This observation is consistent across different datasets. The speed-up of all the approaches drops as the recall@1 rises from 0.8 to 0.9. The speed-up degradation is more significant for approaches such as PQ and FLANN. No considerable speed-up is observed for SRS on any of the datasets. This basically indicates SRS is not suitable for the tasks which require high NN search quality. Another interesting observation is that the performance gap between graph based approaches and the rest is wider on the “easy” dataset than that of “hard”. Compared to the approaches of other categories, the NN search based on the graph makes good use of the sub-space structures latent in a dataset. Since the intrinsic dimension of “easy” dataset is low [8], the hill-climbing is actually undertaken on these low-dimensional sub-spaces. The lower is the intrinsic dimension the higher is the speed-up that graph-based approaches achieve. In contrast, there is no specific strategy in other type of approaches exploits on such latent structures in the data.

On one hand, the high search speed-up is observed from LGD+ on data types such SIFT, GIST and deep features. With such efficiency, it is possible to realize an image search system with instant response on billion level dataset by a single PC. On the other hand, it is still too early to say NN search on high-dimensional data has been solved. As shown on Rand1M and NUSW datasets, where both the data dimension and intrinsic data dimension are high, the efficiency achieved by our approach is still limited. Highly efficient NN search on these types of data (i.e., intrinsic dimension above 50) is still an open issue.

**VI. CONCLUSION**

We have presented our solution for both k-NN graph construction and approximate nearest neighbor search. These two issues have been addressed under a unified framework. Namely, the NN search and NN graph construction are designed as an interdependent procedure that one is built upon another. The advantages of this design are several folds. First of all, the k-NN graph construction is an online procedure. It therefore allows the samples to be inserted in or dropped out from the graph dynamically, which is undesirable from most of the existing solutions. Moreover, no sophisticated
indexing structure is required to support this online approach. Furthermore, the solution has no specification on the distance measure, which makes it a generic approach both for k-NN graph construction and NN search. The effectiveness of the proposed solution both as a k-NN graph construction approach and NN search has been extensively studied. Superior performance is observed in both cases under different test configurations.

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