Towards Efficient Index Construction and Approximate Nearest Neighbor Search in High-Dimensional Spaces

Technical Report

ABSTRACT

The approximate nearest neighbor (ANN) search in high-dimensional spaces is a fundamental but computationally very expensive problem. Existing solutions can be mainly categorized into LSH-based methods and graph-based methods. The LSH-based methods can be costly to reach high query quality due to the hash-boundary issues, while the graph-based methods can achieve better query performance by greedy expansion in an approximate proximity graph (APG). However, the construction cost of these APGs can be one or two orders of magnitude higher than that for building hash-based indexes. In addition, they fail short in incrementally maintaining APGs as the underlying dataset evolves. In this paper, we propose a novel approach named LSH-APG to build APGs and facilitate fast ANN search using a lightweight LSH framework. LSH-APG builds an APG via consecutively inserting points based on their nearest neighbor relationship with an efficient and accurate LSH-based search strategy. A high-quality entry point selection technique and an LSH-based pruning condition are developed to accelerate index construction and query processing by reducing the number of points to be accessed during the search. LSH-APG support fast maintenance of APGs in lieu of building them from scratch as dataset evolves. And its maintenance cost and query cost for a point is proven to be less affected by dataset cardinality. Extensive experiments on real-world and synthetic datasets demonstrate that LSH-APG incurs significantly less construction cost but achieves better query performance than existing graph-based methods.

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The source code, data, and/or other artifacts have been made available at https://github.com/Jacyhust/LSH-APG-SourceCode/tree/main/cppCode/LSH-APG.

1 INTRODUCTION

Given a dataset and a distance function, the nearest neighbor (NN) search problem aims to find the point in the dataset with the minimum distance to a given query point. It has applications in a wide range of areas such as machine learning [4], pattern recognition [39] and data mining [41]. It is well known that finding the exact NN in large high-dimensional datasets can be very time-consuming[24]. A more efficient and potentially more practical alternative is to perform an approximate nearest neighbor (ANN) search, which has been widely studied in the database community [2, 7, 10, 24]. Existing methods for efficient ANN search in high-dimensional spaces can be broadly divided into two categories: locality-sensitive hashing (LSH)-based methods [2, 17, 19, 33, 40, 42] and graph-based methods [16, 21, 36]. The LSH-based methods are known for their robust theoretical guarantee on query result accuracy and simple and efficient implementation. By mapping points in a high-dimensional space to low-dimensional spaces via a set of LSH functions, it is possible to find a high-quality result with a guaranteed high probability by only checking the points around the query point in low-dimensional spaces[2, 19]. On the other hand, the graph-based methods build an approximate proximity graph (APG) where each data point is represented as a vertex in the graph, and there is an edge between two vertices if the corresponding points are sufficiently close to each other in the original space. When the query q comes, the search begins from an arbitrary point o (*i.e.,* the entry point) in the APG and computes the distance between o's neighbors and q. The closest neighbor to q is chosen as the next entry point. The process repeats until it reaches a point v, which is closer to q than any of its neighbors in the APG .

The graph-based methods have been extensively studied due to their higher query accuracy than the LSH-based methods in practice [16, 43]. Compared with LSH-based methods that may suffer from the problem of hash-boundary issues (*i.e.,* some points that are close in the original space may be mapped into different hash buckets, thus not being identified by LSH-based approaches as neighbors) [17, 19, 42], the graph-based methods can achieve much higher accuracy [16, 43]. However, the cost of APG construction can be one or two orders of magnitude higher than that of LSH-based methods for very large datasets [3, 30], as such an approach will require finding proper neighbors for every point in the dataset. To address this issue, many heuristic strategies such as NN-Descent [11] and HCNNG [37] have been proposed for reducing the construction cost of APGs. However, such strategies cannot guarantee the quality of built APG is good enough and lowers the query performance. In addition, dataset in our real life is dynamic in nature, but existing graph-based methods fail short in incrementally maintaining APGs as the underlying dataset evolves.

Motivated by the above observations, in this paper, we propose LSH-APG, a novel approach to build APGs from lightweight LSH indexes and facilitate efficient ANN query processing. By exploiting the properties of LSH functions and analyzing the problem using different structures of proximity graphs, LSH-APG can overcome the drawbacks of both LSH (*i.e.,* the hash-boundary issues) and graph-based methods (*i.e.,* high graph construction time and poor maintainability for dynamic datasets). It adopts LSH indexes to quickly retrieve some query results as the entry point for a search in a proximity graph, followed by using graph-based techniques to further improve the accuracy of the query result. To boost query processing efficiency, an accurate and scalable pruning strategy is proposed to filter out neighbors which are far away from the query point. This strategy can significantly reduce the number of points

that need to be accessed during the search on the graph. A consecutive insertion strategy is used to build the graph index. It handles the high construction cost issue with the help of the LSH framework. All points are consecutively inserted into the index structure where each point is regarded as a query point and inserted into the graph index based on its nearest neighbors. This strategy not only reduces the construction cost due to improved search efficiency using the LSH framework but also enables a formal correctness and complexity analysis for our approach.

In summary, our main contributions in this paper include:

- Based on a comprehensive analysis of state-of-the-art LSH-based methods and graph-based methods, a new solution named LSH-APG is developed for efficient index construction and ANN query in high-dimensional spaces. LSH-APG adopts a well-designed LSH framework to accelerate indexing and query processing for proximity graphs with higher-quality entry point selection and LSH-based pruning conditions. LSH-APG has a much lower construction cost without scarifying query efficiency or query quality.
- We provide a cost model to demonstrate the effectiveness of LSH-APG, which shows the expected query cost of LSH-APG is nearly independent on the cardinality of the dataset. The effectiveness of the LSH framework is also theoretically proven.
- Based on our construction strategy and index structure, an efficient update strategy is designed to maintain index structures as the database evolves. The expected cost of deleting/inserting a point is also nearly independent on the cardinality of the dataset.
- Extensive experiments show that LSH-APG can greatly reduce indexing cost and achieve the best trade-off between query processing efficiency and query accuracy compared with the existing methods for ANN queries.

The rest of the paper is organized as follows. Section 2 reviews the related work. Section 3 introduces the problem definition, basic concepts and analyzes the limitations in the existing methods. The framework of LSH-APG is presented in Section 4. The pruning condition and update strategies are discussed in Section 5 and Section 6. Section 7 reports experimental results. We conclude this paper in Section 8.

2 RELATED WORK

The ANN search algorithms mainly come from the tree-based methods [5, 6, 45], quantization-based methods [18, 20, 26], LSH-based methods and graph-based methods. However, tree-based methods are not suitable for efficient ANN search in high-dimensional spaces due to the "curse of dimensionality". Quantization-based methods are data-dependent and thus bring a higher construction cost compared to LSH-based methods. Moreover, quantization-based methods are difficult to achieve a high query accuracy due to the quantization errors and cannot provide the quality guarantee theoretically. Therefore, we mainly discuss LSH-based and graph-based methods for ANN search in high-dimensional spaces.

2.1 LSH-based Methods

LSH-based method is originally proposed in [10, 19, 24]. In these methods, LSH functions map data points in the high-dimensional space into several low-dimensional hash buckets and the ANN query is answered by checking the buckets where the query falls. However, to guarantee a high query accuracy and sub-linear query cost, these methods require preparing multiple suit of LSH indexes with different bucket width, which causes undesirably large index sizes and limits their applications. [40] and [17] addressed this issue via the *virtual rehashing* technique, but they are hard to achieve a very high query quality due to the hash boundary issue, a shortcoming shared by all static LSH-based methods. To relieve the hash boundary issue, recent studies focus on designing dynamic LSH methods that dynamically construct query-centric hash buckets for every query point via novel LSH frameworks, such as collision counting based strategy [23, 33, 34] and metric based strategy [32, 47]. However, their query cost is no longer sub-linear due to the overhead of dynamic bucketing. In this year, Tian et al. combined the dynamic query strategy with the static LSH framework and proposed DB-LSH, which achieved the best query complexity theoretically among the existing LSH-based methods [42].

2.2 Graph-based Methods

Graph-based methods use the proximity graphs to facilitate ANN search and have shown better query performance compared to other methods, in terms of both accuracy and efficiency recently [36, 37, 43]. However, the construction cost of exact proximity graphs, *e.g.,* Delaunay graph (DG) [28], relative neighborhood graph (RNG) [25], minimum spanning tree (MST) [37] and kNN graph (KNNG) [11], is at least $O(n^2)$, which is unaffordable for large-scale datasets.

To lower the construction cost, several indexing strategies tried to build an approximate proximity graph (APG) at the cost of a bit of query quality. Dong et al.[11] proposed NN-Descent that approximates KNNG. In this method, an APG is built from a random graph and the edges for each point are updated by conducting local search iteratively among close neighbors of the query. The construction complexity of NN-Descent is lowered to $\tilde{O}(n^{1.14})$. Due to its efficiency compared to the brute-force manner, NN-Descent algorithm is used in many graph based methods, such as EFANNA [14], NSG [16] and others [31, 46] and some derivatives are developed [7]. However, it needs iterating about 10 times to find the high-quality neighbors, which is still time-consuming. NSW [35] builds the approximate KNNG and DG via consecutive insertion strategy, where the point to be inserted is regarded as a query in the current graph, and connected to its neighbors to finish the insertion. This construction manner is very efficient, but it can cause hubness issue, *i.e.,* high out-degrees for some vertexes, which makes the query inefficient. HNSW [36] adopts the same strategy as NSW but limits the maximum degree for each point to alleviate the hubness issue. HCNNG [37] and VRLSH [12] cluster or partition the data into many subgroups, and then build an APG in each subgroup. It could reduce the construction cost of graph index to $O(n)$ but requires building the graph multiple times to achieve a good performance.

To further boost query efficiency, many studies proposed the neighbor selection strategies to diversify the distribution of neighbors [16, 21, 30, 36]. In this manner, the similar edges will be cut off to reduce the average degree of the graph based on some occlusion rules. NSG [16] and HNSW consider the distribution of neighbors by their distance. In these two methods, for any two neighbors u and v of o, the value of $dist(u, v)$ must be larger than $dist(o, u)$

Table 1: List of Key Notations.

Notation	Description
$\mathbb{R}^d$	d-dimensional Euclidean space
$\mathcal{D}$	The dataset
n	The cardinality of dataset
d_i	The local intrinsic dimensionality of dataset
o, v, u	A data point
q	A query point
$\|o_1, o_2\|$	The distance between o_1 and o_2
$e = (o_1, o_2)$	The directed edge from o_1 to o_2
$h^*(o), h(o)$	Hash function
$\chi^2(m)$	The χ^2 distribution with freedom m
C_Q	The expected number of points accessed per query

and $dist(o, v)$. Otherwise, the longer edge between (o, u) and (o, v) would be discarded. DPG [30] and NSSG [15] consider the distribution of neighbors by the angle between two edges (o, u) and (o, v). DPG maximizes the average angle between any two edges of o and NSSG limits the angle between two edges no less than a given threshold. These strategies demonstrate better query performance, but all of them bring much larger construction costs due to the extra computation cost for occlusion rules.

3 PRELIMINARIES

In this section, we first introduce the problem definition, the concepts of LSH and graph-based methods. Then, a comprehensive analysis of limitations in the existing ANN methods is presented, which inspires us to design LSH-APG. Frequently used notations are summarized in the Table 1.

3.1 Problem Definition

In this paper, we study the c-ANN and (c, k)-ANN queries in the Euclidean space. Let $\mathcal{D}$ be a set of points in d-dimensional Euclidean space $\mathbb{R}^d$ with cardinality $|\mathcal{D}| = n$. Let $\|o_1, o_2\|$ denote the Euclidean distance between points $o_1, o_2 \in \mathcal{D}$.

Definition 1 ((c, k)-ANN Query [42]). *Given a query point q, an approximation ratio $c > 1$ and a positive integer k, a (c, k)-approximate nearest neighbor query returns k points $o_1, \ldots, o_k$ that are sorted in ascending order w.r.t. their distances to q. If o_i^* is the i-th nearest neighbor of q in $\mathcal{D}$, it satisfies that $\|q, o_i\| \leq c \cdot \|q, o_i^*\|$.*

Remark 1. *The c-ANN query is the (c, k)-ANN query with $k = 1$.*

Remark 2. *In the graph-based methods, we usually do not explicitly use c to control the query quality. Without confusion, we abbreviate (c, k)-ANN as kANN for simplicity.*

3.2 Locality Sensitive Hashing

Definition 2 (Locality Sensitive Hashing (LSH) [42, 47]). *Given a distance r and an approximation ratio $c > 1$, a family of hash functions $\mathcal{H} = \{h : \mathbb{R}^d \to \mathbb{R}\}$ is called (r, cr, p_1, p_2)-locality-sensitive, if for $\forall o_1, o_2 \in \mathbb{R}^d$, it satisfies both conditions below:*

(1) If $\|o_1, o_2\| \leq r$, $\Pr[h(o_1) = h(o_2)] \geq p_1$;
(2) If $\|o_1, o_2\| > cr$, $\Pr[h(o_1) = h(o_2)] \leq p_2$,

where $h \in \mathcal{H}$ is chosen at random, p_1, p_2 are collision probabilities and $p_1 > p_2$.

A typical LSH family in the Euclidean space is defined as follows [23]:

$$h^*(o) = \vec{a} \cdot \vec{o}, \tag{1}$$

where $\vec{o}$ is the vector representation of a point $o \in \mathbb{R}^d$ and $\vec{a}$ is a d-dimensional vector where each entry is chosen independently from the standard normal distribution.

Lemma 1. *Let $P(o) = (h_1^*(o), \ldots, h_m^*(o))$ be an m-dimensional vector where h_i^* is chosen from the LSH family in Eq. 1. Then, for $\forall o_1, o_2 \in \mathcal{D}$, we have $\frac{\|P(o_1), P(o_2)\|^2}{\|o_1, o_2\|^2} \sim \chi^2(m)$.*

Proof. The proof of this lemma can be found in [47]. □

Another commonly used LSH family in the Euclidean space is defined as follows [10]:

$$h(o) = \left\lfloor \frac{h^*(o) + b}{w} \right\rfloor, \tag{2}$$

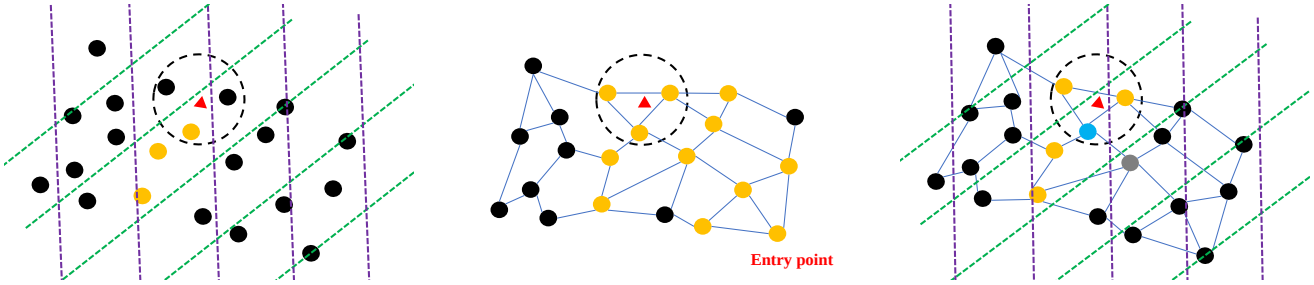
where w is a pre-defined integer and b is a real number chosen uniformly from $[0, w)$. To distinguish these two LSH families, we call h^* as the projected function and h as the hash function.

3.3 Graph based Methods

The foundational structure of graph-based methods is a proximity graph, denoted as $G = (V, E)$, where the vertex set V represents all data points in the dataset $\mathcal{D}$, and the edge set E is the collection of all edges between vertexes if the corespondent points are sufficiently close to each other in the original space. There are mainly three strategies to build the proximity graph [43].

- **Cluster & Merge [37].** The dataset $\mathcal{D}$ is clustered into several small groups and the exact proximity graph is built in each group. Then, we obtain the approximate proximity graph by merging the all subgraphs.
- **Iteration [11, 16].** The APG is built from an initial random graph. For each vertex, we iteratively update its neighbors according to the local information. The final APG is obtained when the iteration converges.
- **Consecutive Insertion [35, 36].** In this manner, the graph is built by inserting the point one by one, like that in R-Tree.

The number of edges directly affects the query performance [43]. Intuitively, the more the out-edges of a vertex, the more candidates and computations need to be performed, and the slower the query processing will be. There are two commonly used neighbor selection strategies to control the distribution of edges, *i.e.,* the simple selection strategy and the heuristic selection strategy. The simple selecting strategy is to choose the closest M neighbors, where M is a pre-defined threshold. In the heuristic selecting strategy, neighbors are chosen based on the distribution so as to preserve their diversity. Take HNSW and NSG for example, if the point o has two edges (o, u) and (o, v) that satisfies $\|o, u\| < \|u, v\| < \|o, v\|$, the edge (o, v) is said to be conflicted to (o, u) and the longer edge (o, v) will be discarded. The behind idea is that edges (o, u) and (o, v) are too similar, and thus there is no need to store both of them.



(a) Search in the LSH-Based Method (b) Search in the Graph-Based Method (c) Search in LSH-APG

Figure 1: Difference in the LSH-based method, graph-based method and LSH-APG. The red triangle is the query point q. The three points in the black dashed circle are the 3NN of q. The orange points denote those that are accessed during the search.

3.4 Limitations in the existing ANN methods

In this subsection, we analyze the drawbacks of the LSH-based and graph-based methods.

LSH-based methods. Figure 1(a) shows the framework of the LSH-based methods, where the data points are mapped into several hash buckets (parallelograms formed by purple and green lines). Then, the points in the 2-dimensional projected space are indexed by some simple structures, such as hash table, B+-Tree and R-Tree, which makes the LSH indexes easy to be maintained for dynamic datasets. To answer the ANN query, we only check the points in the bucket where the query point falls, *i.e.,* the 3 orange points in Figure 1(a). Both the LSH family in Equation 1 and 2 satisfy that the collision probability decreases monotonically with the distance between points. Thus, LSH-based methods provide a guarantee of query quality. However, it is hard for these methods to achieve a very high recall due to their simple query strategy and hash boundary issue. As shown in the Figure 1(a), 2 of 3-NN results are not found by this LSH index. To find them, it requires to build more LSH indexes, and thus incurs higher query cost.

Graph-based methods. Figure 1(b) shows the framework of the graph-based methods, where each vertex in the graph has 2-4 neighbors. The query procedure begins from the bottom right point (a random entry point) and approaches to the correct results via the greedy search in the APG. The orange points are the points accessed during the search for the 3ANN of q. Although these methods hardly offer a theoretical guarantee, they always perform better than LSH-based methods. Experimental results show that to reach the recall of 0.95, the cost of DB-LSH is about 100 times higher than that of graph-based methods. The bottleneck of graph-based methods, however, comes from their huge construction cost. In the cluster and merge strategy, the subgraphs built for each cluster are disconnected and their graph quality is unsatisfactory since many close point pairs are divided into different clusters. Thus, we need to repeat the cluster and merge operations several times to improve the graph quality, which is time-consuming. Moreover, the graph built via this strategy requires being reconstructed as the data evolves since the clusters inevitably evolve with the data. In the iteration strategy, the construction cost is high because it requires updating the neighbors for every vertex in each iteration and the number of iterations to convergence increases with the data cardinality. Compared to them, the consecutive insertion strategy is more efficient and can be easily adapted to support the index maintenance for dynamic dataset, since the index are built point by point. However, the construction cost and graph quality of APG built via this strategy depends heavily on a well-designed query strategy. Besides, the neighbor selection strategies have a significant impact on the construction cost. The heuristic selection strategy greatly increases the computational cost since we need to compare every two neighbors. To lower its cost, some methods, such as HNSW [36], only adopt the heuristic selection strategy to cut off the edges of a vertex when its degree reaches a given maximum capacity. The simple selecting strategy is more efficient, but some edges could be similar especially when the data is in a dense region, which incurs the unnecessary computational cost in the query processing.

4 LSH-APG FRAMEWORK

Observe that LSH indexes have a relatively low recall although they can be quickly built and maintained as the underlying dataset evolves; while graph-based methods perform well in terms of query processing, they suffer from the high construction cost due to the complex construction strategy and edge selection strategy. To address this dilemma, we propose a novel framework called LSH-APG that can reduce the construction cost without sacrificing query performance for ANN search. The main idea is to quickly build APGs via a consecutive insertion and simple selection strategy, based on which the LSH framework is further adopted to accelerate the construction of APGs and the query processing by providing a closer entry point and filtering out some irrelevant edges. Consider Figure 1(c), LSH-APG selects the closest point to the query point q in the bucket where the q falls as the entry point (*i.e.,* the blue point), and thus the number of hops is reduced to 2, half of that in Figure 1(b). Then, it adopts the LSH-based pruning condition to avoid accessing all the neighbors during the search. In the figure, the grey point is one of neighbors of the red point, but we do not need to check it since its distance to q is much larger than that of the red point. Compared to existing methods, LSH-APG has the following advantages:

(1) *Low construction cost.* As the APG is built via the consecutive insertion strategy without considering the distribution of edges, the distance computation cost is greatly reduced. In addition,

Algorithm 1: Building Naive-APG($\mathcal{D}, T, T'$)

Input: Dataset $\mathcal{D}$ and parameter T, T'
Output: $\mathcal{I}_G$

1 $\mathcal{I}_G \leftarrow \emptyset$;
2 **for** *each point* $o \in \mathcal{D}$ **do**
3 $candidates \leftarrow T$ ANN results of o found in $\mathcal{I}_G$;
4 **for** *each* $e \in candidates$ **do**
5 $\mathcal{I}_G \leftarrow \mathcal{I}_G \cup \{(o, e), (e, o)\}$;
6 **if** $e.degree > T'$ **then**
7 $o_f \leftarrow e$'s furthest neighbor in $\mathcal{I}_G$;
8 $\mathcal{I}_G \leftarrow \mathcal{I}_G - \{(e, o_f)\}$;
9 **return** $\mathcal{I}_G$;

Algorithm 2: Building LSH-APG($\mathcal{D}, T, T'$)

Input: Dataset $\mathcal{D}$ and parameter T, T'
Output: LSH-APG index $\mathcal{I}_G$ and $\mathcal{I}_H$

1 $\mathcal{I}_H \leftarrow \emptyset, \mathcal{I}_G \leftarrow \emptyset$;
2 **for** *each point* $o \in \mathcal{D}$ **do**
3 $candidates \leftarrow$ **call** kANN-Query($o, \mathcal{I}_G, \mathcal{I}_H, p_\tau = 0.95, T$);
4 **for** *each* $e \in candidates$ **do**
5 $\mathcal{I}_G \leftarrow \mathcal{I}_G \cup \{(o, e), (e, o)\}$;
6 **if** $e.degree > T'$ **then**
7 $o_f \leftarrow e$'s furthest neighbor in $\mathcal{I}_G$;
8 $\mathcal{I}_G \leftarrow \mathcal{I}_G - \{(e, o_f)\}$;
9 Insert o into the corresponding LSB-Tree in the $\mathcal{I}_H$;
10 **return** $\mathcal{I}_H$ and $\mathcal{I}_G$;

LSH framework further helps reduce the construction cost to nearly $O(n)$.

(2) *Guaranteed query cost and quality.* LSH-APG adopts a suit of lightweight LSH indexes to quickly find a better entry point for the query in the graph, which reduces the number of hops required to terminate the algorithm and ensures the worst query quality is bounded.
(3) *Accurate pruning condition.* LSH-APG filters out some edges during the search by an accurate yet efficient LSH-based pruning condition for reducing the unnecessary distance computations.
(4) *Incremental index maintenance.* LSH-APG supports incremental index maintenance in a low cost as the data evolves.

In what follows, we begin with a basic framework called Naive-APG (see Section 4.1), which can achieve (1). Then, we further develop LSH-APG by integrating the LSH framework with Naive-APG to realize (2) and (3) (Section 4.2– Section. 5). To accomplish (4), we present the index updating strategy (see Section 6) for incrementally maintaining the indexes as the underlying dataset evolves.

4.1 Naive-APG: the Basic Structure

The index of Naive-APG, denoted as $\mathcal{I}_G = (V, E)$, is a directed NN graph. $V = \mathcal{D}$ is the dataset and $E = (u, v)$ is the edge set where v is an approximate nearest neighbor of u in the dataset. Unlike the NN graph where each vertex connects to the unified number of edges, we allow the degree to vary in a range $[T, T']$ to better fit the data distribution, where T is the initial degree and T' is the maximum degree. An intuition explanation is that: The data points in dense regions are difficult to be differentiate from its nearby points, and thus requires more edges than data points in sparse regions. We build $\mathcal{I}_G$ via the consecutive insertion strategy as described in Algorithm 1. In this strategy, we find T ANN results for the incoming point o in the current graph index (Line 3). Next, we mutually connect o with its each ANN result e (Line 5). Finally, we check whether the degree of e reaches the maximum capacity T'. If so, we select the closest T' points to o_i in $N(o_i)$, following the simple neighbor selection strategy (Line 6-8).

Remark 3. *When $T' = T$, all vertices in $\mathcal{I}_G$ will have a unified number of edges, as that in most NN graph. However, we find such a structure has a low performance due to the following reasons: 1) The real-world dataset is usually distributed unevenly and this setting does not consider this difference totally; 2) The points inserted earlier will often be accessed when we insert the points later. So, providing them more edges help the points coming later find the better ANN result. However, a too large T' will increases the number of distance computation during the search and incurs a high query cost. Considering these factors, we set $T' = 2T$ by default. More discussion about settings of T and T' is reported in the experiments (see Sec. 7.2.)*

4.2 LSH-APG: Optimized by LSH Indexes

Algorithm 1 guarantees the APG can be build in a rather low cost since the required distance computations just comes from finding ANN results for o and graph-based index has a low query cost. However, an underlying problem in this strategy is that the graph quality is not guaranteed. If we cannot find good enough ANN results for o, the o's edge quality is limited; in turn, a low-quality edge selection of o will prevent us from finding the high-quality ANN results for next-coming points. To address this issue, we adopt a suit of lightweight LSH indexes to quickly find a better entry point for the query in the graph to guarantee the query quality.

The chosen LSH indexes $\mathcal{I}_H$ need to be built quickly and answer an NN query efficiently. Since the final ANN results will be refined in the graph index, its query quality is not supposed to be very high, which is in line with the property of LSH indexes. To achieve this goal, we build our hash indexes $\mathcal{I}_H$ following the idea in [40]: first, we randomly choose K LSH functions $h_1, \ldots, h_K$ as described by Eq. 2. For a point o to be inserted, we compute its K hash values $h_1(o), \ldots, h_K(o)$ and consider them as a K-dimensional point $H(o) = (h_1(o), \ldots, h_K(o))$. Then, we transform $H(o)$ into a one-dimensional value $z(H(o))$ via the Z-order curve [9] and store the $z(H(o))$ in a B+-Tree (other sorted indexes are also suitable). Repeating this process L times, we build L B+-Trees, which forms $\mathcal{I}_H$. For the convenience, we denote the K LSH functions used the for i-th projected space as $H_i = \{h_{i,1}, \ldots, h_{i,K}\}, i = 1, \ldots, L$, *i.e.,* there are total $L \times K$ LSH functions used. Algorithm 2 describes how to build $\mathcal{I}_H$ and $\mathcal{I}_G$ in the same time, which is much more efficient than building them independently.

Algorithm 3: kANN Query($q, \mathcal{I}_G, \mathcal{I}_H, p_\tau, k$)

Input: A query point q, LSH-APG index $\mathcal{I}_G$ and $\mathcal{I}_H$, L, K, p_τ, k
Output: k nearest points to q

1 Compute q's projected values $h^*_1(q), \ldots, h^*_{L\times K}(q)$;
2 EPs$\leftarrow$ the set of k approximate nearest points to q in $\mathcal{I}_H$;
3 $V \leftarrow$ the set of visited points during the above search;
4 $R \leftarrow EP$s; //the result set of k best results found so far
5 $m \leftarrow K$, $P(q) \leftarrow (h^*_1(q), \ldots, h^*_m(q))$;
6 $t \leftarrow \sqrt{\chi^2_{p_\tau}(m)}$;
7 **while** $|EPs| > 0$ **do**
8 $e_p \leftarrow$ pop the nearest element in EPs to q;
9 $R_k \leftarrow$ the furthest points in R to q;
10 **if** $\|e_p, q\| > \|q, R_k\|$ **then**
11 **break**;
12 **for** *each* $o \in N(e_p)$ **do**
13 **if** $o \notin V$ **then**
14 $V \leftarrow V \cup \{o\}$;
15 **if** $\|P(q), P(o)\| < t \cdot \|q, R_k\|$ **then**
16 Compute $\|q, o\|$;
17 update R and EPs;
18 **return** R;

4.3 ANN Query in LSH-APG

The query algorithm not only decides the efficiency and accuracy of ANN search, but also affects the index quality and indexing efficiency. Algorithm 3 outlines the ANN query processing, which consists of two parts: find entry points using $\mathcal{I}_H$ (Line 1 - 4) and improve query quality using $\mathcal{I}_G$ (Line 5 - 18). The algorithm starts by computing the hash values of q (Line 1). Then, we can conduct a kANN search for q using $\mathcal{I}_H$ (Line 2). Since the search procedure in $\mathcal{I}_H$ is the same as that in the LSB-Tree [40], we do not give detailed description here due to the space limitation. According to the property of LSH, we can obtain high-quality results in $O(L)$ costs [40]. Next, we take points in EPs as the entry points to conduct a kANN query in $\mathcal{I}_G$. Specifically, in each iteration (hop), the nearest point e_p in EPs to q is popped from EPs (Line 8) and we denote the current found k-th NN as R_k (Line 9). If the distance between q and e_p is already greater than that between q and R_k, the algorithm terminates immediately (Line 10). Otherwise, we continue the search from e_p by checking its neighbors. To further boost query efficiency, we design an LSH-based pruning condition (Line 15) to reduce the number of neighbors checked. That is, for each neighbor o of e_p, if $\|P(q), P(o)\| > t \cdot \|q, R_k\|$, we filter out o without computing the distance $\|q, o\|$. According to Lemma 7, to be introduced in Section 5, we can guarantee that $\|q, o\| > \|q, R_k\|$ with the high probability p_τ, and thus it is reasonable to prune o directly. By updating EPs and the result set R iteratively, we get kANN of q finally. Generating entry points via the LSH framework greatly reduces the initial search radius. The reduction of the initial search radius can lower the hop numbers required to terminate the algorithm, and thus improve the query efficiency. Moreover, a closer entry point decreases the probability that the query terminates at a local minimal where the final search radius is still very high.

4.4 Cost Model of LSH-APG

We provide a cost model to analyze the construction cost, query cost and query quality of LSH-APG via the expected query cost C_Q and the final search radius, *i.e.,* the search radius when the query terminates. Here, the search radius r is the distance between the query point q and the current entry point o. We aim to find a model to analyze the correctness and cost of LSH-APG via C_Q and the final search radius. To compute C_Q and the final search radius, we consider the the hop numbers l and the final search radius s are the functions of the initial search radius r, and denote them as the $l(r)$ and $s(r)$, respectively.

The models of $l(r)$ and $s(r)$. We assume that the length of the edges in $\mathcal{I}_G$ is r_o, and for each vertex, its neighbors are uniformly distributed around it. The hop number l depends on the initial search radius r. Given the entry point e_p with $\|q, e_p\| = r$, we denote as $l(r)$ the hop numbers of query processing starting with e_p. To solve $l(r)$, we need to know how fast the search radius decreases and where the query terminates. We define $p(r)$ as the probability that the query terminates when the search radius is r and $\delta(r) = r - r'$ as the hop length, where r' is the search radius of the next hop.

Lemma 2. *Assume that $l(r) \gg \delta(r)$ and $l(r)$ is differentiable, $l(r)$, $p(r)$ and $\delta(r)$ satisfy the following equation:*

$$[1 - p(r)]\delta(r)l'(r) + p(r)l(r) = 1, \tag{3}$$

where $l'(r)$ is the derivative of $l(r)$ with respect to r.

We can derive a similar conclusion for $s(r)$ as follows.

Lemma 3. *Assume that $s(r) \gg \delta(r)$ and $s(r)$ is differentiable, $s(r)$, $p(r)$ and $\delta(r)$ satisfy the following equation:*

$$[1 - p(r)]\delta(r)s'(r) + p(r)s(r) = rp(r), \tag{4}$$

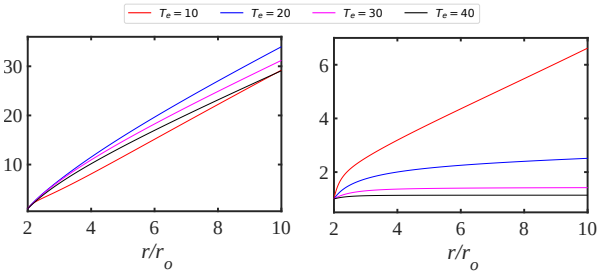
where $s'(r)$ is the derivative of $s(r)$ with respect to r.

Proof. Due to the space limitation, we put the proofs of these two lemmas in our technical report [38]. □

The correctness and the query cost of LSH-APG. It is impossible to obtain the closed-form expressions of $l(r)$ and $s(r)$ from Eq. 3 and 4 since the expressions of $\delta(r)$ and $p(r)$ are extremely complex. Due to the space limitation, the details are in the technical report [38]. Here we give the final conclusions about them.

Theorem 1. *Assume that the expected edge length in LSH-APG is r_o and for each vertex its neighbors are uniformly distributed around it, the query cost of LSH-APG is expected to depend only on the local intrinsic dimensionality of the dataset. Moreover, the final search radius s is expected to be bounded by $(1 + \gamma)r_o$ where $\gamma < 1$.*

Figure 2 shows the curves of $l(r)$ and $s(r)$ with varying r where T_e is the average degree. From Figure 2(a) we can see that $l(r)$ is nearly linear with r when $r > 2$. We can estimate the value of $\varphi(d_i)$ according to the curve. From Figure 2(b) we can see that $s(r)$ converges to the maximum value s_{max} when r increases and a larger T_e incurs a smaller s_{max}. For a given LID, we can reduce the value of s_{max} to at most $2r_o$ by increasing T_e, *i.e.,* $\gamma < 1$.



(a) $l(r)$ (b) $s(r)/r_o$

Figure 2: The curves of $l(r)$ and $s(r)$

The benefit from $\mathcal{I}_H$. Since $l(s)$ depends on the initial search radius r_i. By using $\mathcal{I}_H$, we can obtain the closer entry point o_h, which essentially reduces the initial search radius. Assume that $\|q, o_h\| = r_1$ and a random entry point has the distance r_2 to q ($r_0 < r_1 < r_2$). Then, the benefit from $\mathcal{I}_H$ is $B_{\mathcal{I}_H} = l(r_2) - l(r_1)$. To demonstrate the $\mathcal{I}_H$ is effective, we first prove the results returned from $\mathcal{I}_H$ is good enough.

Lemma 4 (Theorem 1 of [40]). *By setting $K = O(\log n)$ and $L = n^\rho$ where $\rho = O(1/c')$, $\mathcal{I}_H$ can answer a c'^2-ANN ($c' \geq 2$) in $O(dL)$ query cost with at least constant probability of $1/2 - 1/e$.*

The lemma indicates that we can find a c'^2-ANN result with a small query cost $O(dL)$. As stated in [40], even single LSB-Tree is also expected to return results with high quality. In our method, $c' = 2$ and we set $K = O(1)$ and $L = O(1)$ following the mainstream LSH methods [34, 42].

Lemma 5. *Let $\Delta r = r_2 - r_1$ be the reduction of the initial search radius compared to the random entry point, the expected $B_{\mathcal{I}_H}$ is $\frac{\Delta r}{\lambda r_o}$ where $\lambda < 1$ and depends on LID and the average degree T_e.*

Proof. Due to the space limitation, we put the proof in our technical report [38]. □

This lemma indicates that the benefit of the entry point selection is $O(\Delta r)$, which is in line with Figure 2(a). When $r > r_1$, $\delta(r)$ is nearly a constant and the search radius decreases slowly, which incurs a large query cost in the graph-based methods. On the contrary, although the LSH-based methods are hard to achieve as a high query performance as graph-based methods, they can quickly find a point o with $\|q, o\| = r_1 \leq c'r$, and thus improve the query performance of LSH-APG.

Remark 4. *In our cost model, we assume that for each vertex, its neighbors are uniformly distributed around it. This assumption determines the concrete formation of $\delta(r)$, but does not affect the correctness of our method and the upper bound of C_Q. The neighbors of each vertex depend mostly on the points close to it rather than all the dataset, which indicates that $\delta(r)$ is hardly influenced by n. This is in line with our conclusion that C_Q is affected little by n.*

4.5 Complexity Analysis

Following the mainstream graph-based methods [16, 36, 37], we consider T and T' as a constant. According to Theorem 1, we have the following conclusion:

Theorem 2. *LSH-APG has the space complexity of $O(n)$ and can be built in $O(nd\varphi(d_i))$ time, where d_i is the LID of $\mathcal{D}$ and $\varphi(d_i)$ is the expectation of C_Q. The query cost of LSH-APG is $O(d\varphi(d_i))$.*

5 LSH-BASED PRUNING CONDITION

The query cost of a graph-based method comes from the number of distance computations between q and the neighbors of e_p when accessing e_p. The previous query strategy checks all e_p's neighbors, which is unnecessary and time-consuming since some neighbors are obviously far away from q and unlikely to be the required result. Hence, we design an LSH-based pruning condition as follow to filter out some neighbors that might be far:

$$\|P(q), P(o)\| < \sqrt{\chi^2_{p_\tau}(m)} \cdot d_k, \tag{5}$$

where $P(o)$ is the m-dimensional projected vector defined as in Lemma 1, $\chi^2_p(m)$ is the quantile of $\chi^2(m)$ distribution at p_τ and d_k is the current found k-th best NN result. The intuition of the pruning condition is that when $\|o, q\|$ is greater than d_k, $\|P(q), P(o)\|$ will also be greater than $\sqrt{\chi^2_{p_\tau}(m)} \cdot d_k$ with high probability p_τ. Then, it is reasonable to discard o without computing the distance $\|q, o\|$.

Lemma 6 (Lemma 4 in [47]). *Given a query q, an approximation ratio c and parameter t, we define the following two events:*

- ***E1:** For a point o that $\|q, o\| \leq r$, its projected distance to q, $\|P(q), P(o)\|$, is smaller than tr.*
- ***E2:** There are fewer than βn ($\beta > \alpha_2$) points whose distances to q exceed cr but projected distances to q are smaller than tr.*

Then, we have that the probability that E1 occurs is at least α_1, and the probability that E2 occurs is at least $1 - \frac{\alpha_2}{\beta}$, where $\alpha_1 = F(t^2; m)$ and $\alpha_2 = F(t^2/c^2; m)$.

Lemma 6 reveals that $\|P(q), P(o)\|$ can be a proper estimator of $\|q, o\|$. Based on it, we have:

Lemma 7. *With the LSH-based pruning condition, the probability that a point o is filtered increases with $\|q, o\|$. Assume $p_\tau = \frac{1}{2}$ and the current search radius is r, for any $c > 1$, the point whose distance to q is less than r will not be filtered with at least the probability of $\frac{1}{2}$ and we access at most $O(n^\alpha)$ points whose distance to q is greater than cr, where $\alpha = 1 - \frac{9\kappa(c^{-2/3}-1)^2}{4}$ and $\kappa = \frac{m}{\log n}$.*

Proof. According to the Lemma 6, those points whose distance to q exceed cr are very likely to have projected distances to q larger than tr. The total number of this kind of points is less than $2\alpha_2 n$ and the total number of points to be verified is at most $2\alpha_2 n + k$. We try to bound α_1 and $2\alpha_2 n + k$ where $p_\tau = \alpha_1$. By using the Wilson–Hilferty transformation [27, 44], for a random variable $X \sim \chi^2(m)$, $\sqrt[3]{X/k}$ is approximately distributed with $N(1 - \frac{2}{9m}, \frac{2}{9m})$, and thus $Y = \frac{\sqrt[3]{X/k} - (1 - \frac{2}{9m})}{\sqrt{\frac{2}{9m}}} \sim N(0, 1)$. Consider $t^2 = m(1 - \frac{2}{9m})^3$, $\alpha_1 = \Pr[X \leq m(1 - \frac{2}{9m})^3] = \Pr[Y \leq 0] = 0.5 = p_\tau$, which is coincident with our setting. Likewise, $\alpha_2 = \Phi(c_1(\sqrt{m} - \frac{2}{9}\sqrt{1/m}))$, where $c_1 = \sqrt{\frac{9}{2}}(c^{-2/3} - 1) < 0$ and $\Phi(x)$ is the cumulative distribution function of the standard normal distribution. Next, we prove that α_2 can be bounded by $\exp(-\frac{c_1^2 m}{2})$. Denote $g(u) = \Phi(c_1(u - \frac{2}{9u})) - \exp(-\frac{c_1^2 u^2}{2})$,

it is easy to demonstrate that $g(u)$ first decreases and then increases with u in $(0, +\infty)$, so $g(\sqrt{m}) < \max\{g(0), g(+\infty)\}$. $g(0) = g(+\infty) = 0$ and thus $g(\sqrt{m}) < 0$, which implies $\alpha_2 < \exp(-\frac{c_1^2 m}{2})$. Considering that $m = \kappa \log n$, we have $\exp(-\frac{c_1^2 m}{2}) = n^{-\frac{\kappa c_1^2}{2}}$ and the total number of points to be verified is at most $2n^{1-\frac{\kappa c_1^2}{2}} + k$. □

This lemma indicates the point whose distance to q is less than the search radius r will be checked with at least the probability of $\frac{1}{2}$. On the contrary, the farther a point is to q, the more likely it is filtered out. The number of checked points whose distances to q are greater than cr is bounded by $O(n^{\alpha})$, which depends on the values of c, n and m. The total number of points filtered by the pruning condition depends on how many "far" points we meet. This pruning condition helps reduce the query cost and still guarantees the query quality. Usually, a large p_τ is used to better balance the query quality and query efficiency. We only prove this lemma with $p_\tau = \frac{1}{2}$ as an example. For other values of p_τ, α is also bounded.

6 INDEX MAINTENANCE

As the data evolves, we need to update LSH-APG by reconstructing some edges for related points. The updates of LSH-APG includes the insertion and deletion. It is simple and natural to insert a new point into LSH-APG since LSH-APG is built via the consecutive insertion strategy. Therefore, we focus on designing an efficient deletion strategy. To delete a point o, we need to discard all the out-edges and in-edges of o in $\mathcal{I}_G$ and remove o from $\mathcal{I}_H$. It is trivial to remove a point from the $\mathcal{I}_H$, but it is challenging to delete in-edges in $\mathcal{I}_G$ since they are not recorded in the graph.

Let $RN(o) = \{v | (v, o) \in E\}$ be the set of reverse neighbors of o in $\mathcal{I}_G$ and $d_m = \max_{v \in RN(o)} \|o, v\|$ be the maximum length. We store the in-degree of o, $|RN(o)|$, and d_m in LSH-APG to facilitate the deletion, which is much space-saving than storing all the in-edges. To delete o, we first mark o and all the out-edges of o as the Deleting status. Then, we conduct a range search in LSH-APG with the search radius d_m from o's closest neighbor in $\mathcal{I}_G$. Once a point u is found, we check whether u is in the $RN(o)$. If so, (u, o) is discarded and the in-degree of o is decreased by one. Moreover, we increase the number of u's neighbors to T' by finding points in neighbors of u's neighbors once the degree of u is less than T. By this manner, we maintain the degree of each vertex in the range $[T, T']$ and reduce the influence of the deletion on the graph quality.

However, d_m could be very large in some cases and it is costly to check all the points whose distance to q is within d_m. Moreover, $\mathcal{I}_G$ is a directed graph and some points in $RN(o)$ is unreachable from o. Hence, we first set a maximum search cost C_{Dm} to control the cost of the range search during the deletion. The larger C_{Dm}, the more likely it is to find an in-edge, but it incurs a higher cost. Then, for an in-edge of o not found in the range search, we leave it to the deletion procedure in the following queries. If it is found during an ANN query later, we discard it and decrease the in-degree of o by one. Once the in-degree of o becomes 0, we discard all the out-edges of o and o itself. Finally, to avoid some in-edges not being found for a long time and thus wasting the space, we also traverse the graph and discard all the edges to be deleted when their amount reaches 10% of the total number of edges in $\mathcal{I}_G$.

The deletion cost of LSH-APG includes the cost of finding o's in-edges, adding new neighbors for some points and C_{Dm}. Due to the property of the NN-graph, *i.e.,* neighbors are more likely to be neighbors of each other [11], $C_{Dm} = C_Q$ can ensure that the most of in-edges are found. To add new neighbors for a point u, it is sufficient to find points in neighbors of e's neighbors rather than conduct a query for u. C_{Dm} is bounded by C_Q and thus we have the following conclusion as follows:

Theorem 3. *The expected deletion cost of LSH-APG only depends on the local intrinsic dimensionality of the dataset.*

As our graph updating strategy is developed on top of the indexing strategy, *i.e.,* the consecutive insertion strategy, the graph structure can maintain its high-quality as the dataset evolves. However, the graph indexes built via cluster & merge strategy and iteration strategy cannot implement such strategies, since the addition or deletion of a batch of points affects the clustering results or edge selection of original points. The indexing strategy shapes the index structure, and the index structure determines what a suitable indexing and updating strategy should be. If we simply implement the similar updating strategies on these APGs, it is difficult to ensure their graph quality. On the contrary, the query performance of LSH-APG remains steady after updating, as shown in Sec. 7.5.

7 EXPERIMENTAL STUDY

In this section, we conduct extensive experiments on real-world and synthetic datasets to provide a comprehension analysis on LSH-APG. We implement LSH-APG[1] and the competitors in C++ compiled with g++ using -Ofast optimization and openMP for parallelism. All experiments are run on a Ubuntu server with 2 Intel(R) Xeon(R) Gold 5218 CPUs @ 2.30GHz (64 threads) and 254 GB RAM.

7.1 Experimental Settings

Datasets. We employ 8 datasets varying in cardinality and dimensionality, whose information is summarized in Table 2 in the ascending order of their sizes. **LID.**[2] in the table is used to measure the difficulty of answering NN queries in the dataset [1]. A larger LID implies that it is harder to find NN on the dataset. Among the datasets, Six are real-world datasets widely used in NN search methods[16, 36, 42, 43], including our competitors. The rest 2 synthetic datasets, **Rand10M** and **Gauss10M** are generated from uniform distribution $U(-1, 1)$ and Gaussian distribution $N(0, 1)$ on each dimensionality independently. For NN queries, we randomly select 100 points as query points and remove them from the datasets.

Competitors. To demonstrate the indexing and query performance of LSH-APG, we compare it with the best existing NN search methods, including LSH-based and graph-based methods. Among LSH-based methods, DB-LSH [42] is proven to have the lowest query complexity. Among graph-based methods, a comprehensive experimental comparison of graph-based methods [43] has shown that HNSW [36], HCNNG [37] and NSG [16] are always the best three ones in terms of the query performance. Therefore, we choose DB-LSH, HNSW, HCNNG and NSG as our competitor algorithms.

[1] https://github.com/Jacyhust/LSH-APG-SourceCode/tree/main/cppCode/LSH-APG

[2] There is no unified method to compute the LID and we compute it according to the Definition 1 in [1] with x being the average distance between the query points and their 50-th NN.

Table 2: Summary of Datasets

Datasets	Cardinality	Dim.	LID.	Size (GB)
MNIST	60,000	784	12.7	0.184
Deep1M	1,000,000	256	26.0	1.00
Gauss10M	10,000,000	32	26.3	1.19
Rand10M	10,000,000	32	23.9	1.19
Gist1M	1,000,000	960	36.2	3.58
SIFT10M	10,000,000	128	22.0	4.77
SIFT100M	100,000,000	128	23.7	47.7
Tiny80M	79,302,017	384	44.6	113

Table 3: Parameter Settings of Algorithms

Algorithm	Parameters
LSH-APG	$K = 16, L = 2, T = 24, T' = 2T, p_\tau = 0.95$
DB-LSH	$c = 1.5, K = 12, L = 5$
HNSW	$M = 48, ef = 80$
HCNNG	$MC = 500, NC = 10$
NSG	$L = 40, R = 50, C = 500$

Parameter Settings. We consider the (c, k)-ANN queries with $k = 50$ for all algorithms in the default settings. Following the settings in the paper or source code of our competitors, we adopt the fixed parameters for each algorithm as shown in Table 3. For HCNNG, MC is the maximum size of the cluster and NC is the number executions of hierarchical clustering procedures.

Evaluation Metric. We compare the algorithms from four aspects: indexing quality, indexing efficiency, query quality and query efficiency. We report the average degrees, the range of degrees, the standard deviation of degrees of each graph index and evaluate the quality of them by using the normalized maximum common subgraph (NMCS). Maximum common subgraph (MCS) is used to measure the similarity of two graphs [13]. Here, we adopt **NMCS**, a derived definition from MCS, to compute the similarity between a graph index G for the ANN query and the exact NN graph, which is defined as follow,

Definition 3 (NMCS (Normalized maximum common subgraph)). *Let $G = (V, E)$ be an APG and $G_E = (V, E')$ be the exact NN graph of V that satisfies:*

- *For any a point $v \in V$, $|G(v)| = |G_E(v)|$ where $G(v)$ is the neighbors of v in G;*
- *Let $k' = |G_E(v)|$. $G_E(v)$ is the k'-NN result of v in $V - \{v\}$.*

Then

$$NMCS = \frac{\sum_{v \in V} |G(e) \cap G_E(e)|}{\sum_{v \in V} |G(e)|} \tag{6}$$

Since the exact NN graph is nearly impossible to compute, we randomly choose 200 vertexes in V to estimate the NMCS.

We evaluate the query quality via recall. Given a query point q, for a (c, k)-ANN query, assume that the algorithm return the set $R = \{o_1, \ldots, o_k\}$ and the exact kNN of q is $R^* = \{o_1^*, \ldots, o_k^*\}$, then recall is defined as follows [42]

$$Recall = \frac{|R \cap R^*|}{k}. \tag{7}$$

Since all algorithms except DB-LSH adopt openMP parallelizing, their running times are unstable and liable to be affected by the current system status. Therefore, we use the number of distance computations per insertion (**CPI**) and the number of distance computations per query (**CPQ**) instead of the running time to evaluate the indexing and query efficiency, respectively. For fairness, we consider the cost of computing hash values as a part of distance computations in LSH-APG.

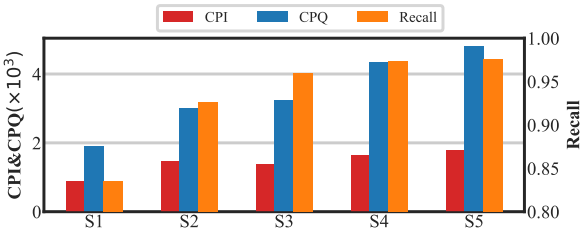


Figure 3: Performance on DEEP1M when Varying T and T'

7.2 Self Evaluation

In this subsection, we demonstrate the effectiveness of the LSH framework on LSH-APG and analysis the effect of p_τ.

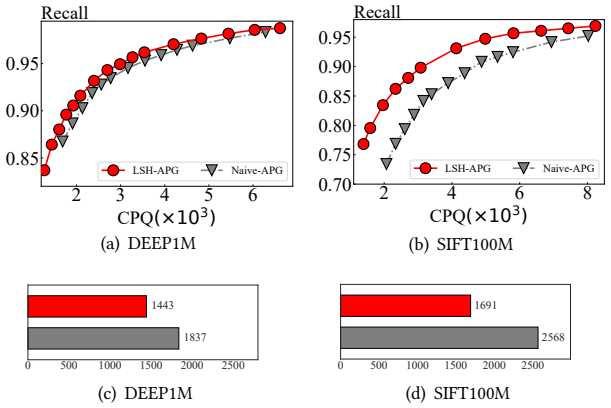
Evaluation of the LSH framework. To demonstrate the functionality of the LSH framework, we compare Naive-APG with LSH-APG. Here we report the results on DEEP1M and SIFT100M for brevity, as shown in Figure 4. To compare their query performance, we plot their Recall-CPQ curves. The results show that to reach a given recall, LSH-APG reduce about 20% CPQ on DEEP1M and 50% CPQ on SIFT100M, which demonstrates the improvement of the LSH framework on query processing. To compare their indexing performance, we notice that LSH-APG and Naive-APG have nearly the same graph indexes and LSH framework only affects the indexing cost. Thus, we report the CPIs of LSH-APG and Naive-APG. The results show that LSH-APG (the red bar) reduce about 20% CPI on DEEP1M and 60% CPI on SIFT100M, respectively. It indicates that LSH framework plays also an important role in the indexing phase.

Parameter study on p_τ. We discuss the effect of p_τ on query performance by varying p_τ in range $\{0.8, 0.9, 0.95, 0.95, 1.0\}$. Here, we only show results on DEEP1M for brevity. p_τ controls the pruning threshold in the query phase and a smaller p_τ makes it more likely to filter out a neighbor. As shown in Figure 5, both the recall and CPQ increases with p_τ, which indicates that the pruning condition in LSH-APG can reduce the query cost but slightly damages the query quality to some extent because it inevitably filter out some exact results. Taking both query efficiency and quality into consideration, we set $p_\tau = 0.9$.

Parameter study on T and T'. In this set of experiment, we discuss the effect of T and T' on performance of LSH-APG by setting (T, T') as $S1 = (24, 24)$, $S2 = (48, 48)$ $S3 = (24, 48)$, $S4 = (24, 72)$ and $S5 = (24, 96)$, respectively. Here, we only show the results on DEEP1M for brevity. As shown in Figure 3, when comparing $S2$ and $S3$, we can find that the setting of $T' = 2T$ achieves surprisingly a higher recall with nearly a same CPQ. The setting of $T = T' = 48$ has a higher CPI than the setting of $T = 24, T' = 48$ but achieves a worse query performance. When fixing T as 24, a higher T' incurs a higher CPI, CPQ and Recall (see $S1, S3, S4, S5$). The CPI and CPQ increase nearly linearly with T'; while Recall has been almost steady when $T' = 2T$. Hence, $T' = 2T$ is a good choice.

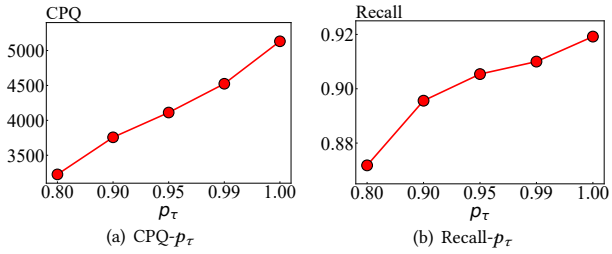
Table 4: Overview of index information.

		(μ, σ)	Range	NMCS	CPI			(μ, σ)	Range	NMCS	CPI
MNIST	**LSH-APG**	(37.51,9.19)	[24,48]	0.7655	583.59	**GIST1M**	**LSH-APG**	(32.43,9.33)	[24,48]	0.4159	1864.0
	HNSW	(17.21,8.83)	[1,48]	0.4006	928.50		**HNSW**	(10.07,9.86)	[1,48]	0.1159	2144.3
	NSG	(18.19,5.72)	[1,50]	0.4499	3801.7		**NSG**	(16.50,12.53)	[1,77]	0.2929	7027.1
	HCNNG	(11.39,3.03)	[1,26]	0.5353	4801.9		**HCNNG**	(17.50,5.63)	[1,30]	0.1375	5091.8
	DB-LSH	-	-	-	60		**DB-LSH**	-	-	-	60
DEEP1M	**LSH-APG**	(35.84,9.42)	[24,48]	0.5915	1442.9	**SIFT10M**	**LSH-APG**	(36.61,9.31)	[24,48]	0.5194	1476.8
	HNSW	(23.55,10.84)	[1,48]	0.3036	2138.8		**HNSW**	(25.84,10.80)	[1,48]	0.3018	2578.5
	NSG	(20.96,9.17)	[1,50]	0.4510	6291.6		**NSG**	(21.11,9.29)	[1,51]	0.4143	4782.5
	HCNNG	(17.49,4.35)	[2,30]	0.2786	5091.8		**HCNNG**	(17.83,4.09)	[1,30]	0.2163	3341.7
	DB-LSH	-	-	-	50		**DB-LSH**	-	-	-	60
Gauss10M	**LSH-APG**	(32.47,9.21)	[24,48]	0.3645	2266.4	**SIFT100M**	**LSH-APG**	(36.31,9.36)	[24,48]	0.5110	1691.3
	HNSW	(25.43,13.00)	[1,48]	0.2463	8776.5		**HNSW**	(26.68,11.05)	[24,48]	0.2577	3262.2
	NSG	(24.31,13.95)	[1,51]	0.3365	7279.9		**NSG**	(26.84,12.07)	[1,52]	0.3734	7024.7
	HCNNG	(19.68,6.09)	[6,30]	0.0793	3341.8		**HCNNG**	(18.18,4.17)	[1,30]	0.1719	4164.7
	DB-LSH	-	-	-	50		**DB-LSH**	-	-	-	60
Rand10M	**LSH-APG**	(35.76,9.21)	[24,48]	0.5508	2159.2	**Tiny80M**	**LSH-APG**	(32.18,9.15)	[24,48]	0.3159	2494.6
	HNSW	(33.92,9.41)	[1,48]	0.4544	9547.2		**HNSW**	(13.34,10.97)	[1,48]	0.0698	3567.6
	NSG	(36.02,11.78)	[2,50]	0.4126	6573.0		**NSG**	/	/	/	/
	HCNNG	(19.58,4.92)	[7,30]	0.1005	3341.8		**HCNNG**	(17.75,5.99)	[1,30]	0.1436	6380.3
	DB-LSH	-	-	-	60		**DB-LSH**	-	-	-	60



(a) DEEP1M (b) SIFT100M (c) DEEP1M (d) SIFT100M

Figure 4: Comparison of LSH-APG and Naive-APG



(a) CPQ-p_τ (b) Recall-p_τ

Figure 5: Performance of LSH-APG when varying p_τ

7.3 Evaluation of Indexing Performance

We study the index quality and indexing efficiency of all algorithms with the default settings. The results are shown in Table 4. In this table, μ and σ denote the average of degrees and the standard deviation of degrees. **Range** is the interval where degrees distribute. NSG fails to build the index on Tiny80M due to the out of memory issue, so we do not report its results (including the query results) on Tiny80M. From the table we have the following observations when comparing each evaluation metric:

(1) LSH-APG have the the large average degrees. It is because LSH-APG adopt the simple neighbor selection strategy and does not discard the similar edges. HNSW has the extremely low degree on Gist1M and Tiny80M, although these two datasets have high LIDs. This abnormal phenomenon is caused by the heuristic neighbor selection and will damage the query performance to some extent. Comparing the degree among different datasets, we find the distribution of degrees on LSH-APG changes little but the distributions on other graph indexes do not. It is hard to say which is better.

(2) LSH-APG always has the highest NMCS among the graph based algorithms, which indicates it is more similar as an exact NN graph and has the highest-quality edges, which benefits the query quality since it is more likely that we find the exact NN in the APG.

(3) DB-LSH achieves the smallest CPI among the graph-based methods on all datasets since it just needs to compute a small number of hash functions. Among the graph-based algorithms, LSH-APG has the smallest CPI and only HNSW's CPI is comparable with it. NSG and HCNNG both have the larger CPIs. The reason of this phenomenon is that: First, LSH-APG avoids many unnecessary distance computation by the better entry point selection and LSH-based pruning condition when insertion. Second, LSH-APG does not adopt the time-consuming heuristic selection strategy like that in HNSW or NSG. In NSG, half the CPI comes from building an approximation kNN graph with a large degree K via NN-Descent strategy. Moreover, the CPI of building the NSG on top of an NNG is also high due to the heuristic selection strategy. HCNNG requires computing the distance between any two points in a group and conducts hierarchical clustering procedures multiple times, which incurs a large CPI.

(4) Comparing the NMCS and CPI among different datasets, we can find all the algorithms follows the similar tendency. For example, LSH-APG has the smaller CPI and higher NMCS on DEEP1M than that on GIST1M. Then, HNSW, NSG and HCNNG all have the smaller CPI and higher NMCS on DEEP1M than that on GIST1M, respectively. Moreover, the CPI and NMCS of each algorithm vary with the datasets. For LSH-APG, the CPI increase gradually with the data cardinality when comparing that on SIFT10M and SIFT100M. The CPI and NMCS of LSH-APG are greatly influenced by LID. A larger LID incurs a higher CPI and a smaller NMCS. For other algorithms, their NMCS and CPI are influenced by data cardinality and LID. Astonishingly, HNSW has the highest CPIs on Gauss10M and Rand10M (8776.5 and 9547.2), which is even much higher than that on SIFT100M and Tiny80M (3262.2 and 3567.6). It indicates HNSW is hard to process the random dataset.

7.4 Evaluation of Query Performance

In these sets of experiments, we study the query performance of all algorithms. We first study how the characteristics of dataset, *i.e.,* data cardinality n and dimensionality d, affect the query performance. Then, we study the effect of k. Finally, we analysis the trade-off between the query quality and query efficiency by increasing the number of checked points. Since DB-LSH always needs the much larger query cost to reach the similar recall than the graph-based methods, we do not report its results in the rest experiments. . For example, the CPQ of DB-LSH to reach a recall of 0.95 is about $8M$, which is 100 times higher than the worst graph-based methods.

7.4.1 ***Effect of*** n. By randomly selecting some points from the original dataset, we compare the query performance of all algorithms in the default settings. Limited by the space, we only report the result on SIFT100M, as shown in Figure 6(a)-(b). The range of the cardinality n is $\{0.2N_0, 0.4N_0, \ldots, N_0\}$, where N_0 is the cardinality of the original datasets. As shown in the figures, for each algorithm, the CPQ (resp. recall) increases (resp. decreases) with the value of n. But the increase on CPQ of LSH-APG is rather slight, which is in line with our conclusion that the query cost LSH-APG is less affected by the data cardinality.

7.4.2 ***Effect of*** k. We compare the query performance of all algorithms when varying k of (c, k)-ANN query in $\{1, 10, 20, \ldots, 100\}$. Limited by the space, we only report the result on SIFT100M, as shown in Figure 6(c)-(d). From the figures we can see that CPQ of each algorithm increases nearly linearly with k but LSH-APG has the smallest slope. Moreover, LSH-APG always achieves the smallest CPQ and the highest recall, which indicates it performs best on query processing among the competitor algorithms. NSG and HNSW achieves the surprisingly close recall and their CPQ-k curves also have about the same slope, which further demonstrate the similarity between them.

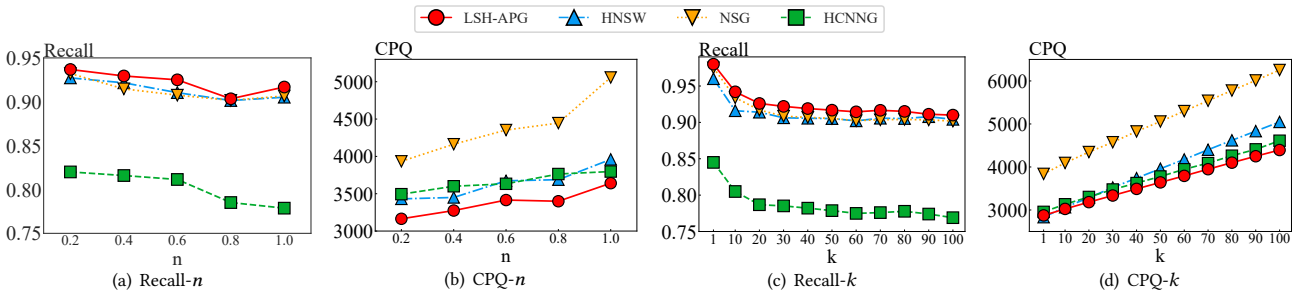
7.4.3 ***Effect of*** d. In the default settings, we compare the query performance of all algorithms when varying the dimensionality d of datasets. Due to the unbalanced distribution in real-world datasets, it is not meaningful to pick up parts of dimensionality on them. So, we only compare the algorithms on two synthetic datasets, Rand10M and Gauss10M with the range of d $\{8, 16, 32, 64, 128\}$. The results are shown in Figure 7. As shown in the figures, the CPQ of each algorithm increases with d. The increasing tendencies of LSH-APG, HNSW and HCNNG are sublinear but that of NSG are nearly linear, which indicates NSG is more likely to be affected by the dimensionality. As for the recall, we surprisingly find that the recall of each algorithm decreases very rapidly with d. When d is 8 or 16, all algorithms can reach the recall of nearly 1.0; when d comes to 32, recalls all declines to about 0.6 on Gauss10M and 0.75 on Rand10M; when d reaches 64 or even 128, recalls have gone down to less than 0.3. This results show that the effect of the dimensionality on the recall is much greater than that of the cardinality. This result can be explained by the "curse of dimensionality",*i.e.,* when the dimensionality is large enough, the distance between any two points is almost identical and it becomes very difficult to differentiate the NNs and other points for any query. The "curse of dimensionality" phenomenon becomes very obvious on the random datasets than that on the real-world datasets, even when d is only 64 or 128. This is because with the same dimensionality, the random datasets have the much higher LID than the real-world datasets.

7.4.4 ***Recall-CPQ Curve***. For any ANN method, a more accurate result can be obtained by increasing the number of checked points, which consequently damages the query efficiency. Therefore, there is a trade-off between the query quality and query efficiency. In this set of experiments, we analyze the trade-off between them via the Recall-CPQ Curve. To reach the same target recall, the algorithm with the smaller CPQ has a higher query performance. Figure 8 present the results on four datasets.

From the figures we have the following observations: (1) As the CPQ increases, all algorithms achieve the higher recall, which is in line with the philosophy of ANN methods, *i.e.,* trading accuracy for efficiency. Moreover, the required CPQ to reach a given recall *Rec* increases nearly exponentially with *Rec*, which indirectly demonstrates that finding the exact NNs is extremely hard and time-consuming. (2) Among all algorithms, LSH-APG requires the smallest CPQ to reach the same recall, which indicates LSH-APG achieves the best trade-off between the query quality and query efficiency. As analyzed in the previous part, the advantages of LSH-APG are due to the better entry point selection found in the LSH indexes and the pruning condition that enables us to filter out some neighbors. (3) NSG and HNSW always exhibit the similar tendency and even nearly the same curve on Rand10M, which demonstrates that they may have the similar structure since they adopt the totally identical heuristic selection strategy (This is proven in [43]). However, in the most cases, HNSW is the better algorithm. (4) HCNNG always achieves the worst query performance. On Gauss10M and Rand10M, to reach the same recall, HCNNG requires nearly 4 times as large CPQ as LSH-APG. This can be explianed that: HCNNG adopts the cluster-based approach to construct subgraphs. However, the data in the high-dimensional space are not "well" clustered and we could not find proper clusters.

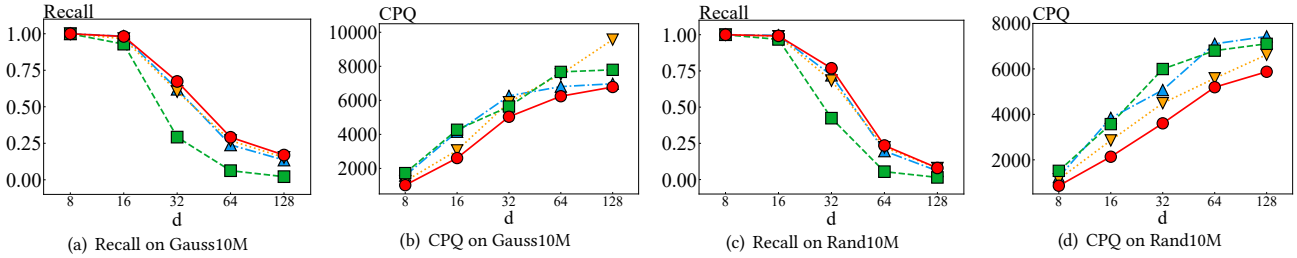
7.5 Evaluation of Updating

We follow [22] and evaluate the update performance of LSH-APG via a batch insertion or deletion. Given the graph index of LSH-APG, $\mathcal{I}_G = (V_0, E_0)$, we denote a batch insertion (resp. deletion) of the APG as $Y\%$ update where $Y = \frac{|V|-|V_0|}{|V_0|}$ and $|V|$ is the number of points in the graph after insertion or deletion. In this set of



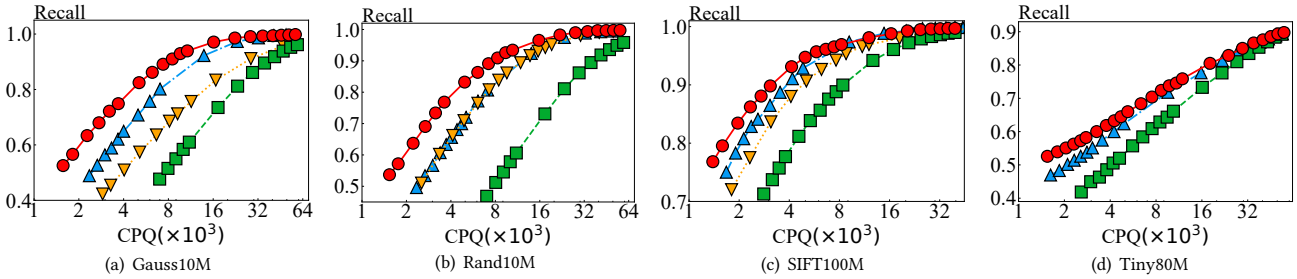
(a) Recall-n (b) CPQ-n (c) Recall-k (d) CPQ-k

Figure 6: Performance on SIFT100M when Varying n and k



(a) Recall on Gauss10M (b) CPQ on Gauss10M (c) Recall on Rand10M (d) CPQ on Rand10M

Figure 7: Performance on Rand10M and Gauss10M when Varying d



(a) Gauss10M (b) Rand10M (c) SIFT100M (d) Tiny80M

Figure 8: Recall-CPQ Curves on all Datasets

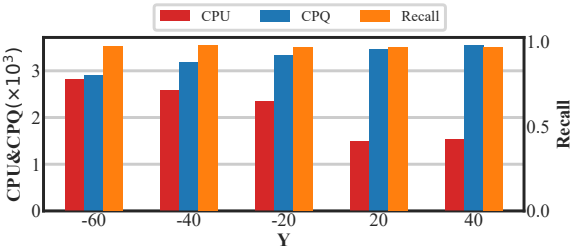


Figure 9: Performance on DEEP1M when Updating

experiments, we study the the effect of Y on DEEP1M with $V_0 = 600K$ when varying Y in $\{-60, -40, -20, 20, 40\}$ ($Y < 0$ denotes the deletion operation) and report the query performance and the cost per update (CPU) on Figure 9. As for the updating cost, the insertion cost is obvious smaller than the deletion cost and 40% insertion has the higher cost than 20% insertion. The deletion cost increases slightly with $|Y|$, which can be explained that the total number of points in the graph decreases and The probability that a vertex connecting to the points to be deleted increases, and thus it takes more time to add the new edges. For the query performance, we find the recall is steady and CPQ gradually increases with Y since the number of the points increases. It indicates that the update operations do not damage the query performance.

8 CONCLUSION

In this paper, we have proposed a novel approach, called LSH-APG, to efficiently build an APG and facilitate ANN query processing in high-dimensional spaces with quality guarantees. LSH-APG handles the high construction cost issue in the graph-based methods by designing an efficient and accurate LSH-based query strategy to consecutively insert data points in the APG. A high-quality entry point selection technique and LSH-based pruning condition have been developed to reduce the number of points to be checked in the search. The expected query cost has been proven to be less affected by dataset cardinality, allowing us to simultaneously reduce the query processing time and the indexing time. Therefore, LSH-APG is well positioned to deal with large-scale datasets. In addition, it is proven that LSH-APG can be maintained incrementally in a low cost as the dataset evolves. A thorough range of experiments showed that LSH-APG can reduce the average construction cost by 40% compared to the best competitor, HNSW, while still maintain the best query performance.

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APPENDIX: PROOFS

A. Proof of Lemma 2

Proof. When the query starts with search radius r, the query could terminate with the probability $p(r)$ and go to the next hop with the probability $1 - p(r)$. If the query terminates, $l(r) = 1$; otherwise, $l(r) = l(r - \delta(r)) + 1$. Hence,

$$l(r) = p(r) \cdot 1 + [1 - p(r)][l(r - \delta(r)) + 1] \tag{8}$$

Considering that $l(r) \gg \delta(r)$, we have

$$\frac{l(r) - l(r - \delta(r))}{\delta(r)} \approx l'(r)$$

Thus, $l(r - \delta(r)) = l(r) - \delta(r)l'(r)$ and

$$l(r) = p(r) \cdot 1 + [1 - p(r)][l(r) - \delta(r)l'(r) + 1] \tag{9}$$

Simplifying the above equation, we prove the lemma. □

B. Proof of Lemma 3

Proof. As that in Proof 8, we have

$$s(r) = p(r) \cdot r + [1 - p(r)]s(r - \delta(r)) \tag{10}$$

Considering that

$$\frac{s(r) - s(r - \delta(r))}{\delta(r)} \approx s'(r)$$

Thus,

$$[1 - p(r)]\delta(r)s'(r) + p(r)s(r) = rp(r) \tag{11}$$

□

C. Solving $\delta(r)$ and $p(r)$.

We now begin to solve $\delta(r)$. Let o_n be the closest points to q among ep's neighbors and θ_m be the vectorial angle between $\vec{e_pq}$ and $\vec{e_po_n}$. We have the following observation:

Observation 1. *$\delta(r)$ satisfies $\delta(r) = r - \sqrt{r^2 + r_o^2 - 2rr_0\cos\theta_m}$. When $r \gg r_0$, $\delta(r) = r_0\cos\theta_m$.*

Proof. Since $\|e_p, q\| = r$, $\|e_p, o_n\| = r$ and the vectorial angle between $\vec{e_pq}$ and $\vec{e_po_n}$ is θ_m. According to the law of cosines, $\|o_n, q\| = \sqrt{r^2 + r_o^2 - 2rr_0\cos\theta_m}$. Thus, $\delta(r) = \|e_p, q\| - \|o_n, q\| = r - \sqrt{r^2 + r_o^2 - 2rr_0\cos\theta_m}$. □

To analyze the distribution of θ_m, we first consider the distribution of the vectorial angle θ_o between $\vec{e_pq}$ and $\vec{e_po}$, where o is one of neighbors of e_p. Since e_p's neighbors are uniformly distributed around it, θ_o follows the distribution of the vectorial angle between any two random vectors in $\mathbb{R}^{d_i}$, where d_i is the local intrinsic dimensionality (LID) of $\mathcal{D}$ [1].

Lemma 8 (Theorem 1 in [8]). *The probability density function of θ_o is*

$$f_{\theta_o}(\theta) = \frac{\Gamma(\frac{d_i}{2})sin^{d_i-2}\theta}{\sqrt{\pi}\Gamma(\frac{d_i-1}{2})}, \tag{12}$$

where $\Gamma(x)$ is the Gamma function [29].

Then, the cumulative distribution function of θ_o can be written as $F_{\theta_o}(\theta) = \int_0^\theta f_{\theta_o}(t)dt$. Assume e_p has T_e neighbors. Based on the above assumptions, $\vec{e_po_n}$ is the edge that has the minimal angle to $\vec{e_pq}$. Then, θ_m is the minimal one among T_e vectorial angles, and thus we have

Corollary 1. *The cumulative distribution function of θ_m is*

$$F_{\theta_m}(\theta) = 1 - [1 - F_{\theta_o}(\theta)]^{T_e}, \tag{13}$$

Correspondingly, the probability density function of θ_m can be written as $f_{\theta_m}(\theta) = F'_{\theta_m}(\theta)$.

We now compute $p(r)$ and $p(r)$ is the probability that the query terminates, which indicates that $\delta(r) < 0$. Hence, we have

Lemma 9. *$p(r)$ satisfies*

$$p(r) = 1 - F_{\theta_m}(\arccos\frac{r_0}{2r}). \tag{14}$$

Proof. $p(r) = \Pr[\delta(r) < 0] = \Pr[\cos\theta_m < \frac{r_0}{2r}] = \Pr[\theta_m > \frac{r_0}{2r}] = 1 - F_{\theta_m}(\arccos\frac{r_0}{2r})$. □

D. Proof of Lemma 5

Proof. When $r > r_1$, the query is very unlikely to terminate and when can consider $p(r) = 0$. Thus, Eq. 3 can be simplified as $\delta(r)l'(r) = 1$ and we have

$$l(r) = \int_{r_1}^{r} \frac{1}{\delta(r)}dr + l(r_1).$$

Then, $B_{\mathcal{I}_H} = l(r_2) - l(r_1) = \int_{r_1}^{r_2} \frac{1}{\delta(r)}dr$. Further, consider $r \gg r_o$, we approximate $\delta(r)$ as

$$\begin{aligned}\delta(r) =& r - r\sqrt{1 + (\frac{r_o}{r})^2 - 2\frac{r_o}{r}\cos\theta_m} \\ \approx& r - r[1 + \frac{r_o^2}{2r^2} - \frac{r_o}{r}\cos\theta_m] \approx r_o\cos\theta_m\end{aligned}$$

Hence, we have $B_{\mathcal{I}_H} = \frac{r_2 - r_1}{r_o\cos\theta_m}$ and $r_2 - r_1 = \Delta r$. Therefore, the expected $B_{\mathcal{I}_H}$ is $\frac{\Delta r}{r_o\mathbb{E}[\cos\theta_m]}$. Denote $\lambda = \mathbb{E}[\cos\theta_m]$, which satisfies $\lambda < 1$, we prove the lemma. □

E. Proof of Theorem 1

Proof. Since $p(r)$ and $\delta(r)$ are independent on n, $l(r)$ and $s(r)$ will also be independent on n and only affected by the local intrinsic dimensionality of the dataset. Hence, the query cost of LSH-APG is expected to depend only on the local intrinsic dimensionality of the dataset. Next, we prove that the final search radius s is expected to be bounded by $(1 + \gamma)r_o$ where $\gamma < 1$.

Consider that $r > r_o$ and we express $s(r)$ as $s(r) = \int_{r_o}^{r_i} s'(r)dr + s(r_o)$. Since $s(r_o) \le r_o$, denote $\int_{r_o}^{r_i} s'(r)dr = \beta r_o$ and we prove that β is bounded.

According to Lemma 3, we have

$$[1 - p(r)]\delta(r)s'(r) < rp(r). \tag{15}$$

$p(r)$ decreases monotonically with r and thus $1 - p(r) > 1 - p(r_o)$. From the proof of Lemma 5 we know that $\delta(r) \approx \lambda r_o$ where $\lambda = \mathbb{E}[\cos\theta_m]$. Hence,

$$s'(r) < \frac{rp(r)}{[1 - p(r_o)]r_o\cos\theta_m}.$$

Then,

$$\beta r_o = \int_{r_o}^{r_i} s'(r)dr < \frac{\int_{r_o}^{r_i} rp(r)dr}{[1 - p(r_o)]r_o\cos\theta_m}$$

$p(r) = 1 - F_{\theta_m}(\arccos\frac{r_0}{2r}) = [1 - F_{\theta_o}(\arccos\frac{r_0}{2r})]^{T_e}$. Let $u = r/r_o$ and $u_i = r_i/r_o$, we have

$$\beta < \frac{\int_1^{u_i} u[1 - F_{\theta_o}(\arccos\frac{1}{2u})]^{T_e}du}{\lambda[1 - p(r_o)]}.$$

Although it is hard to compute this integral, we can find it can be reduced by increasing T_e. Since $\lim_{T_e\to=\infty}\beta = 0$, we can guarantee that $\beta < 1$ when given a large enough T_e. □