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Efficient and accurate nearest neighbor and closest pair search in high-dimensional space — Source link

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Efficient and Accurate Nearest Neighbor and Closest Pair Search in High Dimensional Space

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Nearest neighbor (NN) search in high dimensional space is an important problem in many applications. From the database perspective, a good solution needs to have two properties: (i) it can be easily incorporated in a relational database, and (ii) its query cost should increase *sub-linearly* with the dataset size, regardless of the data and query distributions. *Locality sensitive hashing* (LSH) is a well-known methodology fulfilling both requirements, but its current implementations either incur expensive space and query cost, or abandon its theoretical guarantee on the quality of query results.

Motivated by this, we improve LSH by proposing an access method called the *locality sensitive B-tree* (LSB-tree) to enable fast, accurate, high-dimensional NN search in relational databases. The combination of several LSB-trees forms a *LSB-forest* that has strong quality guarantees, but improves dramatically the efficiency of the previous LSH implementation having the same guarantees. In practice, the LSB-tree itself is also an effective index, which consumes linear space, supports efficient updates, and provides accurate query results. In our experiments, the LSB-tree was faster than (i) *iDistance* (a famous technique for exact NN search) by two orders of magnitude, and (ii) *MedRank* (a recent approximate method with non-trivial quality guarantees) by one order of magnitude, and meanwhile returned much better results.

As a second step, we extend our LSB technique to solve another classic problem, called closest pair (CP) search, in high dimensional space. The long-term challenge for this problem has been to achieve *sub-quadratic* running time at very high dimensionalities, which fails most of the existing solutions. We show that, using a LSB-forest, CP search can be accomplished in (worst-case) time significantly lower than the quadratic complexity, yet still ensuring very good quality. In practice, accurate answers can be found using just two LSB-trees, thus giving a substantial reduction in the space and running time. In our experiments, our technique was faster (i) than *distance browsing* (a well-known method for solving the problem exactly) by several orders of magnitude, and (ii) than *D-shift* (an approximate approach with theoretical guarantees in low-dimensional space) by one order of magnitude, and at the same time, outputs better results.

Categories and Subject Descriptors: H2.2 [**Database Management**]: Access Methods; H3.3 [**Information Storage and Retrieval**]: Information Search and Retrieval

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General Terms: Theory, Algorithms, Experimentation
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1. INTRODUCTION

Nearest neighbor (NN) search is a classic problem with tremendous impacts on artificial intelligence, pattern recognition, information retrieval, and so on. Let $\mathcal{D}$ be a set of points in d-dimensional space. Given a query point q, its NN is the point $o^* \in \mathcal{D}$ closest to q. Formally, there is no other point $o \in \mathcal{D}$ satisfying $\|o, q\| < \|o^*, q\|$, where $\|, \|$ denotes the distance of two points.

In this paper, we consider *high-dimensional* NN search. Some studies [Beyer et al. 1999] argue that high-dimensional NN queries may not be meaningful. On the other hand, there is also evidence [Bennett et al. 1999] that such an argument is based on restrictive assumptions. Intuitively, a meaningful query is one where the query point q is much closer to its NN than to most data points. This is true in many applications involving high-dimensional data, as supported by a large body of recent works [Andoni and Indyk 2006; Athitsos et al. 2008; Ciaccia and Patella 2000; Datar et al. 2004; Fagin et al. 2003; Ferhatosmanoglu et al. 2001; Gionis et al. 1999; Goldstein and Ramakrishnan 2000; Har-Peled 2001; Houle and Sakuma 2005; Indyk and Motwani 1998; Li et al. 2002; Lv et al. 2007; Panigrahy 2006].

Sequential scan trivially solves a NN query by examining the entire dataset $\mathcal{D}$, but its cost grows linearly with the cardinality of $\mathcal{D}$. From the database perspective, a good solution should satisfy two requirements: (i) it can be easily implemented in a relational database, and (ii) its query cost should increase *sub-linearly* with the cardinality for *all* data and query distributions. Despite the bulk of NN literature (see Section 8), with a single exception to be explained shortly, we are not aware of any existing solution that is able to fulfill both requirements at the same time. Specifically, a majority of them (e.g., those based on new indexes [Arya et al. 1998; Goldstein and Ramakrishnan 2000; Har-Peled 2001; Houle and Sakuma 2005; Lin et al. 1994]) demand non-relational features, and thus cannot be incorporated in a commercial system. There also exist relational solutions (such as *iDistance* [Jagadish et al. 2005] and *MedRank* [Fagin et al. 2003]), which are experimentally shown to perform well for some datasets and queries. Their drawback is that they may incur expensive query cost on other datasets.

Locality sensitive hashing (LSH) is the only known solution that satisfies both requirements (i) and (ii). It supports *c-approximate NN search*. Formally, a point o is a c-approximate NN of q if its distance to q is at most c times the distance from q to its exact NN o^*, namely, $\|o, q\| \leq c\|o^*, q\|$, where $c \geq 1$ is the *approximation ratio*. It is widely recognized that approximate NNs already fulfill the needs of many applications [Andoni and Indyk 2006; Arya et al. 1998; Athitsos et al. 2008; Datar et al. 2004; Ferhatosmanoglu et al. 2001; Gionis et al. 1999; Har-Peled 2001; Houle and Sakuma 2005; Indyk and Motwani 1998; Krauthgamer and Lee 2004; Li et al. 2002; Lv et al. 2007; Panigrahy 2006]. LSH was originally proposed as a theoretical method [Indyk and Motwani 1998] with attractive asymptotical space and query

performance. As elaborated in Section 3, its practical implementation can be either rigorous or adhoc. Specifically, *rigorous-LSH* ensures good quality of query results (i.e., small approximation ratio c), but requires expensive space and query cost. Although *adhoc-LSH* is more efficient, it abandons quality control, i.e., the neighbor it outputs can be *arbitrarily* bad. In other words, no LSH implementation is able to ensure both quality and efficiency simultaneously, which is a serious problem severely limiting the applicability of LSH.

Motivated by this, we propose an access method called *locality sensitive B-tree* (LSB-tree) that enables fast high-dimensional NN search with excellent quality. The combination of several LSB-trees leads to a structure called the *LSB-forest* that combines the advantages of both *rigorous-* and *adhoc-LSH*, without sharing their shortcomings. Specifically, the LSB-forest has the following features. First, its space consumption is the same as *adhoc-LSH*, and significantly lower than *rigorous-LSH*, typically by a factor over an order of magnitude. Second, it retains the approximation guarantee of *rigorous-LSH* (recall that *adhoc-LSH* has no such guarantee). Third, its query cost is substantially lower than *adhoc-LSH*, and as an immediate corollary, sub-linear to the dataset size. Finally, the LSB-forest adopts purely relational technology, and hence, can be easily incorporated in a commercial system.

All LSH implementations require replicating the database multiple times, and therefore, entail large space consumption and update overhead. Many applications prefer an index that consumes only linear space, and supports insertions/deletions efficiently. The LSB-tree itself meets all these requirements, by storing every data point once in a conventional B-tree. Based on real datasets, we experimentally compared the LSB-tree to *iDistance* [Jagadish et al. 2005], which is a famous technique for exact NN search, and to *MedRank* [Fagin et al. 2003], which is a recent approximate method with non-trivial quality guarantees. The LSB-tree outperformed *iDistance* by two orders of magnitude, well confirming the advantage of approximate retrieval. Compared to *MedRank*, our technique was consistently superior in both query efficiency and result quality. Specifically, the LSB-tree was faster by one order of magnitude, and at the same time, returned neighbors with much better quality.

As a second step, we tackle another classic problem, called *closest pair* (CP) search, in high-dimensional space. Here, given a set $\mathcal{D}$ of points, the goal is to find two points whose distance is the smallest among all pairs of points in $\mathcal{D}$. This problem has abundant applications in geographic information systems, clustering, and numerous matching problems (such as stable marriage [Wong et al. 2007]), and has been very well solved in low dimensional space [Corral et al. 2000; Hjaltason and Samet 1998; Lenhof and Smid 1992]. When the dimensionality increases, the challenge has been to achieve *sub-quadratic* running time, namely, faster than the naive approach that simply examines each pair of points in $\mathcal{D}$. Algorithms that work well in low-dimensional space generally see their computation cost quickly climb to quadratic even at a moderate dimensionality. The c-approximate version of the CP problem is to return a pair of points with distance at most c times the distance of the closest pair. The dimensionality curse haunts this approximate version, too. For example, when the dimensionality can be viewed as a constant, Lopez and Liao

[Lopez and Liao 2000] propose an algorithm, which we call *D-shift*, with a constant approximation ratio (i.e., $c = O(1)$). As the dimensionality grows, however, their approximation ratio increases super-linearly, and thus, becomes unattractive very soon.

We conquer the above challenge in this paper by giving an algorithm that runs in time significantly lower than the quadratic complexity and meanwhile, gives a very good worst-case guarantee on the quality of results (approximation ratio around 2), regardless of the dimensionality. As in the NN context, although such nice theoretical performance demands a full LSB-forest, in practice only 2 LSB-trees are already sufficient to return accurate results, thus substantially reducing the space and query cost. In the experiments, we compared the proposed algorithms against *distance browsing* [Corral et al. 2000], which is a well-cited exact solution, and the *D-shift* algorithm mentioned earlier. Our technique was faster than *distance browsing* by several orders of magnitude, and than *D-shift* by one order of magnitude. Moreover, our solutions returned much more accurate answers than *D-shift*.

The rest of the paper is organized as follows. Section 2 presents the problem settings and our objectives. Section 3 points out the defects of the existing LSH implementations. Section 4 explains the construction and NN search algorithms of the LSB-tree, and Section 5 establishes its performance guarantees. Section 6 extends the LSB-tree to provide additional tradeoffs between space/query cost and the quality of query results. Section 7 explains how to use LSB-trees for closest pair search. Section 8 reviews the previous work directly related to ours. Section 9 contains an extensive experimental evaluation. Finally, Section 10 concludes the paper with a summary of our findings.

2. PROBLEM SETTINGS

Without loss of generality, we assume that each dimension has a range $[0, t]$, where t is an integer. Following the LSH literature [Datar et al. 2004; Gionis et al. 1999; Indyk and Motwani 1998], in analyzing the quality of query results, we assume that all coordinates are integers, so that we can put a lower bound of 1 on the distance between two different points. In fact, this is not a harsh assumption because, with proper scaling, we can convert the real numbers in most applications to integers. In any case, this assumption is needed only in theoretical analysis; neither the proposed structure nor our query algorithms rely on it.

We consider that distances are measured by ℓ_p norm, which has extensive applications in machine learning, physics, statistics, finance, and many other disciplines. Moreover, as ℓ_p norm generalizes or approximates several other metrics, our technique is directly applicable to those metrics as well. For example, in case all dimensions are binary (i.e., having only 2 distinct values), ℓ_1 norm is exactly Hamming distance, which is widely employed in text retrieval, time-series databases, etc. Hence, our technique can be immediately applied in those applications, too.

The main problem studied is *c-approximate NN search*, where c is a positive integer. As mentioned in Section 1, given a point q, such a query returns a point o in the dataset $\mathcal{D}$, such that the distance $\|o, q\|$ between o and q is at most c times the distance between q and its real NN o^*. We assume that q is not in $\mathcal{D}$. Otherwise, the NN problem becomes a lookup query, which can be easily solved

by standard hashing. A direct extension of NN queries is *kNN search*, which finds the k points in D closest to q. The c-approximate version of kNN search aims at returning k points, where the i-th ($1 \leq i \leq k$) one is a c-approximation of the real i-th nearest neighbor. Formally, let o_1^*, ..., o_k^* be the real k NNs in ascending order of their distances to q. Then, a set of points o_1, ..., o_k (also sorted in the same way) is a *c-approximate answer* if $\|o_i, q\| \leq c\|o_i^*, q\|$ for all $i \in [1, k]$.

We consider that the dataset $\mathcal{D}$ resides in external memory where each page has B words. Furthermore, we follow the convention that every integer or real number is represented with one word. Since a point has d coordinates, the entire $\mathcal{D}$ occupies totally dn/B pages, where n is the cardinality of $\mathcal{D}$. In other words, all algorithms, which do not have provable sub-linear cost growth with n, incur I/O complexity $\Omega(dn/B)$. Our objective is to design a *relational* solution beating this complexity.

The second problem solved in this paper is *c-approximate CP search*. Specifically, let us define the closest pair in $\mathcal{D}$ to be the pair of points (o_1^*, o_2^*) having the minimum distance among all pairs of points in $\mathcal{D}$. Then the goal of c-approximate CP search is to return a pair of points (o_1, o_2) in $\mathcal{D}$ whose distance is at most c times the distance of the closest pair, namely, $\|o_1, o_2\| \leq c\|o_1^*, o_2^*\|$. A naive solution examines all pairs of points, and thus, has time complexity quadratic to n. Note that the CP problem has a *bichromatic* counterpart, which includes two datasets $\mathcal{D}_1$ and $\mathcal{D}_2$. Here, the exact answer (o_1^*, o_2^*) is the one with the smallest distance in the cartesian product $\mathcal{D}_1 \times \mathcal{D}_2$, and a c-approximate answer is a pair $(o_1, o_2) \in \mathcal{D}_1 \times \mathcal{D}_2$ such that $\|o_1, o_2\| \leq c\|o_1^*, o_2^*\|$. These two CP problems can also be extended to *kCP search*, whose c-approximate version can be defined in the same fashion as c-approximate kNN.

We denote by M the amount of available memory, measured in number of words. Unless specifically stated, M can be as small as $3B$ for our algorithms to work (i.e., there are at least 3 memory pages). This, however, excludes the memory needed to store the query results. Specifically, a set of kNN or kCP result requires $O(kd)$ extra words in memory, which we assume can be afforded.

Our theoretical analysis assumes that a point can fit in a constant number of disk pages (i.e., $d = O(B)$), which is almost always true in reality. For instance, we may set the constant to 10, thus comfortably supporting dimensionality up to $10B$. Also, to simplify the resulting bounds, we assume that the dimensionality d is at least $\log(n/B)$ (all the logarithms, unless explicitly stated, have base 2). This is reasonable because, for practical values of n and B, $\log(n/B)$ seldom exceeds 20, whereas $d = 20$ is barely "high-dimensional".

3. THE PRELIMINARIES

Our solutions leverage LSH as the building brick. In Sections 3.1 and 3.2, we discuss the drawbacks of the existing LSH implementations, and further motivate our methods. In Section 3.3, we present the technical details of LSH that are necessary for our discussion.

3.1 Rigorous-LSH and ball cover

As a matter of fact, LSH does not solve c-approximate NN queries directly. Instead, it is designed [Indyk and Motwani 1998] for a different problem called *c-approximate ball cover* (BC). Let $\mathcal{D}$ be a set of points in d-dimensional space. Denote by $B(q, r)$

a ball that centers at the query point q and has radius r. A c-approximate BC query returns the following result:

(1) If $B(q, r)$ covers at least one point in $\mathcal{D}$, return a point whose distance to q is at most cr.
(2) If $B(q, cr)$ covers no point in $\mathcal{D}$, return nothing.
(3) Otherwise, the result is undefined.

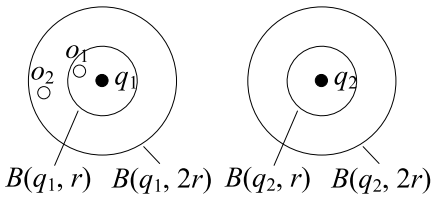


Fig. 1. Illustration of ball cover queries

Figure 1 shows an example where $\mathcal{D}$ has two points o_1 and o_2. Consider first the 2-approximate BC query q_1 (the left black point). The two circles centering at q_1 represent balls $B(q_1, r)$ and $B(q_1, 2r)$ respectively. Since $B(q_1, r)$ covers a data point o_1, the query will have to return a point, but it can be either o_1 or o_2, as both of them fall in $B(q_1, 2r)$. Now, consider the 2-approximate BC query q_2. Since $B(q_2, 2r)$ does not cover any data point, the query must return empty.

Interestingly, an approximate NN query can be reduced to a number of approximate BC queries with different radii r [Har-Peled 2001; Indyk and Motwani 1998]. The rationale is that: *if ball $B(q, r)$ is empty but $B(q, cr)$ is not, then any point in $B(q, cr)$ is a c-approximate NN of q.* Consider the query point q in Figure 2. Here, ball $B(q, r)$ is empty, but $B(q, cr)$ is not. It follows that the NN of q must have a distance between r and cr to q. Hence, any point in $B(q, cr)$ (i.e., either o_1 or o_2) is a c-approximate NN of q.

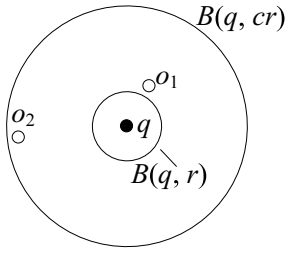


Fig. 2. The rationale of the reduction from nearest neighbor to ball cover queries

Based on this idea, Indyk and Motwani [Indyk and Motwani 1998] propose a structure that supports c-approximate BC queries at $r = 1, c, c^2, c^3, ..., x$ respectively, where x is the smallest power of c that is larger than or equal to td (recall that t is the greatest coordinate on each dimension). They give an algorithm [Indyk and Motwani 1998] to guarantee an approximation ratio of c^2 for

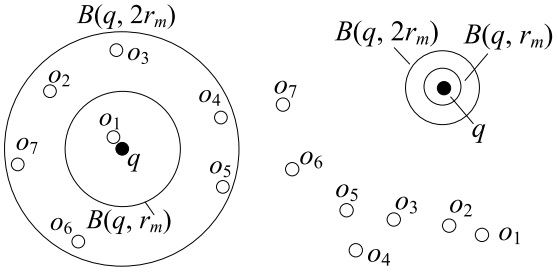
NN search (in other words, we need a structure for $\sqrt{c}$-approximate BC queries to support c-approximate NN retrieval). Their method, which we call *rigorous-LSH*, consumes $O((\log_c t + \log_c d) \cdot (dn/B)^{1+1/c})$ space, and answers a query in $O((\log_c t + \log_c d) \cdot (dn/B)^{1/c})$ I/Os. Note that t can be a large value, thus making the space and query cost potentially very expensive. Our LSB-tree will eliminate the factor $\log_c t + \log_c d$ completely.

Finally, it is worth mentioning that there exist complicated NN-to-BC reductions [Har-Peled 2001; Indyk and Motwani 1998] with better complexities. However, those reductions are highly theoretical, and are difficult to implement in relational databases.

3.2 Adhoc-LSH

Although *rigorous-LSH* is theoretically sound, its space and query cost is prohibitively expensive in practice. The root of the problem is that it must support BC queries at too many (i.e., $\log_c t + \log_c d$) radii. Gionis et al. [Gionis et al. 1999] remedy this drawback with a heuristic approach, which we refer to as *adhoc-LSH*. Given a NN query q, they return directly the output of *the* BC query that is at location q and has radius r_m, where r_m is a "magic" radius pre-determined by the system. Since only one radius needs to be supported, *adhoc-LSH* improves *rigorous-LSH* by requiring only $O((dn/B)^{1+1/c})$ space and $O((dn/B)^{1/c})$ query time.

Unfortunately, the cost saving of *adhoc-LSH* trades away the quality control on query results. To illustrate, consider Figure 3a, where the dataset $\mathcal{D}$ has 7 points o_1, o_2, ..., o_7, and the black point is a NN query q. Suppose that *adhoc-LSH* is set to support 2-approximate BC queries at radius r_m. Thus, it answers the NN query q by finding a data point that satisfies the 2-approximate BC query located at q with radius r_m. The two circles in Figure 3a represent $B(q, r_m)$ and $B(q, 2r_m)$ respectively. As $B(q, r_m)$ covers some data of $\mathcal{D}$, (by the definition stated in the previous subsection) the BC query q may return *any* of the 7 data points in $B(q, 2r_m)$. It is clear that no bounded approximation ratio can be ensured, as the real NN o_1 of q can be *arbitrarily* close to q.



(a) r_m too large (b) r_m too small

Fig. 3. Drawbacks of *adhoc-LSH*

The above problem is caused by an excessively large r_m. Conversely, if r_m is too small, *adhoc-LSH* may not return any result at all. To see this, consider Figure 3b. Again, the white points constitute the dataset $\mathcal{D}$, and the two circles are $B(q, r_m)$

and $B(q, 2r_m)$. As $B(q, 2r_m)$ is empty, the 2-approximate BC query q must not return anything. As a result, *adhoc-LSH* reports nothing too, and is said to have *missed* the query [Gionis et al. 1999].

Adhoc-LSH performs well if r_m is roughly equivalent to the distance between q and its exact NN, which is why *adhoc-LSH* can be effective when given the right r_m. Unfortunately, finding such an r_m is non-trivial. Even worse, such r_m may not exist at all because an r_m good for some queries may be bad for others. Figure 4 presents a dataset with two clusters whose densities are drastically different. Apparently, if a NN query q falls in cluster 1, the distance from q to its NN is significantly smaller than if q falls in cluster 2. Hence, it is impossible to choose an r_m that closely captures the NN distances of all queries. Note that clusters with different densities are common in real datasets [Breunig et al. 2000].

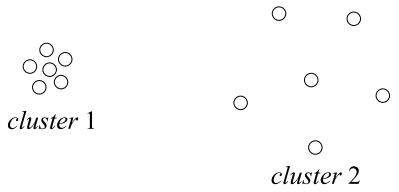


Fig. 4. No good r_m exists if clusters have different densities

Recently, [Lv et al. 2007] present a variation of *adhoc-LSH* with less space consumption. This variation, however, suffers from the same drawback (i.e., no quality control) as *adhoc-LSH*, and entails higher query cost than *adhoc-LSH*.

In summary, currently a practitioner, who wants to apply LSH, faces a dilemma between space/query efficiency and approximation guarantee. If the quality of the retrieved neighbor is crucial (as in security systems such as finger-print verification), a huge amount of space is needed, and large query cost must be paid. On the other hand, to meet a tight space budget or stringent query time requirement, one would have to sacrifice the quality guarantee of LSH, which somewhat ironically is exactly the main strength of LSH.

3.3 Details of hash functions

Let $h(o)$ be a hash function that maps a d-dimensional point o to a one-dimensional value. It is *locality sensitive* if the chance of mapping two points o_1, o_2 to the same value grows as their distance $\|o_1, o_2\|$ decreases. Formally:

Definition 1 (LSH). Given a distance r, approximation ratio c, probability values p_1 and p_2 such that $p_1 > p_2$, a hash function $h(.)$ is (r, cr, p_1, p_2) *locality sensitive* if it satisfies both conditions below:

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

LSH functions are known for many distance metrics. For ℓ_p norm, a popular LSH function is defined as follows [Datar et al. 2004]:

$$h(o) = \left\lfloor \frac{\vec{a} \cdot \vec{o} + b}{w} \right\rfloor. \tag{1}$$

Here, $\vec{o}$ represents the d-dimensional vector representation of a point o; $\vec{a}$ is another d-dimensional vector where each component is drawn independently from a so-called *p-stable* distribution [Datar et al. 2004]; $\vec{a} \cdot \vec{o}$ denotes the dot product of these two vectors. w is a sufficiently large constant, and finally, b is uniformly drawn from $[0, w)$.

Equation 1 has a simple geometric interpretation. To illustrate, let us consider $p = 2$, i.e., ℓ_p is Euclidean distance. In this case, a 2-stable distribution can be just a normal distribution (mean 0, variance 1), and it suffices to set $w = 4$ [Datar et al. 2004]. Assuming dimensionality $d = 2$, Figure 5 shows the line that crosses the origin, and its slope coincides with the direction of $\vec{a}$. For convenience, assume that $\vec{a}$ has a unit norm, so that the dot product $\vec{a} \cdot \vec{o}$ is the projection of point o onto line $\vec{a}$, namely, point A in the figure. The effect of $\vec{a} \cdot \vec{o} + b$ is to shift A by a distance b (along the line) to a point B. Finally, imagine we partition the line into intervals with length w; then, the hash value $h(o)$ is the ID of the interval covering B.

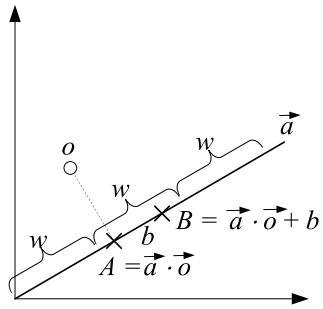


Fig. 5. Geometric interpretation of LSH

The intuition behind such a hash function is that, if two points are close to each other, then with high probability their shifted projections (on line $\vec{a}$) will fall in the same interval. On the other hand, two faraway points are very likely to be projected into different intervals. The following is proved in [Datar et al. 2004]:

LEMMA 1 (PROVED IN [DATAR ET AL. 2004]). Equation 1 is $(1, c, p_1, p_2)$ locality sensitive, where p_1 and p_2 are two constants satisfying $\frac{\ln 1/p_1}{\ln 1/p_2} \leq \frac{1}{c}$. □

4. LSB-TREE

This section includes everything that a practitioner needs to know to apply LSB-trees. Specifically, Section 4.1 explains how to build a LSB-tree, and Section 4.2 gives its NN algorithm. We will leave all the theoretical analysis to Section 5,

including its space, query performance, and quality guarantee. For simplicity, we will assume ℓ_2 norm but the extension to arbitrary ℓ_p norms is straightforward.

4.1 Building a LSB-tree

The construction of a LSB-tree is very simple. Given a d-dimensional dataset $\mathcal{D}$, we first convert each point $o \in \mathcal{D}$ to an m-dimensional point $G(o)$, and then, obtain the *Z-order value* $z(o)$ of $G(o)$. Note that $z(o)$ is just a simple number. Hence, we can index all the resulting Z-order values with a conventional B-tree, which is the LSB-tree. The coordinates of o are stored along with its leaf entry. Next, we clarify the details of each step.

From o to $G(o)$. We set the dimensionality m of $G(o)$ as

$$m = \log_{1/p_2}(dn/B) \tag{2}$$

where p_2 is the constant given in Lemma 1 under $c = 2$, n is the size of dataset $\mathcal{D}$, and B is the page size. As explained in Section 5, this choice of m makes it rather unlikely that the $G(o_1)$ and $G(o_2)$ of two far-away points o_1, o_2 are similar on all m dimensions. Note that, the choice of $c = 2$ is not compulsory, and our technique can be adapted to any integer $c \geq 2$, as discussed in Section 6.

The derivation of $G(o)$ is based on a *family* of hash functions:

$$H(o) = \vec{a} \cdot \vec{o} + b^*. \tag{3}$$

Here, $\vec{a}$ is a d-dimensional vector where each component is drawn independently from the normal distribution (mean 0 and variance 1). Value b^* is uniformly distributed in $[0, 2^f w)$, where w is any constant at least 4, and

$$f = \lceil \log d + \log t \rceil. \tag{4}$$

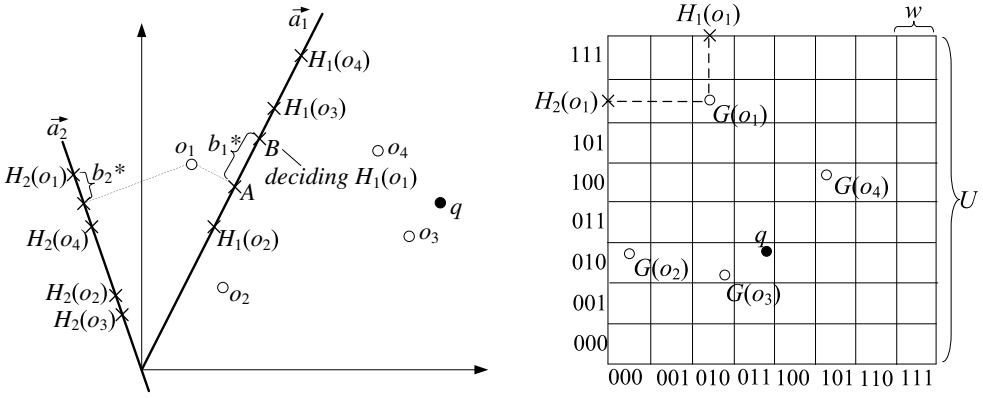
Recall that t is the largest coordinate on each dimension. Note that while $\vec{a}$ and w are the same as in Equation 1, b^* is different, which is an important design underlying the efficiency of the LSB-tree (as elaborated in Section 5 with Lemma 2).

We randomly select m functions $H_1(.)$, ..., $H_m(.)$ independently from the family described by Equation 3. Then, $G(o)$ is the m-dimensional vector:

$$G(o) = \langle H_1(o), H_2(o), ..., H_m(o) \rangle. \tag{5}$$

From $G(o)$ to $z(o)$. Let U be the axis length of the m-dimensional space $G(o)$ falls in. As explained shortly, we will choose a value of U such that U/w is a power of 2. Computation of a Z-order curve requires a hyper-grid partitioning the space. We impose a grid where each cell is a hyper-square with side length w; therefore, there are U/w cells per dimension, and totally $(U/w)^m$ cells in the whole grid. Given the grid, calculating the Z-order value $z(o)$ of $G(o)$ is a standard process well-known in the literature [Gaede and Gunther 1998]. Let $u = \log(U/w)$. Each $z(o)$ is thus a binary string with um bits.

Example. To illustrate the conversion, assume that the dataset $\mathcal{D}$ consists of 4 two-dimensional points o_1, o_2, ..., o_4 as shown in Figure 6a. Suppose that we select $m = 2$ hash functions $H_1(.)$ and $H_2(.)$. Let $\vec{a}_1$ ($\vec{a}_2$) be the "$\vec{a}$-vector" in function $H_1(.)$ ($H_2(.)$). For simplicity, assume that both $\vec{a}_1$ and $\vec{a}_2$ have norm 1.



(a) Computing hash values (b) Computing Z-order values

Fig. 6. Illustration of data conversion

In Figure 6a, we slightly abuse notations by also using $\vec{a}_1$ ($\vec{a}_2$) to denote the line that passes the origin, and coincides with the direction of vector $\vec{a}_1$ ($\vec{a}_2$).

Let us take o_1 as an example. The first step of our conversion is to obtain $G(o_1)$, which is a 2-dimensional vector with components $H_1(o_1)$ and $H_2(o_2)$. The value of $H_1(o_1)$ can be understood in the same way as explained in Figure 5. Specifically, first project o_1 onto line $\vec{a}_1$, and then move the projected point A (along the line) by a distance b_1^* to a point B. $H_1(o_1)$ is the distance from B to the origin[1]. $H_2(o_2)$ is computed similarly on line $\vec{a}_2$ (note that the shifting distance is b_2^*).

Treating $H_1(o_1)$ and $H_2(o_2)$ as coordinates, in the second step, we regard $G(o_1)$ as a point in a data space as shown in Figure 6b, and derive $z(o_1)$ as the Z-order value of point $G(o_1)$ in this space. In Figure 6b, the Z-order calculation is based on a 8×8 grid. As $G(o_1)$ falls in a cell whose (binary) horizontal and vertical labels are 010 and $\underline{110}$ respectively, $z(o_1)$ equals $0\underline{1}1\underline{1}0\underline{0}$ (in general, a Z-order value interleaves the bits of the two labels, starting from the most significant bits [Gaede and Gunther 1998]).

Choice of U. In practice, U can be any value making U/w a sufficiently large power of 2. For theoretical reasoning, next we provide a specific choice for U. Besides U/w being a power of 2, our choice fulfills another two conditions: (i) $U/w \geq 2^f$, and (ii) $|H_i(o)|$ is confined to at most $U/2$ for any $i \in [1, m]$.

In the form of Equation 3, for each $i \in [1, m]$, write $H_i(o) = \vec{a}_i \cdot \vec{o} + b_i^*$. Denote by $\|\vec{a}_i\|_1$ the ℓ_1 norm[2] of $\vec{a}_i$. Remember that o distributes in space $[0, t]^d$, where t is the largest coordinate on each dimension. Hence, $|H_i(.)|$ is bounded by

$$H_{\max} = \max_{i=1}^{m}(\|\vec{a}_i\|_1 \cdot t + b_i^*). \tag{6}$$

We thus determine U by setting U/w to the smallest power of 2 that bounds both

[1]Precisely speaking, it is $|H_1(o_1)|$ that is equal to the distance. $H_1(o_1)$ itself can be either positive or negative, depending on which side of the origin B lies on.

[2]Given a d-dimensional vector $\vec{a} = \langle a[1], a[2], ..., a[d] \rangle$, $\|\vec{a}\|_1 = \sum_{i=1}^{d} |a[i]|$.

2^f and $2H_{\max}/w$ from above.

4.2 Nearest neighbor algorithm

In practice, a single LSB-tree already produces query results with very good quality, as demonstrated in our experiments. To elevate the quality to a theoretical level, we may independently build a number l of trees. We choose

$$l = \sqrt{dn/B}. \tag{7}$$

which, as analyzed in Section 5, ensures a high chance for nearby points o_1, o_2 to have close Z-order values in at least one tree.

Denote the l trees as T_1, T_2, ..., T_l respectively, and call them collectively a *LSB-forest*. Use $z_j(o)$ to represent the Z-order value of o in tree T_j ($1 \leq j \leq l$). Without ambiguity, we also let $z_j(o)$ refer to the leaf entry of o in T_j. Remember that the coordinates of o are stored in the leaf entry.

Given a NN query q, we first get its Z-order value $z_j(q)$ in each tree T_j ($1 \leq j \leq l$). As with the Z-order values of data points, $z_j(q)$ is a binary string with um bits. We denote by $LLCP(z_j(o), z_j(q))$ the *length of the longest common prefix* (LLCP) of $z_j(o)$ and $z_j(q)$. For example, suppose $z_j(o) = 100101$ and $z_j(q) = 100001$; then $LLCP(z_j(o), z_j(q)) = 3$. When q is clear from the context, we may refer to $LLCP(z_j(o), z_j(q))$ simply as the *LLCP of* $z_j(o)$.

Figure 7 presents our nearest neighbor algorithm at a high level. The main idea is to visit the leaf entries of all l trees in descending order of their LLCPs, until either enough points have been seen, or we have found a point that is close enough. Next, we explain the details of lines 2 and 3.

Algorithm *NN1*

1. repeat
2. pick, from all the trees T_1, ..., T_l, the leaf entry with the next greatest LLCP
3. until condition $\boldsymbol{E_1}$ or $\boldsymbol{E_2}$ holds (the two conditions will be clarified later)
4. return the nearest point found so far

Fig. 7. The NN algorithm

Finding the next greatest LLCP. This can be done by a synchronous bi-directional expansion at the leaf levels of all trees. Specifically, recall that we have obtained the Z-order value $z_j(q)$ in each tree T_j ($1 \leq j \leq l$). Search T_j to locate the leaf entry $e_{j\vdash}$ with the lowest Z-order value at least $z_j(q)$. Let $e_{j\dashv}$ be the leaf entry immediately preceding $e_{j\vdash}$. To illustrate, Figure 8 gives an example where each Z-order value has $um = 6$ bits, and $l = 3$ LSB-trees are used. The values of $z_1(q)$, $z_2(q)$, and $z_3(q)$ are given next to the corresponding trees. In T_1, for instance, $z_1(o_1) = 011100$ is the lowest among all the Z-order values at least $z_1(q) = 001110$. Hence, $e_{1\vdash}$ is $z_1(o_1)$, and $e_{1\dashv}$ is the entry $z_1(o_3) = 001100$ preceding $z_1(o_1)$.

The leaf entry with the greatest LLCP must be in the set $S = \{e_{1\vdash}, e_{1\dashv}, ..., e_{l\vdash}, e_{l\dashv}\}$. Let $e \in S$ be this entry. To determine the leaf entry with the next greatest LLCP, we move e *away* from q by one position in the corresponding tree, and then repeat the process. For example, in Figure 8, the leaf entry with the maximum LLCP is $e_{2\dashv}$ (whose LLCP is 5, as it shares the same first 5 bits with $z_2(q)$). Thus,

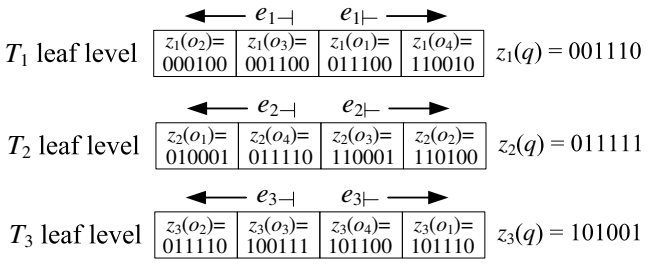


Fig. 8. Bi-directional expansion ($um = 6, l = 3$)

we shift $e_{2\dashv}$ to its left, i.e., to $z_2(o_1) = 010001$. The entry with the next largest LLCP can be found again in $\{e_{1\vdash}, e_{1\dashv}, ..., e_{3\vdash}, e_{3\dashv}\}$.

Terminating condition. Algorithm *NN1* terminates when one of two events $\boldsymbol{E_1}$ and $\boldsymbol{E_2}$ happens. The first event is:

$\boldsymbol{E_1}$: the total number of leaf entries accessed from all l LSB-trees has reached $4Bl/d$.

Event $\boldsymbol{E_2}$ is based on the LLCP of the leaf entry just retrieved from line 2. Denote the LLCP by v, which bounds from above the LLCP of all the leaf entries that have not been processed.

$\boldsymbol{E_2}$: the nearest point found so far (from all the leaf entries already inspected) has distance to q at most $2^{u-\lfloor v/m \rfloor+1}$.

Let us use again Figure 8 to illustrate algorithm *NN1*. Assume that the dataset consists of points o_1, o_2, ..., o_4 in Figure 6a, and the query is the black point q. Notice that the Z-order values in tree T_1 are obtained according to the transformation in Figure 6b with $u = 3$ and $m = 2$. Suppose that $\|o_3, q\| = 3$ and $\|o_4, q\| = 5$.

As explained earlier, entry $z_2(o_4)$ in Figure 8 has the largest LLCP $v = 5$, and thus, is processed first. *NN1* obtains the object o_4 associated with $z_2(o_4)$, and calculates its distance to q. Since $\|o_4, q\| = 5 > 2^{u-\lfloor v/m \rfloor+1} = 4$, condition $\boldsymbol{E_2}$ does not hold. Assuming $\boldsymbol{E_1}$ is also violated (i.e., let $4Bl/d > 1$), the algorithm processes the entry with the next largest LLCP, which is $z_1(o_3)$ in Figure 8 whose LLCP $v = 4$. In this entry, *NN1* finds o_3 which replaces o_4 as the nearest point so far. As now $\|o_3, q\| = 3 \leq 2^{u-\lfloor v/m \rfloor+1} = 4$, $\boldsymbol{E_2}$ holds, and *NN1* terminates by returning o_3.

Retrieving k neighbors. Algorithm *NN1* can be easily adapted to answer kNN queries. Specifically, it suffices to modify $\boldsymbol{E_1}$ to "*the total number of leaf entries accessed from all l LSB-trees has reached $(4Bl/d)+(k-1)l$*", and $\boldsymbol{E_2}$ to "*q is within distance $2^{u-\lfloor v/m \rfloor+1}$ to the k nearest points found so far*". Also, apparently line 4 should return the k nearest points. Finally, the value of l in Equation 7 needs to be increased by $O(\log(n))$ times. All these changes are to ensure strong quality guarantees in theory for any k (as will be analyzed in the next Section). In practice, as long as k is small, only the change to $\boldsymbol{E_2}$ is needed, and $\boldsymbol{E_1}$ and l can remain as they are for $k = 1$.

***k*NN search with a single tree.** Maintaining a forest of l LSB-trees incurs large space consumption and update overhead. In practice, we may prefer an index that has linear space and supports fast data insertions/deletions. In this case, we can build only one LSB-tree, and use it to process kNN queries. Accordingly, we slightly modify the algorithm *NN1* by simply ignoring event $\boldsymbol{E_1}$ in the terminating condition (as this event is designed specifically for querying l trees). Condition $\boldsymbol{E_2}$, however, is retained. As a tradeoff for efficiency, querying only a single tree loses the theoretical guarantees of the LSB-forest (as established in the next section). Nevertheless, this approach is expected to return neighbors with high quality, because the converted Z-order values adequately preserve the proximity of the data points in the original data space.

5. THEORETICAL ANALYSIS

We now proceed to study the theoretical characteristics of the LSB-tree. Denote by $\mathbb{D}$ the original d-dimensional space of the dataset $\mathcal{D}$. Namely, $\mathbb{D} = [0, t]^d$, where t is the maximum coordinate on each axis. Recall that, to construct a LSB-tree, we convert each point $o \in \mathcal{D}$ to an m-dimensional point $G(o)$ as in Equation 5. Denote by $\mathbb{G}$ the space where $G(o)$ is distributed. By the way we select U in Section 4.1, $\mathbb{G} = [-U/2, U/2]^m$.

5.1 Quality guarantee

We begin with an observation on the basic LSH in Equation 1:

OBSERVATION 1. Given any integer $x \geq 1$, define hash function

$$h'(o) = \left\lfloor \frac{\vec{a} \cdot \vec{o} + bx}{w} \right\rfloor \tag{8}$$

where $\vec{a}$, b, and w are the same as in Equation 1. $h'(.)$ is $(1, c, p_1, p_2)$ locality sensitive, and $\frac{\ln 1/p_1}{\ln 1/p_2} \leq 1/c$.

PROOF. We first point out a useful fact. Imagine a line that has been partitioned into consecutive intervals of length w. Let A, B be two points on this line with distance $y \leq w$. Shift both points towards right by a distance uniformly drawn from $[0, w\lambda)$, where λ is any integer. After this, A and B fall in the same interval with probability $1 - y/w$, which is irrelevant to λ.

Consider the hash function $h(o)$ in Equation 1. Use $\vec{a}$ to denote also the line passing the origin containing vector $\vec{a}$. As explained in Section 3.3, $\vec{a} \cdot \vec{o}$ decides a point in Line $\vec{a}$, and $\vec{a} \cdot \vec{o} + b$ shifts the point away from the origin by distance b along the line. Call it the *shifted projection* of o. Let us partition line $\vec{a}$ with intervals of length w. By Equation 1, two objects o_1, o_2 have the same hash value if and only if their shifted projections fall in the same interval.

Now assume that we change the shifting distance from b to bx. Since b is uniformly distributed in $[0, w)$, bx is uniformly distributed in $[0, wx)$. Hence, the change does not alter the probability for the shifted projections of o_1 and o_2 to fall in the same interval. This means that Equation 8 is also $(1, c, p_1, p_2)$ locality sensitive with the same p_1 and p_2 as Equation 1. □

For any $s \in [0, f]$ with f given in Equation 4, define:

$$H^*(o, s) = \left\lfloor \frac{\vec{a} \cdot \vec{o} + b^*}{2^s w} \right\rfloor \tag{9}$$

where $\vec{a}$, b^* and w follow those in Equation 3. We have:

LEMMA 2. $H^*(o, s)$ is $(2^s, 2^{s+1}, p_1, p_2)$ locality sensitive, where p_1 and p_2 satisfy $\frac{\ln 1/p_1}{\ln 1/p_2} \leq 1/2$.

PROOF. Create another space $\mathbb{D}'$ by dividing all coordinates of $\mathbb{D}$ by 2^s. It is easy to see that the distance of two points in $\mathbb{D}$ is 2^s times the distance of their converted points in $\mathbb{D}'$. Consider

$$h''(o') = \left\lfloor \frac{\vec{a} \cdot \vec{o'} + (b^*/2^f w)(2^{f-s} w)}{w} \right\rfloor \tag{10}$$

where o' is a point in $\mathbb{D}'$. As $b^*/(2^f w)$ is uniformly distributed in $[0, w)$, by Observation 1, $h''(.)$ is $(1, 2, p_1, p_2)$ locality sensitive in $\mathbb{D}'$ with $(\ln 1/p_1)/(\ln 1/p_2) \leq 1/2$. Let o be the corresponding point of o' in $\mathbb{D}$. Clearly, $\vec{a} \cdot \vec{o'} = (\vec{a} \cdot \vec{o})/2^s$. Hence, $h''(o') = H^*(o, s)$. The lemma thus holds. □

As shown in Equation 5, $G(o)$ is composed of hash values $H_1(o)$, ..., $H_m(o)$. In the way we obtain $H^*(o, s)$ (Equation 9) from $H(o)$ (Equation 3), let $H_i^*(o, s)$ be the hash function corresponding to $H_i(o)$ $(1 \leq i \leq m)$. Also remember that $z(o)$ is the Z-order value of $G(o)$ in space $\mathbb{G}$, and function $LLCP(.,.)$ returns the length of the longest common prefix of two Z-order values. Now we prove a crucial lemma that is the key to the design of the LSB-tree.

LEMMA 3. Let o_1, o_2 be two arbitrary points in space $\mathbb{D}$. A value s satisfies $s \geq u - \lfloor LLCP(z(o_1), z(o_2))/m \rfloor$ if and only if $H_i^*(o_1, s) = H_i^*(o_2, s)$ for all $i \in [1, m]$.

PROOF. Recall that, for Z-order value calculation, we impose on $\mathbb{G}$ a grid with 2^u cells (each with side length w) per dimension. Refer to the entire $\mathbb{G}$ as a level-u *tile*. In general, a level-s $(2 \leq s \leq u)$ tile defines 2^m level-$(s-1)$ tiles, by cutting the level-s tile in half on every dimension. Thus, each cell in the grid partitioning $\mathbb{G}$ is a level-0 tile.

As a property of the Z-order curve, $G(o_1)$ and $G(o_2)$ belong to a level-s tile, if and only if their Z-order values share at least $m(u-s)$ most significant bits [Gaede and Gunther 1998], namely, $LLCP(z(o_1), z(o_2)) \geq m(u-s)$. On the other hand, note that a level-s tile is a hyper-square with side length $2^s w$. This means that $G(o_1)$ and $G(o_2)$ belong to a level-s tile, if and only if $H_i^*(o_1, s) = H_i^*(o_2, s)$ for all $i \in [1, m]$. Thus, the lemma follows. □

Lemmas 2 and 3 allow us to rephrase the probabilistic guarantees of LSH using LLCP.

COROLLARY 1. Let r be any power of 2 at most 2^f. Given a query point q and a data point o, we have:

1. If $\|q, o\| \leq r$, then $LLCP(z(q), z(o)) \geq m(u - \log r)$ with probability at least p_1^m.

2. If $\|q, o\| > 2r$, then $LLCP(z(q), z(o)) \geq m(u - \log r)$ with probability at most p_2^m.

Furthermore, $\frac{\ln 1/p_1}{\ln 1/p_2} \leq 1/2$. □

The above result holds for any LSB-tree. Recall that, for NN search, we need a forest of l trees T_1, ..., T_l built independently. Next, we will explain an imperative property guaranteed by these trees. Let q be the query point, and r be any power of 2 up to 2^f such that there is a point o^* in the ball $B(q, r)$. Consider events $\boldsymbol{P_1}$ and $\boldsymbol{P_2}$:

$\boldsymbol{P_1}$: $LLCP(z_j(q), z_j(o^*)) \geq m(u - \log r)$ in at least one tree T_j $(1 \leq j \leq \ell)$.

$\boldsymbol{P_2}$: There are less than $4Bl/d$ leaf entries $z_j(o)$ from all trees T_j $(1 \leq j \leq l)$ such that (i) $LLCP(z_j(q), z_j(o)) \geq m(u - \log r)$, and (ii) o is outside $B(q, 2r)$.

The property guaranteed by the l trees is:

LEMMA 4. $\boldsymbol{P_1}$ and $\boldsymbol{P_2}$ hold at the same time with at least constant probability.

PROOF. Equipped with Corollary 1, this proof is analogous to the standard proof [Gionis et al. 1999] of the correctness of LSH. □

Now we establish an approximation ratio of 4 for algorithm *NN1*. In the next section, we will extend the LSB-tree to achieve better approximation ratios.

THEOREM 1. Algorithm *NN1* returns a 4-approximate NN with at least constant probability.

PROOF. Let o^* be the NN of query q, and $r^* = \|o^*, q\|$. Let r be the smallest power of 2 bounding r^* from above. Obviously $r < 2r^*$ and $r \leq 2^f$ (notice that r^* is at most $td \leq 2^f$ under any ℓ_p norm). If when *NN1* finishes, it has already found o^* in any tree, apparently it will return o^* which is optimal. Next, we assume *NN1* has not seen o^* at termination.

We will show that when both $\boldsymbol{P_1}$ and $\boldsymbol{P_2}$ are true, the output of *NN1* is definitely 4-approximate. Denote by j^* the j stated in $\boldsymbol{P_1}$. Recall that *NN1* may terminate due to the occurrence of either event $\boldsymbol{E_1}$ or $\boldsymbol{E_2}$. If it is due to $\boldsymbol{E_2}$, and given the fact that *NN1* visits leaf entries in descending order of their LLCP, the LLCP v of the last fetched leaf entry is at least $LLCP(z_{j^*}(q), z_{j^*}(o^*)) \geq m(u - \log r)$. It follows that $\lfloor v/m \rfloor \geq u - \log r$. $\boldsymbol{E_2}$ ensures that we return a point o with $\|o, q\| \leq 2r < 4r^*$.

In case the termination is due to $\boldsymbol{E_1}$, by $\boldsymbol{P_2}$, we know that *NN1* has seen at least one point o inside $B(q, 2r)$. Hence, the point returned has distance to q at most $2r < 4r^*$. Finally, Lemma 4 indicates that $\boldsymbol{P_1}$ and $\boldsymbol{P_2}$ are true with at least constant probability, thus completing the proof. □

Also, the proof of Theorem 1 actually shows:

COROLLARY 2. Let r^* be the distance from q to its real NN. With at least constant probability, *NN1* returns a point within distance $2r$ to q, where r is the lowest power of 2 bounding r^* from above. □

Remark 1. When defining the problem in Section 2, we restricted point coordinates to integers. In fact, the above analysis holds also for real coordinates as well, as long as the minimum distance between two points in $\mathcal{D}$ is at least 1.

Remark 2. As a standard trick in probabilistic algorithms, by repeating our solution $O(\log(1/p))$ times, we boost the success probability of algorithm *NN1* from constant to at least $1-p$, for any arbitrarily low $p > 0$. In other words, by repeating $O(\log n)$ times (namely, increasing l to $O(\log n\sqrt{dn/B})$), the failure probability of *NN1* can be lowered to at most $1/n$. Using the Union Bound inequality (also called the Boole's inequality), it is easy to show that the kNN algorithm described in Section 4.2 gives a 4-approximate answer with at least constant probability.

5.2 Space and query time

THEOREM 2. We can build a forest of l LSB-trees that consume totally $O((dn/B)^{1.5})$ space. Given these trees, algorithm *NN1* answers a 4-approximate NN query in $O(E\sqrt{dn/B})$ I/Os, where E is the height of a LSB-tree.

PROOF. Each leaf entry of a LSB-tree stores a Z-order value $z(o)$ and the coordinates of o. $z(o)$ has um bits where $u = O(f) = O(\log d + \log t)$ and $m = O(\log(dn/B))$. As $\log d + \log t$ bits fit in 2 words, $z(o)$ occupies $O(\log(dn/B))$ words. It takes d words to store the coordinates of o. Hence, overall a leaf entry is $O(d)$ words long. Hence, a LSB-tree consumes $O((dn/B))$ pages, and $l = \sqrt{dn/B}$ of them require totally $O((dn/B)^{1.5})$ space.

Algorithm *NN1* (i) first accesses a single path in each LSB-tree, and then (ii) fetches at most $4Bl/d$ leaf entries. The cost of (i) is bounded by $O(lE)$. As a leaf entry consumes $O(d)$ words, $4Bl/d$ of them occupy at most $O(l)$ pages. □

By implementing each LSB-tree as a *string B-tree* [Ferragina and Grossi 1999], the height E is bounded by $O(\log_B n)$, resulting in query complexity $O(\sqrt{dn/B}\log_B n)$.

5.3 Comparison with rigorous-LSH

As discussed in Section 3, for 4-approximate NN search, *rigorous-LSH* consumes $O((\log d + \log t)(dn/B)^{1.5})$ space, and answers a query in $O((\log d + \log t)\sqrt{dn/B})$ I/Os. Comparing these complexities with those in Theorem 2, it is clear that the LSB-forest improves *rigorous-LSH* significantly in the following ways.

First, the performance of the LSB-forest is not sensitive to t, the greatest coordinate of a dimension. This is a crucial improvement because t can be very large in practice. As a result, *rigorous-LSH* is suitable only when data are confined to a relatively small space. The LSB-forest enjoys much higher applicability by retaining the same efficiency regardless of the size of the data space.

Second, the space consumption of a LSB-forest is lower than that of *rigorous-LSH* by a factor of $\log d + \log t$. For practical values of d and t (e.g., $d = 50$ and $t = 10000$), the space of a LSB-forest is lower than that of *rigorous-LSH* by more than *an order of magnitude*. Furthermore, note that the LSB-forest is as space efficient as *adhoc-LSH*, even though the latter does not guarantee the quality of query results at all.

Third, the LSB-forest promises higher query efficiency than *rigorous-LSH*. As mentioned earlier, the height E can be strictly confined to $O(\log_B n)$ by resorting

Algorithm *NN2* (r)
1. o = the output of algorithm *NN1* on F
2. o' = the output of algorithm *NN1* on F'
3. return the point between o and o' closer to q

Fig. 9. The 3-approximate algorithm

to the string B-tree. Even if we simply implement a LSB-tree as a normal B-tree, the height E never grows beyond 6 in our experiments. This is expected to be much smaller than $\log d + \log t$, rendering the query complexity of the LSB-forest considerably lower than that of *rigorous-LSH*.

In summary, the LSB-forest outperforms *rigorous-LSH* significantly in applicability, space and query efficiency. It therefore eliminates the reason for resorting to the theoretically vulnerable approach of *adhoc-LSH*. Finally, remember that the LSB-tree achieves all of its nice characteristics by leveraging purely relational techniques.

6. EXTENSIONS

This section presents several interesting extensions to the LSB-tree, which are easy to implement in a relational database, and extend the functionality of the LSB-tree significantly.

Supporting ball cover. A LSB-forest, which is a collection of l LSB-trees as defined in Section 4.2, is able to support 2-approximate BC queries whose radius r is any power of 2. Specifically, given such a query q, we run algorithm *NN1* (Figure 7) using the query point. Let o by the output of *NN1*. If $\|o, q\| \leq 2r$, we return o as the result of the BC query q. Otherwise, we return nothing. By an argument similar to the proof of Theorem 1, it is easy to prove that the above strategy succeeds with high probability.

$(2 + \epsilon)$-approximate nearest neighbors. A LSB-forest ensures an approximation ratio of 4 (Theorem 1). Next we will improve the ratio to 3 with only 2 LSB-forests. As shown earlier, a LSB-forest can answer 2-approximate BC queries with any $r = 1, 2, 2^2, ..., 2^f$ where f is given in Equation 4. We build another LSB-forest to handle 2-approximate BC queries with any $r = 1.5, 1.5 \times 2, 1.5 \times 2^2, ..., 1.5 \times 2^f$. For this purpose, we can create another dataset $\mathcal{D}'$ from $\mathcal{D}$, by dividing all coordinates in $\mathcal{D}$ by 1.5. Then, a LSB-forest on $\mathcal{D}'$ is exactly what we need, noticing that the distance of two points in $\mathcal{D}'$ is 1.5 times smaller than that of their original points in $\mathcal{D}$. The only issue is that the distance of two points in $\mathcal{D}'$ may drop below 1, while our technique requires a lower bound of 1 (see Remark 1 in Section 5.1). This can be easily fixed by scaling up $\mathcal{D}$ first by a factor of 2 (i.e., doubling all the coordinates). Any two points in the new $\mathcal{D}$ have distance at least 2, so any two points in $\mathcal{D}'$ now have distance at least $2/1.5 > 1$.

Denote by F and F' the LSB-forest on $\mathcal{D}$ and $\mathcal{D}'$ respectively. Given a NN query q, we answer it using simple the algorithm *NN2* in Figure 9.

THEOREM 3. Algorithm *NN2* returns a 3-approximate NN with at least constant probability.

PROOF. Let $\mathbb{D}$ be the d-dimensional space of dataset $\mathcal{D}$, and $\mathbb{D}'$ the space of $\mathcal{D}'$. Denote by r^* the distance between q and its real NN o^*. Apparently, r^* must fall in either $(2^x, 1.5 \times 2^x]$ or $(1.5 \times 2^x, 2^{x+1}]$ for some $x \in [0, f]$. Refer to these possibilities as Case 1 and 2, respectively.

For Case 1, the distance $r^{*\prime}$ between q and o^* in space $\mathbb{D}'$ is between $(2^x/1.5, 2^x]$. Hence, by Corollary 2, with at least constant probability the distance between o' and q in $\mathbb{D}'$ is at most 2^{x+1}, where o' is the point output at line 2 of *NN2*. It thus follows that o' is within distance $1.5 \times 2^{x+1} \leq 3r^*$ in $\mathbb{D}$. Similarly, for Case 2, we can show that o (output at line 1) is a 3-approximate NN with at least constant probability. □

The above idea can be easily extended to $(2+\epsilon)$-approximate NN search for any $0 < \epsilon < 2$. Specifically, we can maintain $1 + \lfloor 1/\log(1+\epsilon/2) \rfloor$ LSB-forests, such that the i-th forest ($1 \leq i \leq 1 + \lfloor 1/\log(1+\epsilon/2) \rfloor$) supports 2-approximate BC queries at $r = \alpha, 2\alpha, 2^2\alpha, ..., 2^f\alpha$, where $\alpha = (1+\epsilon/2)^{i-1}$. Given a query q, we run algorithm *NN1* on all the forests, and return the nearest point found. By an argument similar to proving Theorem 3, we have:

THEOREM 4. For any $0 < \epsilon < 2$, we can build $O\left(\frac{1}{\log(1+\epsilon)}\right)$ LSB-forests that consume totally $O\left((dn/B)^{1.5}\frac{1}{\log(1+\epsilon)}\right)$ space, and answer a $(2+\epsilon)$-approximate NN query in $O\left(E\sqrt{dn/B}\frac{1}{\log(1+\epsilon)}\right)$ I/Os, where E is the height of a LSB-tree. □

$(c+\epsilon)$-approximate nearest neighbors. In practice, an application may be able tolerate an approximation ratio higher than that of the basic LSB-forest. In this case, it is possible to further reduce the space and query cost. In the sequel, we generalize the LSB-tree to offer any approximation ratio arbitrarily close to c, for any integer $c \geq 3$.

We make several changes in building a LSB-tree:

—Recall that m equals $\log_{1/p_2}(dn/B)$ in Section 4.1. For $c \geq 3$, the expression for m remains identical, but p_2 is the constant as given in the Lemma 1 for the value of c we are considering.

—In Equation 3, b^* will be uniformly drawn from $[0, c^f w)$, where f, instead of following Equation 4, is set to $\lceil \log_c d + \log_c t \rceil$.

—We will decide U (i.e., the axis length of the m-dimensional space of $G(o)$) by setting U/w to the smallest power of c that bounds both c^f and $2H_{\max}/w$ from above, where $H_{\max}$ is given in Equation 5.

The last change lies in the way a Z-order value $z(o)$ is calculated from $G(o)$. Let us denote by $\mathbb{G}$ the m-dimensional space where $G(o)$ is distributed. Impose a hyper-grid over $\mathbb{G}$ where each cell is a hyper-square with side length w. As mentioned earlier, U/w is a power of c; therefore, the grid has totally x^{cm} cells, for some integer x. Figure 10 shows an example where $\mathbb{G}$ has $m = 2$ dimensions, $c = 3$, and $\mathbb{G}$ is partitioned by a $3^2 \times 3^2$ grid.

We utilize the grid to compute $z(o)$ as follows. Recall that the grid partitions each dimension of $\mathbb{G}$ into c^x intervals. Number these intervals consecutively using

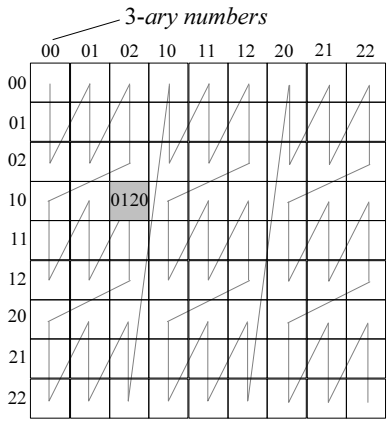


Fig. 10. Computing Z-order values for the order-3 LSB-tree

c-ary values. For instance, in Figure 10, each dimension of $\mathbb{G}$ is cut into $3^2 = 9$ intervals, which are numbered from 00 to 22. Then, the Z-order value of each cell in the grid is obtained by interleaving its c-ary digits on all dimensions. For example, the grey cell in Figure 10 is numbered 02 and 10 on the horizontal and vertical dimensions, respectively. Hence, its Z-order value is 0120, taking the first digits of 02 and 10, then followed by their second digits. $z(o)$ equals the Z-order value of the cell that $G(o)$ falls in. By the Z-order values thus calculated, we impose an ordering of the cells as depicted by the zigzag line in the figure.

We call the adapted LSB-tree an *order-c LSB-tree*, and build a forest of $l = (dn/B)^{1/c}$ such trees independently. Call it an *order-c LSB-forest*. The query algorithm *NN1* in Section 4.2 can be deployed directly on the forest, except that the number $2^{u-\lfloor v/m \rfloor+1}$ in event $\boldsymbol{E_2}$ should be replaced by $c^{u-\lfloor v/m \rfloor+1}$. By an argument similar to the one in Section 5, we can show:

THEOREM 5. We can build a set of order-c LSB-trees that consume totally $O((dn/B)^{1+1/c})$ space. Given a query, *NN1* returns a c^2-approximate NN in $O(E(dn/B)^{1/c})$ I/Os, where E is the height of an order-c LSB-tree. □

Notice that the order-c LSB-forest captures the basic LSB-forest as a special case with $c = 2$. Recall that a basic LSB-forest is able to answer 2-approximate BC queries with r being powers of 2. Likewise, an order-c LSB-forest is able to answer c-approximate BC queries with $r = 1, c, c^2, ...$ To lower the approximation ratio to $c + \epsilon$, we can build $1 + \lfloor \frac{c}{\log(1+\epsilon/c)} \rfloor$ order-c LSB-forests. Specifically, the i-th $(1 \leq i \leq 1 + \lfloor \frac{c}{\log(1+\epsilon/c)} \rfloor)$ forest is responsible for c-approximate BC queries with radius $r = \alpha, c\alpha, c^2\alpha, ...,$ where $\alpha = (1 + \epsilon/c)^{i-1}$. Following the way of establishing Theorem 4, we can prove:

THEOREM 6. For any $0 < \epsilon < c^2 - c$, we can build $O\left(\frac{c}{\log(1+\epsilon/c)}\right)$ order-c LSB-trees that consume totally $O\left((dn/B)^{1+1/c}\frac{c}{\log(1+\epsilon/c)}\right)$ space, and answer a $(c + \epsilon)$-approximate NN query in $O\left(E(dn/B)^{1/c}\frac{c}{\log(1+\epsilon/c)}\right)$ I/Os, where E is the height

of an order-c LSB-tree. □

Note that, for $c \geq 3$, the complexities in the above theorem are strictly smaller than those in Theorem 4 because the polynomials in Theorem 6 have lower exponents.

7. CLOSEST PAIR SEARCH

In this section we will extend the LSB technique to solve the CP problem. There is a straightforward solution. Specifically, assume that a LSB-forest has been built on dataset $\mathcal{D}$. First, for every point $o \in \mathcal{D}$, run algorithm *NN1* (Figure 7) to find its NN o'. Then, among all such pairs (o, o'), report the one with the smallest distance. This will give us a 4-approximate answer with high probability.

In main memory, the solution is quite efficient, requiring only $O(n^{1.5} \log(n))$ time [Datar et al. 2004]. In external memory where an access unit is a page of B words, the running time becomes $O(n\sqrt{dn/B} \log_B n)$, which can be even worse than the trivial bound $O((dn/B)^2)$. Next, we will propose a different approach that requires only $O((dn/B)^{1.5})$ I/Os. As will be clear shortly, the analysis of this approach's running time is drastically different from that in [Datar et al. 2004].

7.1 Ball pair search

As explained in Section 3.1, LSH approaches NN search with ball cover. Similarly, we attack the CP problem with another problem we call *ball pair* (BP) search, which can be regarded as the counterpart of ball cover in the CP context. Formally, given a radius r, a *c-approximate BP* query on $\mathcal{D}$ returns the following:

(1) If there is a pair of points in $\mathcal{D}$ with distance at most r, return a pair of points in $\mathcal{D}$ with distance at most cr.
(2) If no two points in $\mathcal{D}$ have distance at most cr, return nothing.
(3) Otherwise, the result is undefined.

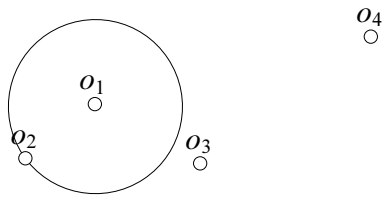


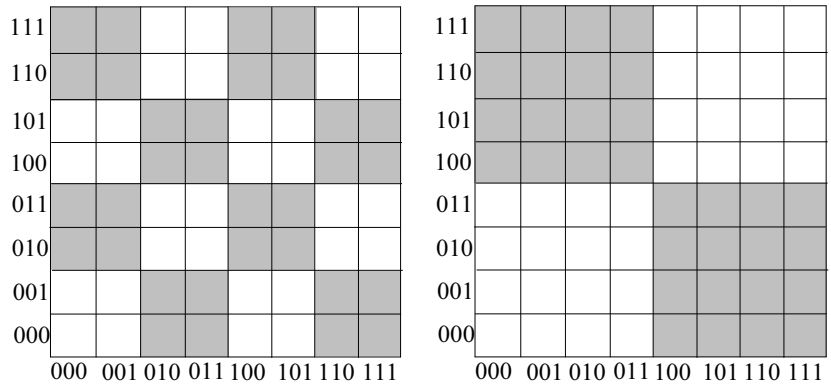
Fig. 11. Illustration of the ball pair problem

For example, consider Figure 11 where $\mathcal{D}$ has 4 points. Let r be the distance between o_1 and o_2. Then, a 2-approximate BP query must return a pair of points within distance $2r$. In our example, there are two such pairs: (o_1, o_2), (o_1, o_3), either of which is a correct result. On the other hand, for any $r < \frac{1}{2}\|o_1, o_2\|$, a 2-approximate BP query must not return anything at all.

Our discussion will focus on radius r that is a power of 2 between 1 and 2^f, where f is given in Equation 4. In the sequel, let $\lambda = \log r$. We will first target an approximation ratio of $c = 2$, and then extend to other ratios later. For $c = 2$, we need

a LSB-forest with l trees built in exactly the way described in Section 4.1. Next, we will first clarify the algorithm for BP search, and then analyze its theoretical properties.

Algorithm. Let us first concentrate on a single LSB-tree T. Remember that each leaf entry carries a Z-order value. Two points o_1, o_2 are said to be in the same *bucket* if they share the first $m(u-\lambda)$ bits in their Z-order values, namely, $LLCP(z(o_1), z(o_2)) \geq m(u-\lambda)$ — see the definitions of m, u, and $LLCP(.)$ in Section 4. Intuitively, a bucket is essentially a hyper-square with $2^{\lambda m}$ cells in the grid partitioning the space $\mathbb{G}$ (that is used to define Z-values). For example, (same as Figure 6b) Figure 12a shows a space $\mathbb{G}$ with $m = 2$ dimensions, the coordinates of which are encoded with $u = 3$ bits. For $\lambda = 1$, there are 16 buckets, each with $2^{\lambda m} = 4$ cells that share same first $m(u-\lambda) = 4$ bits in their Z-order values. Figure 12b demonstrates the case of $\lambda = 2$, where there are 4 buckets each with 16 cells. Note that a bucket of $\lambda = 2$ encloses 4 buckets of $\lambda = 1$. This is true in general: every time λ grows by 1 (i.e., r doubles), a new bucket covers 2^m old buckets. Also notice that, in any case, the cells of a bucket always have continuous Z-order values.



(a) 16 buckets when $\lambda = 1$ (b) 4 buckets when $\lambda = 2$

Fig. 12. Coverage of buckets in space $\mathbb{G}$ ($m = 2, u = 3$)

Let us divide the leaf entries of tree T based on the buckets they belong to. Apparently, points of the same bucket must come together in *adjacent* leaf nodes, as illustrated in Figure 13. Note that a bucket may span multiple leaf nodes, but may also be so small that several buckets can fit in a single leaf. In any case, the important fact is that by scanning the leaf level from the leftmost node rightwards, we can easily determine the bucket boundaries, by comparing the Z-order values of consecutive leaf entries.

Now, let us take back the entire forest of l trees, since we are ready to elaborate the algorithm for BP search, which is fairly simple as presented in Figure 14. For each tree, we scan its leaf level from left to right, starting from the leftmost leaf. For every bucket I encountered during the scan, evaluate the distances of all the pairs of points in I bruteforcely in $O(\lceil d|I|/B \rceil^2)$ I/Os. Meanwhile, we keep track

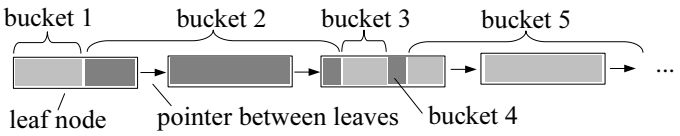


Fig. 13. Buckets at the leaf level of a LSB-tree

of the total number of pairs evaluated (from all trees) so far, namely, the count increases by $|I|(|I|-1)$ after processing a bucket I. The algorithm terminates as soon as the count reaches $2Bnl/d$ (where n is the size of $\mathcal{D}$) — this includes even the duplicate pairs discovered from different trees. At termination, we return the closest pair (among all the pairs evaluated) if its distance is at most $2r$. Otherwise, we return nothing.

Algorithm *BP*(*r*)
/* assume that the LSB-forest has trees T_1, ..., T_l */
1. for $i = 1$ to l
2. scan from the leaf nodes of T_i rightwards, starting from the leftmost one
3. for each bucket I encountered
4. evaluate the $O(|I|^2)$ pairs of points in I
5. break, as soon as $2Bnl/d$ pairs have been evaluated (from all trees)
6. if the closest pair found so far has distance at most $2r$ then return it
7. else return nothing

Fig. 14. The BP algorithm

Analysis. Next we will first establish the quality guarantee of our algorithm *BP*, and then analyze its running time.

LEMMA 5. *BP* returns a 2-approximate answer with at least constant probability.

PROOF. The proof is an adaptation of the standard LSH analytical framework for NN search; we will focus on the differences in the CP context. Given two points in a bucket of a tree, we say that they form a *bad pair* if their distance is larger than $2r$. In the sequel, we will assume the existence of a pair (o_1^*, o_2^*) within distance at most r (the proof is similar if such a pair does not exist). Observe that *BP* finds a 2-approximate answer if both of the following hold:

$\boldsymbol{P_1'}$: There are less than $2Bnl/d$ bad pairs in all the l trees in the LSB-forest.
$\boldsymbol{P_2'}$: (o_1^*, o_2^*) appear in at least one bucket of a LSB-tree.

The rest of the proof will show that they hold at the same time with at least constant probability.

Recall that two points o_1, o_2 fall in the same bucket of some LSB-tree T_j ($1 \leq j \leq l$) if and only if $LLCP(z(o_1), z(o_2)) \geq m(u-\lambda)$. By Corollary 1, if $\|o_1, o_2\| > 2r$, they form a bad pair in T_j with probability at most p_2^m. Hence, in all l trees, the expected number of bad pairs is at most $l \cdot n(n-1)p_2^m$, which is smaller than Bnl/d with the choice of m in Equation 2. By Markov Inequality, the probability for the

total number of bad pairs in all l trees to be at least $2Bnl/d$ is at most $1/2$, that is, $\boldsymbol{P_1'}$ fails with probability at most $1/2$.

By the same reasoning in the standard LSH framework, with the choice of l in Equation 7, $\boldsymbol{P_2'}$ fails with probability at most $1/e$. Hence, the probability that at least one of $\boldsymbol{P_1'}$ and $\boldsymbol{P_2'}$ fails is bounded by $1/2 + 1/e = 0.87$ from above, implying that they hold with probability at least 0.13. □

Although the proof of quality generally follows the LSH framework, the running time analysis is substantially different.

LEMMA 6. *BP* performs $O((dn/B)^{1.5})$ I/Os.

PROOF. We consider only buckets with more than B/d points. Each bucket with at most B/d points fits in at most 2 pages; so examining all pairs of points in each of these buckets takes linear I/Os, namely $O((dn/B)^{1.5})$ I/Os.

Without loss of generality, assume that at the time *BP* finishes, it has encountered J buckets in this order: I_1, I_2, ..., I_J (they may come from different trees). Note that, except the last one I_J, all the other buckets have been *fully* processed. Namely, if we denote by x_i $(1 \leq i \leq J-1)$ the size of bucket I_i, I_i contributed $x_i(x_i-1)$ pairs to the count *BP* is maintaining. As for the last bucket I_J, assume that *BP* scanned x_J points in it. Hence, I_J contributed at least $(x_J-1)(x_J-2)$ to the count. It suffices to consider $x_J \geq 3 + B/d$ (otherwise, we can ignore I_J but add only $O(1)$ I/Os to the overall cost). As totally *BP* evaluates no more than $2Bnl/d$ pairs, we have:

$$(x_J-1)(x_J-2) + \sum_{i=1}^{J-1} x_i(x_i-1) \leq 2Bnl/d. \tag{11}$$

Since $x_i \geq 1 + B/d$ $(1 \leq i \leq J-1)$ and $x_J \geq 3 + B/d$, Inequality 11 implies

$$\sum_{i=1}^{J}(x_i \cdot B/d) < (x_J-1)(x_J-2) + \sum_{i=1}^{J-1} x_i(x_i-1) \leq 2Bnl/d.$$

Hence,

$$\sum_{i=1}^{J} x_i \leq \frac{2Bnl/d}{B/d} = O(nl). \tag{12}$$

From Inequalities 11 and 12, we have:

$$\sum_{i=1}^{J} x_i^2 \leq 2Bnl/d + 3\sum_{i=1}^{J} x_i = O(Bnl/d) \tag{13}$$

where the last equality is due to $d = O(B)$. Furthermore, J satisfies

$$J \leq \frac{\sum_{i=1}^{J} x_i}{B/d} = O(dnl/B). \tag{14}$$

A bucket I_i $(1 \leq i \leq J-1)$ with size x_i occupies at most $O(\lceil dx_i/B \rceil)$ pages. Hence, bruteforce examination of all pairs of points in I_i requires $O(\lceil dx_i/B \rceil^2)$

I/Os. Likewise, examining the last bucket I_J takes $O(\lceil dx_J/B \rceil^2)$ I/Os. Thus, the total cost on all buckets is bounded by

$$O\left(\sum_{i=1}^{J} \lceil dx_i/B \rceil^2\right) = O\left(\sum_{i=1}^{J} (dx_i/B + 1)^2\right)$$
$$= O\left(J + \frac{d^2}{B^2}\sum_{i=1}^{J} x_i^2 + \frac{d}{B}\sum_{i=1}^{J} x_i\right)$$

which, by Inequalities 12-14, is bounded by $O(dnl/B) = O((dn/B)^{1.5})$. □

7.2 Solving the closest pair problem

The closest pair problem can be reduced to BP search. A simple approach is to invoke algorithm *BP* (Figure 14) with doubling radius $r = 1, 2, 4$, and so on, until it returns a pair of points whose distance is at most twice the current r. This procedure, referred to as algorithm *CP1*, is formally presented in Figure 15, which can be easily shown to return a 4-approximate answer with at least constant probability.

Algorithm *CP1*

1. $r = 1$
2. repeat
3. call $BP(r)$
4. if the above returns a pair of points (o_1, o_2) and $\|o_1, o_2\| \leq 2r$ then return (o_1, o_2)
5. else $r = 2r$

Fig. 15. The first CP algorithm

The drawback of *CP1* is that its running time may be $O((\log d + \log t)(dn/B)^{1.5})$ in the worst case, where t is the maximum coordinate of a dimension. In the sequel, we give an alternative algorithm that requires only $O((dn/B)^{1.5})$ time, i.e., eliminating the $\log d + \log t$ factor.

An improved algorithm. We refer to our new algorithm as *CP2*. Unlike *CP1* that performs multiple BP search, *CP2* first picks an appropriate value of r, denoted as r_{good}, and then, performs at most *two* BP search at $r = r_{good}/2$ and r_{good}, respectively. As shown later, r_{good} can be found in $O((dn/B)^{1.5})$ I/Os, which is the same cost of one *BP* search, thus making the overall cost $O((dn/B)^{1.5})$ as well. *CP2* is presented in Figure 16. Next we will focus on explaining Line 1.

Recall that, given a particular r, algorithm *BP* examines a number of point pairs in $\mathcal{D}$. Let us denote the number as $C(r)$. Obviously, $C(r)$ is always bounded from above by $2Bnl/d$, as it is the largest number of pairs evaluated by *BP*. It is fairly simple to obtain the exact $C(r)$ by reading (from left to right) the leaf levels of all LSB-trees once as follows. First, set $C(r)$ to 0, and start reading the first tree. At any time, we keep a count x of how many points have been seen in the current bucket being scanned. When the boundary of the bucket is reached, we add $x(x-1)$ to $C(r)$, and then, reset x to 0 for the next bucket. At the time all trees have been

Algorithm *CP2*
1. find an appropriate radius r_{good}
2. call $BP(r_{good}/2)$
3. if the above returns a pair of points with distance greater than r_{good}
4. call $BP(r_{good})$
5. return the closest of all pairs of points examined

Fig. 16. An improved CP algorithm

scanned, $C(r)$ becomes final. Since every leaf node of each tree is read once, the total cost is $O((dn/B)^{1.5})$ I/Os.

A nice feature of the above strategy is that it needs to store only two values in memory at any time: $C(r)$ and x. There are, however, merely $f = \lceil \log d + \log t \rceil$ different values of r. Hence, we can compute the $C(r)$ of all possible r in a *single* pass. The memory size required is only one memory page (as the reading buffer) plus $2f$ integers! Then, r_{good} is decided as

$$r_{good} = \min\{r \mid C(r) \geq 2Bnl/d\} \tag{15}$$

namely, r_{good} is the lowest r such that $C(r) \geq 2Bnl/d$.

THEOREM 7. Algorithm *CP2* returns a 4-approximate answer with at least constant probability.

PROOF. We will make a claim X: every pair whose distance is evaluated by *CP1* is also evaluated by *CP2*. Under the claim, *CP2* never returns a worse answer than *CP1*, which will establish the theorem.

Assume that when *CP1* finishes, the value of r is r'. Clearly, $r' \leq r_{good}$ because algorithm *BP* never evaluates more than $2Bnl/d$ pairs. If $r' = r_{good}$, it means that the best pair *CP1* returns is found by the last BP search, namely, $BP(r')$. Then, X is true because *CP2* also needs to perform the same BP search $BP(r_{good})$ (notice that Line 4 of *CP2* will definitely be executed, i.e., the if-condition at Line 3 will fail).

Now consider $r' < r_{good}$. The crucial fact is that, for any $r_1 < r_2 < r_{good}$ where r_1 and r_2 are powers of 2, the set of point pairs $BP(r_1)$ evaluates is always a subset of the set $BP(r_2)$ evaluates, due to the selection of r_{good}. Hence, whatever is evaluated by $BP(r')$ is also evaluated by $BP(r_{good}/2)$. Hence, X also holds. □

Thus, we arrive at:

THEOREM 8. Given a LSB-forest, we can perform 4-approximate closest pair search in $O((dn/B)^{1.5})$ I/Os as long as the memory size M is at least $\max\{3B, B + 2f\}$ words.

Note that the value of f is smaller than B in practice. As a reference, let $d = 1000$ and $t = 10^{10}$; in this case, $f < 44$, which means $2f$ integers can easily fit in a page of $B = 1024$ words. Thus, the memory size needed to run *CP2* is only 3 pages. In case the LSB-forest does not exist in advance, then the total time increases by a factor of $\log_{M/B}(dn)$, because building all the leaf levels with external sort takes $O((dn/B)^{1.5} \log_{M/B}(dn))$ I/Os (the non-leaf levels are unnecessary).

Extensions. In theory, kCP search can also be supported in a way similar to how kNN is handled. First, we need to increase l to $O(\sqrt{dn/B}\log n)$. Second, the limit on how many point pairs are evaluated by algorithm *BP* should be raised to $2Bnl/d + (k-1)l$. In practice when k is small, no change is required, and we can simply output the k closest pairs among all the pairs *CP2* evaluates during its execution.

So far we have been targeting an approximation ratio of 4, but the ratio can be improved to arbitrarily close to 2 with only a constant blowup in the computation cost. Conversely, one may also opt for a higher ratio as a tradeoff for lower running time. Using the methods explained in Section 6, for any integer $c \geq 2$ and arbitrary ϵ satisfying $0 < \epsilon < c^2 - c$, we can find a $(c+\epsilon)$-approximate answer in $O\left((dn/B)^{1+1/c}\frac{c}{\log(1+\epsilon/c)}\right)$ I/Os. If the LSB-forests need to be built on the fly, the cost is $O(\log_{M/B}(dn))$ times higher.

All the results can be extended to bichromatic CP search as well. In particular, for $k = 1$, a 4-approximate closest pair between $\mathcal{D}_1$ and $\mathcal{D}_2$ can be found with at least constant probability in

$$O\left(\sqrt{d\sqrt{n_1 n_2}/B}\cdot\left((dn_1/B)\log_{M/B}(dn_1) + (dn_2/B)\log_{M/B}(dn_2)\right)\right)$$

I/Os, where n_1 and n_2 are the cardinalities of the participating datasets $\mathcal{D}_1$ and $\mathcal{D}_2$, respectively. Note that when $n_1 = n_2 = n$, this complexity degenerates into the one obtained earlier for a single dataset.

Using a single LSB-tree. As mentioned in Section 4.2, a practical application may choose to maintain only a single LSB-tree, because this consumes only linear space and allows logarithmic update time. Before finishing this section, we give an algorithm, referred to as *CP3*, which performs approximate kCP search using only such a tree.

The rationale behind *CP3* is that a LSB-tree generally captures the proximity of the points in the original space. Namely, if points o_1 and o_2 are close, they tend to have similar Z-values $Z(o_1)$ and $Z(o_2)$. Hence, for each leaf entry, we will evaluate its distances only to its nearby leaf entries. More specifically, at any time, we pinpoint a leaf node N in memory. After computing the distances of all pairs of points in N, we use another memory page N' to scan forward the subsequent leaf pages one by one. Every point in N' has its distances to all points in N computed. This continues until the Z-order value of an entry in N' is "sufficiently faraway" (to be elaborated shortly) from that of the rightmost entry in N (see Figure 17). When this happens, we move N to the leaf node on its right, and repeat the process. The first N pinpointed is the leftmost leaf node.

It remains to clarify what we mean by "two entries $Z(o_1)$ and $Z(o_2)$ are faraway". We adopt a heuristic similar to the one used in Section 4.2 for kNN search. Specifically, let *dist* be the distance of the k-th closest pair of points *CP3* has discovered so far. We rule that $Z(o_1)$ and $Z(o_2)$ are faraway if

$$dist \leq 2^{u-\lfloor LLCP(Z(o_1),Z(o_2))/m\rfloor+1}$$

where u, m, and $LLCP(.,.)$ are as defined in Section 4. The algorithm *CP3* is formally presented in Figure 18.

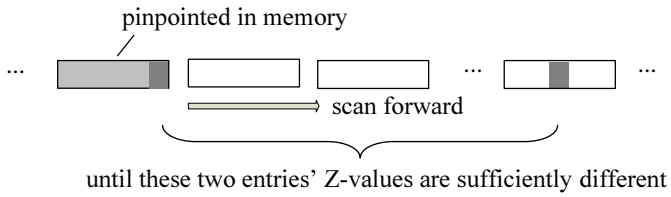


Fig. 17. CP search with only one LSB-tree

Algorithm *CP3*
1. N = the leftmost leaf node
2. repeat
3. compute the distances of all pairs of points in N
4. N' = the leaf node to the right of N
5. repeat
6. compute the distance of each point in N' to each point in N
7. if an entry in N' is sufficiently faraway from the rightmost entry of N
8. break
9. else N' = the leaf node to the right of N'
10. until $N' = \emptyset$
11. N = the leaf node to the right of N
12. until $N = \emptyset$
13. return the k closest pairs found so far

Fig. 18. A CP algorithm using only a single LSB-tree

8. RELATED WORK

NN search is well understood in low dimensional space [Hjaltason and Samet 1999; Roussopoulos et al. 1995]. This problem, however, becomes much more difficult in high dimensional space. Many algorithms (e.g., those based on data or space partitioning indexes [Gaede and Gunther 1998]) that perform nicely on low dimensional data, deteriorate rapidly as the dimensionality increases [Bohm 2000; Weber et al. 1998], and are eventually outperformed even by sequential scan.

Research on high-dimensional NN search can be divided into *exact* and *approximate* retrieval. In the exact category, Lin et al. [Lin et al. 1994] propose the *TV-tree* which improves conventional R-trees [Beckmann et al. 1990; Guttman 1984] by creating MBRs only in selected subspaces. Weber et al. [Weber et al. 1998] design the *VA-file*, which compresses the dataset to minimize the cost of sequential scan. Also based on the idea of compression, Berchtold et al. [Berchtold et al. 2000] develop the *IQ-tree*, combining features of the R-tree and VA-file. Chaudhuri and Gravano [Chaudhuri and Gravano 1999] perform NN search by converting it to range queries. In [Berchtold et al. 2000] Berchtold et al. provide a solution leveraging high-dimensional Voronoi diagrams, whereas Korn et al. [Korn et al. 2001] tackle the problem by utilizing the fractal dimensionality of the dataset. Koudas et al. [Koudas et al. 2004] give a bitmap-based approach. The state of the art is due to Jagadish et al. [Jagadish et al. 2005]. They develop the *iDistance* technique that converts high-dimensional points to 1D values, which are indexed using a B-tree for NN processing. We will compare our solution to *iDistance* experimentally.

In exact search, a majority of the query cost is spent on *verifying* a point as a real NN [Bennett et al. 1999; Ciaccia and Patella 2000]. Approximate retrieval improves efficiency by relaxing the precision of verification. Goldstein and Ramakrishnan [Goldstein and Ramakrishnan 2000] assume that the query distribution is known, and leverage the knowledge to balance the efficiency and result quality. Ferhatosmanoglu et al. [Ferhatosmanoglu et al. 2001] find NNs by examining only the interesting subspaces. Chen and Lin [Chen and Ling 2002] combine sampling with a reduction [Chaudhuri and Gravano 1999] to range search. Li et al. [Li et al. 2002] first partition the dataset into clusters, and then prunes the irrelevant clusters according to their radii. Houle and Sakuma [Houle and Sakuma 2005] develop *SASH* which is designed for memory-resident data, but is not suitable for disk-oriented data due to severe I/O thrashing. Fagin et al. [Fagin et al. 2003] develop the *MedRank* technique that converts the dataset to several sorted lists by projecting the data onto different vectors. To answer a query, *MedRank* traverses these lists in a way similar to the *threshold* algorithm [Fagin et al. 2001] for top-k search. We will also evaluate *MedRank* in the experiments.

None of the aforementioned solutions ensures sub-linear growth of query cost in the worst case. How to achieve this has been carefully studied in the theory community (see, for example, [Har-Peled 2001; Krauthgamer and Lee 2004] and the references therein). Almost all the results there, however, are excessively complex for practical implementation, except LSH. This technique is invented by Indyk and Motwani [Indyk and Motwani 1998] for in-memory data. Gionis et al. [Gionis et al. 1999] adapt it to external memory, but as discussed in Section 3.2, their method loses the guarantee on the approximation ratio. The locality-sensitive hash functions for l_p norms are discovered by Datar et al. [Datar et al. 2004]. Bawa et al. [Bawa et al. 2005] propose a method to tune the parameters of LSH automatically. Their method, however, no longer ensures the same query performance as LSH unless the adopted hash function has a so-called "$(\epsilon, f(\epsilon))$ property" [Bawa et al. 2005]. Unfortunately, no existing hash function for ℓ_p norms is known to possess this property. Charikar [Charikar 2002] investigate LSH for several distance metrics different from ℓ_p norms. LSH has also received other theoretical improvements [Andoni and Indyk 2006; Panigrahy 2006] which cannot be implemented in relational databases. Furthermore, several heuristic variations of LSH have also been suggested. For example, Lv et al. [Lv et al. 2007] reduce space consumption by probing more data in answering a query, while recently Athitsos et al. [Athitsos et al. 2008] introduce the notion of *distance-based hashing*. The solutions of [Athitsos et al. 2008; Lv et al. 2007] guarantee neither sub-linear cost nor good approximation ratios.

CP search is also one of the oldest problems studied in computational geometry. In two-dimensional space, Shamos and Hoey [Shamos and Hoey 1975] give an optimal algorithm that runs in $O(n \log n)$ time. Interestingly, for any fixed dimensionality d, the problem can also be settled optimally in $O(n \log n)$ time, as discovered by Lenhof and Smid [Lenhof and Smid 1992]. The optimality of the above algorithms, however, assumes that d is a constant; when it is not, their running time increases exponentially with d. Avoiding such exponential growth turns out to be a hard problem. Recently, by resorting to matrix multiplication, Indyk et al. [Indyk et al. 2004] give several algorithms with non-trivial bounds that are

applicable to L_1 and L_∞ norms, but not to the other L_p norms. The methods mentioned earlier are rather theoretical. On the practical side, Hjaltason and Samet [Hjaltason and Samet 1998] give a solution, called *distance browsing*, that utilizes R-trees to report point pairs in ascending order of their distances. Following the same idea, Corral et al. [Corral et al. 2000] propose an enhanced algorithm with smaller cost, which will be evaluated in the experiments.

The above solutions aim at solving the CP problem exactly. There have been attempts to address the approximate version, but most of those algorithms require running time that is quadratic to the cardinality n (albeit faster than dn^2); see for example [Kleinberg 1997]. Based on the LSH technique, Datar et al. [Datar et al. 2004] propose an algorithm with sub-quadratic time, but their analysis targets internal memory only. Our discussion in Section 7.1 can in fact also be applied to LSH, and shows that the case of external memory requires a more elaborate reasoning approach. Furthermore, our result in Section 7.2 is actually better (by a logarithmic factor) than the obvious bound adapted from [Datar et al. 2004] (which corresponds to the performance of algorithm *CP1* in Figure 15). Another algorithm worth mentioning is due to Lopez and Liao [Lopez and Liao 2000]. When d is regarded as a constant, their algorithm, which we call *D-shift*, guarantees an answer with constant approximation ratio. Their algorithm can be incorporated in relational databases, and will be compared to our solutions in the experiments.

Finally, it is worth pointing out that this paper substantially extends its preliminary version [Tao et al. 2009] in the following ways. First, in Section 6, we have shown how to modify our NN techniques to achieve approximation $c + \epsilon$ for any integer $c \geq 3$ (only $c = 2$ is discussed in [Tao et al. 2009]), thus giving a stronger tradeoff between the result quality and the query/space efficiency. Second, while the preliminary work concentrates on NN search, the current version contains a full set of results on the CP problem (Section 7), together with the corresponding experiment in the next section.

9. EXPERIMENTS

Next we experimentally evaluate the performance of LSB-trees, using the existing methods as benchmarks. Section 9.1 describes the datasets and queries. Sections 9.2 and 9.3 list the techniques to be examined for NN and CP search, respectively. Section 9.4 explains the computing environments as well as the assessment metrics. Section 9.5 demonstrates the superiority of the LSB-forest over alternative LSH implementations. Then, Section 9.6 (9.7) shows that our techniques significantly outperform the previous methods, in both exact and approximate NN (CP) search.

9.1 Data and queries

We experimented with both synthetic and real datasets. Synthetic data were generated according to a *varden* distribution to be clarified shortly. As for real data, we deployed datasets *color* and *mnist*, which were also used in the papers [Fagin et al. 2003; Jagadish et al. 2005] where *iDistance* and *MedRank* are invented respectively (both methods were included in our experiments). For all datasets, the universe was normalized to have domain $[0, 10000]$ on each dimension.

The distance metric employed was Euclidean distance. Each NN *workload* contained 50 query points that followed the same distribution as the underlying dataset.

CP search takes no query point; it simply finds the k closest pairs in a dataset.

The details of *varden*, *color*, and *mnist* are as follows.

Varden. This distribution contains two clusters with drastically different densities. The sparse cluster has 10 points, whereas all the other points belong to the dense cluster. Furthermore, the dense cluster has the shape of a ring, whose radius is comparable to the average mutual distance of the points in the sparse cluster. The two clusters are well separated. Figure 19 illustrates the idea with a 2D example. We varied the cardinality of a *varden* dataset from 10k to 100k, and its dimensionality from 25 to 100. In the sequel, we will denote a d-dimensional *varden* dataset with cardinality n by *varden-nd*. The corresponding workload of a *varden* dataset had 10 and 40 query points that fell in the areas of the sparse and dense clusters, respectively. No query point coincided with any data point.

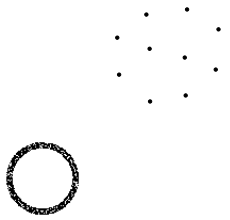


Fig. 19. The *varden* distribution

Color. This is a 32-dimensional dataset[3] with 67,967 points, where each point describes the color histogram of an image in the Corel collection [Jagadish et al. 2005]. We randomly removed 50 points to form a query set. As a result, our *color* dataset has cardinality 67,917.

Mnist. The original *mnist* dataset[4] is a set of 60,000 points. Each point is 784-dimensional, capturing the pixel values of a 28×28 image. Since, however, most pixels are insignificant, we reduced dimensionality by taking the 50 dimensions with the largest variances. After this, we got two identical points so one of them was removed, rendering the final cardinality to be 59,999. The *mnist* collection also contains a test set of 10,000 points [Fagin et al. 2003], among which we randomly picked 50 to form our workload. Obviously, each query point was also projected onto the same 50 dimensions output by the dimensionality reduction.

9.2 Competitors for nearest neighbor search

Sequential scan (*SeqScan*). The bruteforce approach is included because it is known to be a strong competitor in high dimensional NN retrieval. Furthermore, the relative performance with respect to *SeqScan* serves as a reliable way to compare against methods that are reported elsewhere but not in our experiments.

[3] *http://kdd.ics.uci.edu/databases/CorelFeatures/.*
[4] *http://yann.lecun.com/exdb/mnist.*

LSB-forest. As discussed in Section 4.2, this method takes l LSB-trees (l given by Equation 7), and applies algorithm *NN1* (Figure 7) for query processing. For kNN queries with $k > 1$, *LSB-forest* still uses the same l (i.e., no increase in the number of trees) and query algorithm, except that the terminating condition $\boldsymbol{E_2}$ is modified in the way explained in Section 4.2.

LSB-no$\boldsymbol{E_2}$. Same as *LSB-forest* except that it disables condition $\boldsymbol{E_2}$ in algorithm *NN1*. In other words, *LSB-noE_2* terminates on condition $\boldsymbol{E_1}$ only. *LSB-noE_2* is applied only for $k = 1$.

LSB-tree. This method deploys a single LSB-tree (as opposed to l in *LSB-forest*), and hence, requires only linear space and can be updated efficiently. As mentioned at the end of Section 4.2, it disables condition $\boldsymbol{E_1}$, and terminates on $\boldsymbol{E_2}$ only (again, $\boldsymbol{E_2}$ needs to be modified for $k > 1$).

***Rigorous-* [Indyk and Motwani 1998] and *adhoc-LSH* [Gionis et al. 1999].** They are the existing LSH-implementations as reviewed in Sections 3.1 and 3.2, respectively. Recall that both methods are designed for c-approximate BC search. We set c to 2 to match the guarantee of the LSB-forest (see Section 6). *Adhoc-LSH* requires a set of l hash tables, which is used to perform BC queries at a magic radius (to be tuned experimentally later), where l is the same as in Equation 7. *Rigorous-LSH* can be regarded as combining multiple versions of *adhoc-LSH*, one for every radius supported.

***iDistance* [Jagadish et al. 2005].** A famous approach for exact NN search. As mentioned in Section 8, it indexes a dataset using a single B-tree after converting all points to 1D values. As with *LSB-tree*, it consumes linear space and supports data insertions and deletions efficiently.

***MedRank* [Fagin et al. 2003].** A recently proposed method for approximate NN search with a non-trivial quality guarantee. Given a dataset, *MedRank* creates several sorted lists, such that every data point has an entry in each list. More specifically, an entry has the form (id, key), where id uniquely identifies a point, and key is its sorting key (a point has various keys in different lists). Each list is indexed by a B-tree on the keys. Point coordinates are stored in a separate hash table to facilitate probing by id. The number of lists equals $\log n$ (following Theorem 4 in [Fagin et al. 2003]), where n is the dataset cardinality. It should be noted that *MedRank* is not friendly to updates, because a single point insertion/deletion requires updating all the $\log n$ lists.

9.3 Competitors for closest pair search

Quadratic. The naive approach that examines all pairs of points. It serves as a benchmark for comparison with other solutions to the CP problem not included in our experiments.

LSB-forest. This method uses l LSB-trees, where l is given by Equation 7, and applies algorithm *CP2* (Figure 16). The same l and algorithm are also used for kCP search with $k > 1$, except that *CP2* needs to report the k best pairs (instead

of 1).

2LSB-tree. The method uses two LSB-trees; it applies algorithm *CP3* (Figure 18) on each tree separately, and returns the k best pairs after combining the outputs from both trees. Here we are using one more tree than the *LSB-tree* method in the previous subsection, in order to outperform the competitor *D-shift* (to be introduced later) in result quality. Note that using 2 trees does not increase the space and update-time complexities. Namely, *2LSB-tree* still occupies linear space and can be updated in logarithmic time.

Distance browsing (*DistBrowsing*) [Corral et al. 2000]. An extensively-cited solution to exact kCP search. Similar to [Hjaltason and Samet 1998], it leverages an R-tree on the underlying dataset to enumerate point pairs in ascending order of distances.

Diagonal shift (*D-shift*) [Lopez and Liao 2000]. An approximate algorithm with a non-trivial quality guarantee. Given a d-dimensional dataset, it creates d copies of the dataset, where each copy is obtained by shifting the original dataset along the direction of the main diagonal by a different offset (hence the name *D-shift*). Then, the closest pairs are found by sorting and scanning each list once.

9.4 Computing environments and assessment metrics

The page size was fixed to 4,096 bytes. All the experiments were run on a computer equipped with a 3GHz CPU. A memory buffer of 50 pages was adopted in all cases. Under such settings, the running time of all (NN and CP) algorithms was dominated by their I/O overhead. Therefore, we will report the number of I/Os as the computation cost.

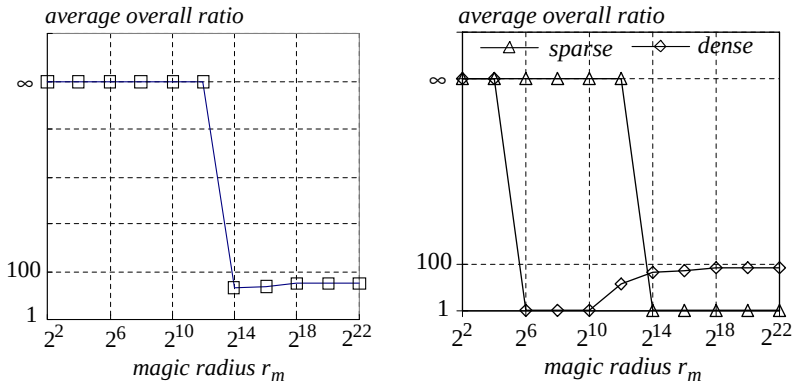
Quality of NN search. We evaluate the quality of a kNN result by how many times farther a reported neighbor is than the real NN. Formally, let o_1, o_2, ..., o_k be the k neighbors that a method retrieves for a query q, in ascending order of their distances to q. Let o_1^*, o_2^* ..., o_k^* be the actual first, second, ..., k-th NNs of q, respectively. For any $i \in [1, k]$, we define the *rank-i* (*approximation*) *ratio*, denoted by $R_i(q)$, as

$$R_i(q) = \|o_i, q\| / \|o_i^*, q\|. \tag{16}$$

The *overall* (*approximation*) *ratio* is the mean of the ratios of all ranks, namely, $(\sum_{i=1}^{k} R_i(q))/k$. When a query result is exact, all ratios are 1.

Given a workload W, define its *average overall ratio* as the mean of the overall ratios of all queries in W. This metric reflects the general quality of all k neighbors, and was used in most experiments. Sometimes we needed to scrutinize the quality of neighbors at individual ranks. In that case, we measured the *average rank-i ratio* ($1 \leq i \leq k$), which is the mean of the rank-i ratios of all queries in W, namely, $(\sum_{\forall q \in W} R_i(q))/|W|$.

Quality of CP search. Also assessed based on *rank-i ratio* and *overall ratio*, both of which are extended from the earlier definitions in a straightforward manner.



(a) Quality vs. r_m (b) Quality of sparse and dense queries

Fig. 20. Magic radius tuning for *adhoc-LSH* (*varden-10k50d*)

9.5 Behavior of LSH implementations

This section explores the characteristic behavior of *LSB-forest*, *LSB-noE_2*, *rigorous-LSH*, and *adhoc-LSH*. For this purpose, we focused on $k = 1$ because the LSH methodology was originally designed in the context of single NN retrieval. Note that, when $k = 1$, the overall ratio of a query is identical to its rank-1 ratio. The data distribution examined was *varden*, as it allowed us to adjust the dimensionality and cardinality. Unless otherwise stated, a *varden* dataset had a default cardinality $n = 10$k and dimensionality $d = 50$.

Recall that *adhoc-LSH* answers a NN query by processing instead a BC query with a magic radius r_m. As argued in Section 3.2, there may not exist an r_m good for all NN queries. To demonstrate this, Figure 20a shows the average overall ratio of *adhoc-LSH* as r_m varied from 2^2 to 2^{22}. For small r_m, the ratio is ∞, implying that *adhoc-LSH missed* at least one query in the workload, namely, returning nothing at all. The ratio improved suddenly to 66 when r_m reached 2^{14}, and stabilized as r_m grew further. It is thus clear that, given any r_m, the result of *adhoc-LSH* was at least 66 times worse than the real NN on average!

As discussed in Section 3.2, if r_m is considerably smaller than the NN-distance of a query, *adhoc-LSH* may return an empty result. Conversely, if r_m is considerably larger, *adhoc-LSH* may output a point much worse than the real NN. We performed an experiment to verify this. Recall that a workload for *varden* has queries in both the sparse and dense clusters. Let us call the former the *sparse* queries, and the latter the *dense* queries. We observed that the average NN distance of a sparse (dense) query was around 12,000 (15). The phenomenon in Figure 20a occurred because *the values of r_m good for sparse queries were bad for dense queries, and vice versa*. To support the claim, Figure 20b plots the average overall ratios of sparse and dense queries separately. When r_m was smaller than or equal to $2^{13} =$ 8,192, it was much lower than the NN-distances of sparse queries; hence, *adhoc-LSH* returned nothing for them, as is why the *sparse* curve in Figure 20b stays at ∞ for all $r_m \leq 2^{13}$. As r_m climbed to 2^{12},*adhoc-LSH* started to return bad results for many dense queries. The situation was worse for larger r_m, so the *dense* curve

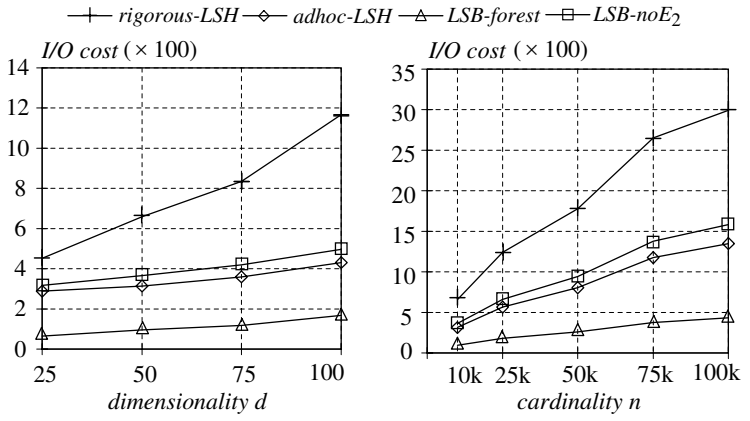
d	25	50	75	100
rigorous-LSH	1			
adhoc-LSH	43	66.4	87	104.2
LSB-forest	1.02	1.02	1.02	1.01
LSB-noE$_2$	1			

(a) Average overall ratio vs. dimensionality d (n = 50k)

n	10k	25k	50k	75k	100k
rigorous-LSH	1				
adhoc-LSH	66.4	68.1	70.3	76.5	87.1
LSB-forest	1.02	1.02	1.03	1.02	1.02
LSB-noE$_2$	1				

(b) Average overall ratio vs. cardinality n (d = 50)

Table I. Result quality on *varden* data



(a) Cost vs. d (n = 50k) (b) Cost vs. n (d = 50)

Fig. 21. Query efficiency on *varden* data

Figure 20b increases continuously from 2^{12}. In all the following experiments, we fixed r_m to the optimal value 2^{14}.

The next experiment compares the result quality of *rigorous-LSH*, *adhoc-LSH*, *LSB-forest*, and *LSB-noE*$_2$. Table Ia (Ib) shows their average overall ratios under different dimensionalities (cardinalities). Both *rigorous-LSH* and *LSB-noE*$_2$ achieved perfect quality, namely, they successfully returned the *exact* NN for all queries. *LSB-forest* incurred slightly higher error because in general it accesses fewer points than *LSB-noE*$_2$, and thus, has a lower chance of encountering the real NN. *Adhoc-LSH* was by far the worst method, and its effectiveness deteriorated rapidly as the dimensionality or cardinality increased.

To evaluate the query efficiency of the four methods. Figure 21a (21b) plots their I/O cost as a function of dimensionality d (cardinality n). *LSB-forest* considerably outperformed its competitors in all cases. Notice that while *LSB-noE*$_2$ was slightly more costly than *adhoc-LSH*, *LSB-forest* entailed only a fraction of the overhead of *adhoc-LSH*. This phenomenon reveals the importance of having terminating condi-

tion $\boldsymbol{E_2}$ in the *NN1* algorithm. *Rigorous-LSH* was much more expensive than the other approaches, which is consistent with its vast asymptotical complexity.

Tables IIa and IIb show the space consumption (in mega bytes) of each solution as a function of d and n, respectively. *LSB-no*E_2 is not included because it differs from *LSB-forest* only in the query algorithm, and thus, had the same space cost as *LSB-forest*. Furthermore, *adhoc-LSH* also occupied as much space as *LSB-forest*, because a hash table of the former stores the same information as a LSB-tree of the latter. As predicted by their space complexities, *rigorous-LSH* required more space than *LSB-forest* by a factor of $\log d + \log t$, where t (the largest coordinate on each dimension) was 10,000 in our experiments.

d	25	50	75	100
rigorous-LSH	382	896	1,563	2,436
adhoc-LSH	24	57	101	159
LSB-forest	24	57	101	159

(a) Space vs. dimensionality d (n = 50k)

n	10k	25k	50k	75k	100k
rigorous-LSH	895	3,624	10,323	18,892	29,016
adhoc-LSH	57	231	660	1,208	1,855
LSB-forest	57	231	660	1,208	1,855

(b) Space vs. cardinality n (d = 50)

Table II. Space consumption on *varden* data in mega bytes

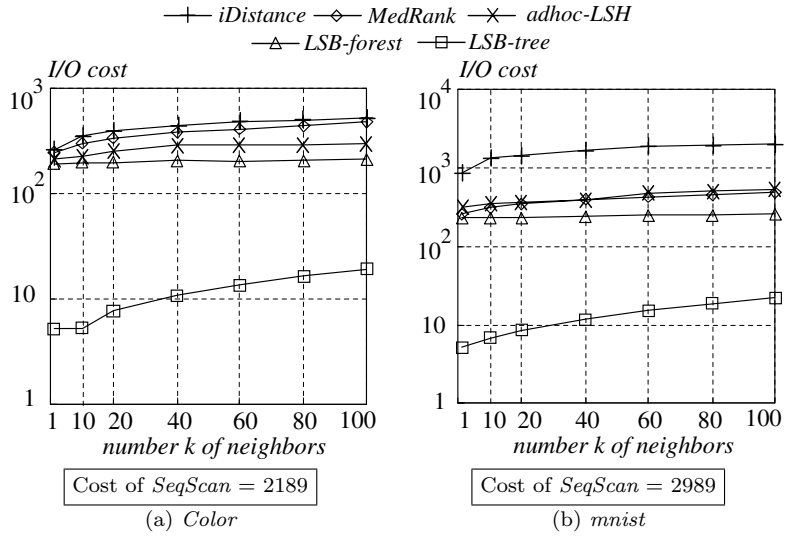
It is evident that *LSB-forest* is overall the best technique in the above experiments. It retains the query accuracy of *rigorous-LSH*, consumes the same space as *adhoc-LSH*, and incurs significantly smaller query cost than both.

9.6 Comparison of NN solutions

Having verified the correctness of our theoretical analysis, in the sequel we assess the practical performance of *SeqScan*, *LSB-tree*, *LSB-forest*, *adhoc-LSH*, *MedRank*, and *iDistance*. *Rigorous-LSH* and *LSB-no*E_2 are omitted because the former incurs gigantic space/query cost, and the latter is merely an auxiliary method for demonstrating the importance of condition $\boldsymbol{E_2}$. Remember that *SeqScan* and *iDistance* return exact NNs, whereas the other methods are approximate.

Only real datasets *color* and *mnist* were adopted in the subsequent evaluation. The workload on *color* (*mnist*) had an average NN distance of 833 (11,422). We set the magic radius of *adhoc-LSH* to the smallest power of 2 that bounds the average NN distance from above, namely, 1,024 and 16,384 for *color* and *mnist*, respectively. The number k of retrieved neighbors varied from 1 to 100.

Let us start with query efficiency. Figure 22a (22b) illustrates the average cost of a kNN query on dataset *color* (*mnist*) as a function of k. *LSB-tree* was by far the fastest method, and outperformed all the other approaches by a factor of at least an order of magnitude. In particular, on *mnist*, *LSB-tree* even achieved a speedup of two orders of magnitude over *iDistance*, justifying the advantages of approximate retrieval. *LSB-forest* was also much faster than *iDistance*, *MedRank*, and *adhoc-LSH*, especially in returning a large number of neighbors.



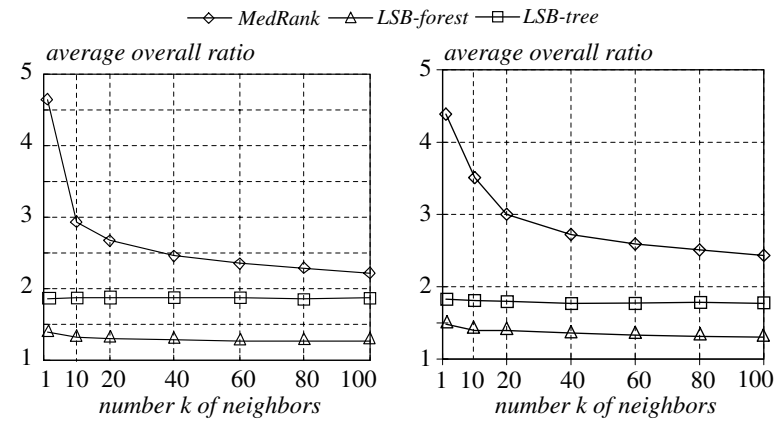
(a) *Color* (b) *mnist*

Fig. 22. Efficiency of kNN search

The next experiment inspects the result quality of the approximate techniques. Focusing on *color* (*mnist*), Figure 23a (23b) plots the average overall ratios of *MedRank*, *LSB-forest*, and *LSB-tree* as a function of k. Since *adhoc-LSH* may *miss* a query (i.e., unable to return k neighbors), we present its results as a table in Figure 23c, where each cell contains two numbers. The number in the bracket indicates how many queries were missed (out of 50), and the number outside is the average overall ratio of the queries that were answered properly. No ratio is reported if *adhoc-LSH* missed more than 30 queries.

LSB-forest incurred low error in all cases (maximum ratio below 1.5), owing to its nice theoretical properties. *LSB-tree* also had good precision (maximum ratio 2), indicating that the proposed conversion (from a d-dimensional point to a Z-order value) adequately preserved the spatial proximity of data points. *MedRank*, in contrast, exhibited much worse precision than the proposed solutions. In particular, observe that *MedRank* was not effective in the important case of single NN search ($k = 1$), for which its average overall ratio was over 4. Finally, *adhoc-LSH* was clearly unreliable due to the large number of queries it missed.

The average overall ratio reflects the general quality of all k neighbors reported. It does not, however, indicate how good the neighbors are at individual ranks. To find out, we set k to 10, and measured the average rank-i ratios at each $i \in [1, 10]$. Figures 24a and 24b demonstrate the results on *color* and *mnist*, respectively (*adhoc-LSH* is not included because it missed many queries). Apparently, both *LSB-forest* and *LSB-tree* provided results significantly better than *MedRank* at all ranks. Observe that the quality of *MedRank* deteriorated considerably at high ranks, whereas our solutions returned fairly good neighbors even at the highest rank. Note that the results in Figure 24 should not be confused with those of Figure 23. For example, the average rank-1 ratio (of $k = 10$) is different from the

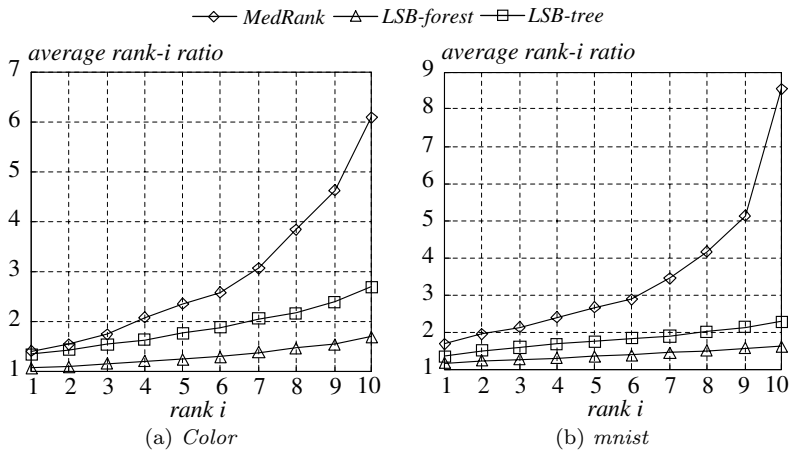


(a) *Color* (b) *Mnist*

k	1	10	20	40	60	80	100
color	1.2 (0)	1.3 (30)	- (42)	- (46)	- (46)	- (47)	- (48)
mnist	1.2 (0)	1.3 (13)	1.3 (19)	1.4 (28)	- (37)	- (39)	- (41)

(c) Results of *adhoc-LSH* (in each cell, the number inside the bracket is the number of missed queries, and the number outside is the average overall ratio of the queries answered properly)

Fig. 23. Average overall ratio vs. k



(a) *Color* (b) *mnist*

Fig. 24. Average ratios at individual ranks for 10NN queries

overall average ratio of $k = 1$[5].

Table III compares the space consumption of different methods. *LSB-tree* required slightly less space than *iDistance* and *MedRank*. We, however, ought to point out that, at least in theory, *LSB-tree* needs to store more information than

[5]The average rank-1 ratio is lower because processing a query with $k = 10$ needs to access more data than a query with $k = 1$, and therefore, has a better chance of encountering the nearest neighbor.

iDistance, so the latter should be more space economical. However, the actual space consumption may contain some extra overhead depending on the concrete implementation. The implementation of *iDistance* we deployed was exactly the one written by the authors of [Jagadish et al. 2005]. Also note that our implementations of *LSB-tree*, *LSB-forest*, and *Adhoc-LSH* have been improved compared to those in the preliminary version [Tao et al. 2009].

	iDistance	*MedRank*	*adhoc-LSH*	*LSB-forest*	*LSB-tree*
color	14	17	573	573	13
mnist	18	19	874	874	16

Table III. Space consumption on real data in mega bytes

Recall that *LSB-forest* utilizes a large number l of LSB-trees, where the number l was 47 and 55 for *color* and *mnist*, respectively. *LSB-tree* represents the other extreme that uses only a single tree. Next, we explore the compromise of these two extremes, by using multiple, but less than l, trees. The query algorithm is the same as the one adopted by *LSB-tree*. In general, leveraging x trees increases the query, space, and update cost by a factor of x. The benefit, however, is that a larger x also improves the quality of results. To explore this tradeoff, Figure 25 shows the average overall ratio of 10NN queries on the two real datasets, when x grew from 1 to the corresponding l of *LSB-forest*. Interestingly, the precision improved dramatically with just a small number of trees. In other words, we can obtain much better results without increasing the space or query overhead considerably, which is especially appealing for datasets that are not updated frequently.

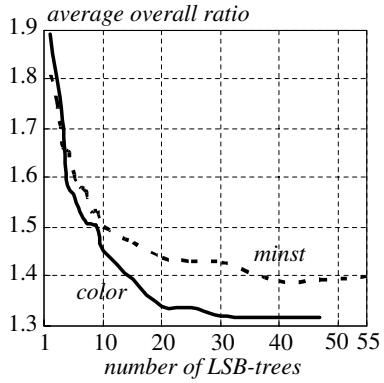
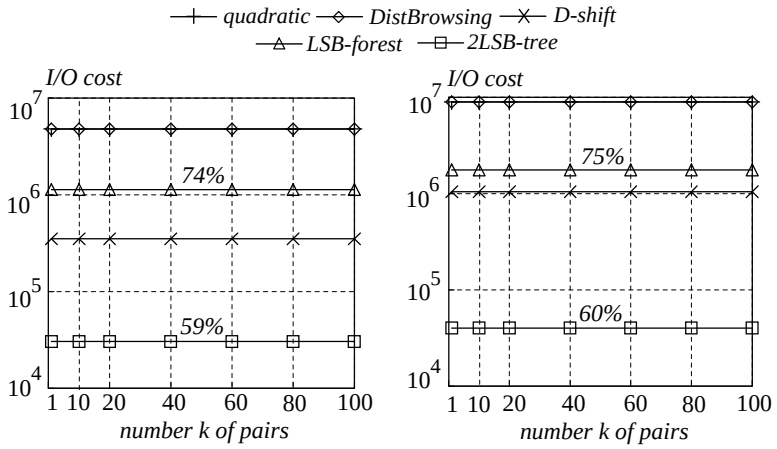


Fig. 25. Benefits of using multiple LSB-trees ($k = 10$)

In summary, our experiment results suggest that an exact solution such as *iDistance* often requires excessively long query response time in practice, confirming the motivation of study approximate solutions. The most serious drawback of *Adhoc-LSH* is that it may fail to report enough neighbors for many queries. In any case, its query overhead is still too high to provide fast response time. *MedRank* is even more expensive than *adhoc-LSH*; furthermore, its result quality is relatively low



(a) *Color* (b) *Mnist*

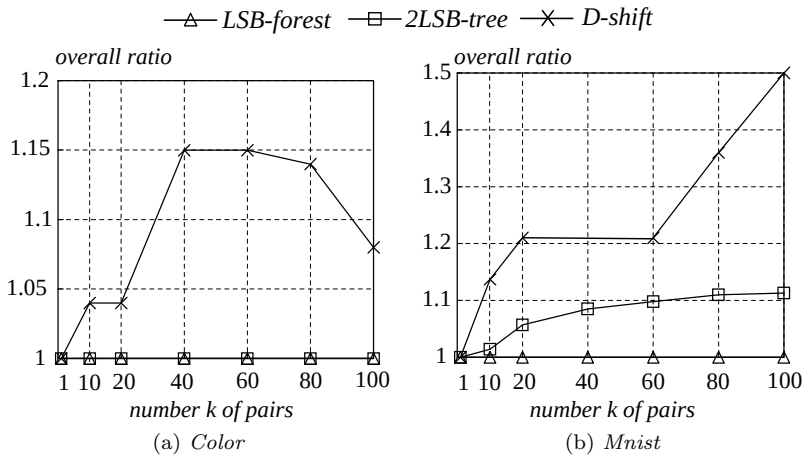
Fig. 26. Cost of kCP search

(i.e., the answers it returns are quite far from the real k NNs). *LSB-forest* is the only (approximate) method that guarantees high result quality and sub-linear query cost in all cases. However, as with *adhoc-LSH* and *MedRank*, it is not friendly to updates. Overall the best solution is *LSB-tree*: it demands only linear space, supports fast updates, returns very accurate results, and is extremely efficient in query processing.

9.7 Comparison of CP solutions

We now proceed to study the methods for closest pair search, using again the real datasets *color* and *mnist*. The first experiment compares their efficiency of finding k closest pair *from scratch*. Namely, we do not assume any pre-computation; if a method requires an index (e.g., an R-tree or LSB-trees), it must construct it on the fly, with the construction time added into its total cost.

Figure 26a (26b) shows the I/O cost of each method on dataset *color* (*mnist*), as the number k of pairs retrieved changed from 1 to 100. *2LSB-tree* was by far the most efficient, and outperformed *D-shift* and *LSB-forest* by more than an order of magnitude. As expected, *LSB-forest* was slower than *D-shift* because the former's time complexity is super-linear with respect to the dataset cardinality n, whereas the latter's is linear [Lopez and Liao 2000]. Nevertheless, as shown shortly, the advantage of *LSB-forest* is that it returned much more accurate answers than *D-shift*. *DistBrowsing* was as expensive as the naive algorithm *quadratic*. This is not surprising because the effectiveness of spatial access methods (particular, R-trees) deteriorates seriously in high dimensional space such that they hardly offer any pruning in distance browsing. The deficiency of exact solutions, once again, confirms the importance of approximate methods. The parameter k, in the tested range of values, did not affect the efficiency of any method. The percentages on the curves of *2LSB-tree* and *LSB-forest* indicate how much of the overall cost was spent on on-the-fly index construction. In other words, if the LSB-trees already existed before the CP search, the costs of *2LSB-tree* and *LSB-forest* would be 60%



(a) *Color* (b) *Mnist*

Fig. 27. Quality of kCP search

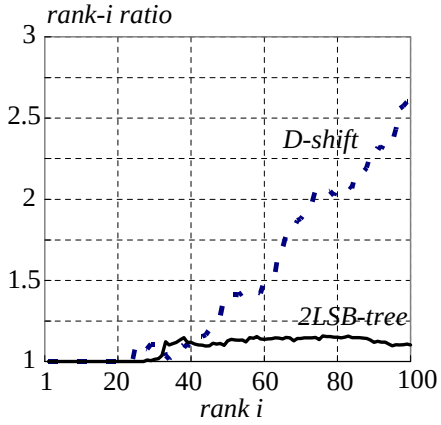


Fig. 28. Quality of individual pairs returned (*minst*, $k = 100$)

and 75% cheaper. Note that stripping 75% from the cost of *LSB-forest* would make it even faster than *D-shift*.

To assess the quality of results, Figure 27a (27b) compares the overall ratios of the three approximate methods in the experiment of Figure 26a (26b). Recall that the overall ratio indicates the average quality of all k pairs returned by a method. *LSB-forest* achieved an overall ratio of 1 on both datasets, meaning that it found the *exact* 100 k closest pairs in both cases. *2LSB-tree* also produced perfectly accurate answers on *color*; on *mnist*, on average the answers it found were worse than the exact ones by merely 10%. The quality of *D-shift* was clearly much worse, thus leaving its expensive computation cost unjustified (see Figure 26).

To zoom into the quality of individual closest pairs, Figure 28 plots the rank-i ratios for all $i \in [1, 100]$, of the results returned by *2LSB-tree* and *D-shift* in performing 100CP on *mnist*. Recall that the rank-i ratio measures how much times worse the i-th pair found by a method is, compared to the exact i-th closest pair.

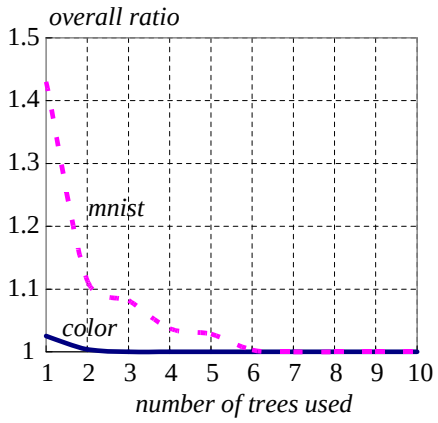


Fig. 29. Benefits of using multiple trees ($k = 100$)

LSB-forest is omitted because, as mentioned earlier, it produced perfect answers. Similarly, we also omit the results on *color* because even *2LSB-tree* was able to achieve perfect accuracy on that dataset. In Figure 28, we can see that all the pairs found by *2LSB-tree* were fairly accurate, whereas the quality of the "high-rank" pairs returned by *D-shift* was rather poor.

We have seen in Section 9.2 that, for NN retrieval, there exists a graceful tradeoff between the result quality and the number of LSB-trees used for query processing. The last experiment aims at identifying a similar phenomenon for CP search. For this purpose, we generalized the strategy of *2LSB-tree*; namely, given x LSB-trees, we ran algorithm *CP3* on each of them, and then, reported the k best pairs among the outputs from all trees. Apparently, the result quality should improve as x increases, but it is most interesting to identify when the quality would improve to perfection, i.e., an overall ratio of 1! The results on *color* and *mnist* are plotted in Figure 29 for $k = 100$. Clearly, the growth of x brought dramatic improvements on the result quality. On *mnist*, only 7 trees were necessary to attain perfect precision (the number was 2 for *color*, as we already knew from Figure 27a).

In summary, our experiments show that an exact solution to CP search such as *DistBrowsing* is not suitable in high-dimensional space due to their prohibitive running time. *D-shift* has the drawbacks that it (i) still entails expensive overhead, and (ii) cannot guarantee accurate answers, especially at high ranks. Same as in NN search, *LSB-forest* is the only (approximate) method able to guarantee excellent result quality in any case. Nevertheless, it still cannot escape the trap of costly execution time. The best approach is to perform CP search using a small (e.g., 2) number of LSB-trees, which is significantly faster than all the other methods (over an order of magnitude), and returns close-to-exact answers in most cases.

10. CONCLUSIONS

Nearest neighbor search in high dimensional space finds numerous applications in a large number of disciplines. This paper develops an access method called the LSB-tree to enable fast NN search with excellent result quality. Our discovery

carries both theoretical and practical significance. In theory, by combining several LSB-trees, we dramatically improve the (asymptotical and actual) space and query efficiency of the previous LSH implementations, without compromising the result quality. In practice, by using a single LSB-tree, we give an effective indexing scheme that can be easily incorporated in a relational database, consumes linear space, supports logarithmic-time updates, and can be used to answer NN queries accurately and efficiently.

As a second step, we have extended our LSB-technique to attack the closest pair problem in high-dimensional space, which is another classic problem with many applications. Our contributions on this topic also have important values in both theory and reality. In particular, we have shown that, in external memory, the closest pair problem can be solved in time strictly lower than the quadratic complexity, regardless of the dimensionality. In practice, our purely-relational solutions can be immediately applied in a commercial system. Furthermore, these solutions can directly leverage the indexing scheme mentioned earlier for NN search. This is a fairly attractive feature because, with only a single structure, one is able to adequately tackle two difficult problems at the same time.

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