A new compressed cover tree guarantees a near linear parameterized complexity for all *k*-nearest neighbors search in metric spaces

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— Abstract

This paper studies the classical problem of finding k nearest neighbors to m query points within a larger set of n reference points in an arbitrary metric space. The well-known work by Beygelzimer, Kakade and Langford in ICML 2006 introduced cover trees and claimed to guarantee a near linear worst-case complexity in the number n of reference points. Section 5.3 of Curtin's PhD (2015) pointed out that the key step in the above work needs to update an estimate $O(\log n)$ for a required number of iterations. This paper describes typical examples when past cover trees need O(n) iterations so that the overall worst-time complexity remains quadratic as for a brute-force search. Despite the same estimate $O(\log n)$ being repeated in numerous subsequent papers, no further analysis was published. A new compressed cover tree is a much smaller structure that resolves the past obstacles for k-nearest neighbor search and guarantees a parameterized complexity that is near linear in the maximum size of both query and reference set for any $k \ge 1$.

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1 History of k-nearest neighbor search, problem statement and overview of results

The search for nearest neighbors was one of the first data-driven problems and led to the neighbor rule for classification [9]. In a modern formulation, the problem is to find all $k \ge 1$ nearest neighbors in a reference set R for all points from a query set Q. Both sets live in an ambient space X with a given distance d satisfying all metric axioms. The simplest example is $X = \mathbb{R}^n$ with the Euclidean metric, where a query set Q can be a single point or a subset of a larger set R.

The exact k-nearest neighbor problem asks for exact (true) k-nearest neighbors of every query point q. Another probabilistic version of the k-nearest neighbor search [22] aims to find exact k-nearest neighbors with a given probability. The approximate version [2], [19],[1],[30] for every query point $q \in Q$, looks for its approximate neighbor $r \in R$ satisfying $d(q,r) \leq (1+\epsilon)d(q, \operatorname{NN}(q))$, where $\epsilon > 0$ is fixed and $\operatorname{NN}(q)$ is the exact first nearest neighbor of q.

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Figure 1 Left: an implicit form of a cover tree defined in 2006 [7, Section 2] for the finite set of reference points $R = \{1, 2, 3, 4, 5\}$. **Right:** a new compressed cover tree in Definition 2.1 corrects the past complexity results for k-nearest neighbors search in R.

The naive approach to find all 1st nearest neighbors of points from Q within R is proportional to the product $|Q| \cdot |R|$ of the sizes of Q, R. Already in 1974 real data was big enough to motivate faster algorithms. Namely, a *quadtree* [13] hierarchically indexed a reference set $R \subset \mathbb{R}^2$ by subdividing its bounding box (a root) into four smaller boxes (children), which are recursively subdivided until final boxes (leaf nodes) contain only a small number of reference points.

The straightforward extension of a quadtree to \mathbb{R}^n leads to an exponential dependence on n, because the n-dimensional box is subdivided into 2^n smaller boxes. The first attempt to overcome this curse of dimensionality was the kd-tree [5] subdividing a subset of R at every level into two subsets instead of 2^n subsets. The nearest search algorithms have positively impacted many related problems: a minimum spanning tree [4], range search [26], k-means clustering [26] and ray tracing [15]. The single-tree structures for finding nearest neighbors in the chronological order are k-means tree [14], R tree [3], ball tree [25], R^* tree [3], vantage-point tree [31], Hilbert R tree [17], TV trees [20], X trees [6], principal axis tree [24], spill tree [21], cover tree [7], cosine tree [16], max-margin tree [28], cone tree [27] and others.

In 2004 the paper [19] attempted to solve the k-nearest neighbor problem in a general metric space in a near-linear time by [19, Theorem 2.7] claiming that all k-nearest neighbors of a query point q can be found in R by using the navigating nets [19, Section 2.1] in time $2^{O(\dim_{KR}(R \cup \{q\})}(k + \log |R|))$, where $\dim_{KR}(R \cup \{q\})$ is the expansion rate from [18] and |R| is the size of the set R. The proof was omitted and the authors did not reply to our request for details.

In 2006 the authors of [7] introduced a cover tree inspired by the navigating nets [19] above. This cover tree was especially designed to prove worst-case bounds on the search complexity in the size |R| and the expansion constant c of the reference set R. In 2015 [12, Section 5.3] pointed out that the proof of [7, Theorem 5] estimated the number of iterations in the nearest neighbor search for k = 1 as $O(c^2 \log n)$ and claimed the final complexity $O(c^{12} \log |R|)$ per query point, though the proposed argument guarantees only $O(c^{12}|R|)$. In the case Q = R, the latter crude estimate gives only a quadratic complexity $O(|R|^2)$ for the all k-nearest neighbor search as in a brute-force approach.

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The similar estimate $O(c^2 \log n)$ was used in several papers later: for a dual-tree based allnearest neighbor search [29, Theorem 3.1], for a Minimum Spanning Tree [23, Theorem 5.1], for a fast exact max-kernel search [11, Lemma 5.2]. The current paper fills the first important gap in the literature and rigorously proves new parametrized time complexities in the singletree case. Another forthcoming paper will similarly correct the more advanced cases above.

To avoid any misunderstanding, we should formally define the k-nearest neighbor set $NN_k(q)$, which might contain several points in a singular case when these reference points have equal distances to a query point q.

▶ **Definition 1.1** (k-nearest neighbor set NN_k). Let Q, R be finite subsets of a metric space (X, d). For any points $q \in Q$ and $r \in R$, the neighborhood $N(q; u) = \{p \in R \mid d(q, p) \leq d(q, u)\}$ consists of all points that are non-strictly closer than u to q. For any integer $k \geq 1$, the k-nearest neighbor set $NN_k(q)$ consists of all points $u \in R$ such that the neighborhood size $|N(q; u)| \geq k$ and any other point $v \in R$ with d(v, q) > d(u, q) has a larger neighborhood of size |N(q; v)| > k.

For $Q = R = \{0, 1, 2, 3\}$, the nearest neighbor sets of 0 are $NN_1(0) = \{1\}$, $NN_2(0) = \{2\}$, $NN_3(0) = \{3\}$. Due to the neighborhoods $N(1;0) = \{0, 1, 2\} = N(1;2)$, both sets $NN_1(1) = \{0, 2\} = NN_2(1)$ consist of two points 0, 2 at equal distance to 1. The 3-nearest neighbor set $NN_3(1) = \{3\}$ is a single point. Because of a potential ambiguity of an exact k-nearest neighbor, Problem 1.2 below allows any neighbors within a set $NN_k(q)$. In the above example, point 0 can be chosen as a 1st neighbor of 1, then 2 as a 2nd neighbor of 1, or these neighbors can be found in a different order.

▶ Problem 1.2 (all k-nearest neighbors search). For any finite subsets Q, R in a metric space (X, d) and any integer $k \ge 1$, design an algorithm to exactly find distinct points $p_i \in NN_i(q) \subseteq R$ for all i = 1, ..., k and all points $q \in Q$ such that the total complexity is near linear in $n = \max\{|Q|, |R|\}$ with hidden constant might depend on some structures of Q, R.

To solve Problem 1.2, Definition 2.1 introduces a compressed cover tree $\mathcal{T}(R)$ on any finite set R with a metric d. Definition 2.11 introduces a new concept of the height $|H(\mathcal{T}(R))|$ that is the number of levels including at least one node in $\mathcal{T}(R)$. The new tree $\mathcal{T}(R)$ in the right hand side picture of Fig. 1 has nodes at levels -1, 0, 1, 2, so its height is 4.

Theorem 4.5 will prove that a compressed cover tree $\mathcal{T}(R)$ can be constructed in time $O(c^8 \cdot |H(\mathcal{T}(R))| \cdot |R|)$, where c is an expansion constant depending on R, see Definition 2.4. Then Corollary 6.6 resolves Problem 1.2 in time $O(c^{10} \cdot k \log(k) \cdot \log_2(\Delta(R)) \cdot (|Q| + |R|))$, where $\Delta(R)$ is the aspect ratio (diameter divided by the minimum inter-point distance in \mathbb{R}), see Definition 2.12. Corollary 7.5 will prove a similar parameterized complexity for an $(1 + \epsilon)$ -approximate k-nearest neighbor search. In all cases we carefully analyze the hidden constants and show typical scenarios when these constants are small. Then all complexities are near linear in the key input size $n = \max\{|Q|, |R|\}$.

2 A new compressed cover tree for *k*-nearest neighbor search in any metric space

▶ Definition 2.1 (A compressed cover tree $\mathcal{T}(R)$). Let R be a finite set in an ambient space X with a metric d. A compressed cover tree $\mathcal{T}(R)$ has the vertex set R with a root $r \in R$ and a *level* function $l : R \to \mathbb{Z}$ satisfying the conditions below.

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Figure 2 For any integer $i \ge 2$, the set $R = \{0, 1, 2^i\}$ has at least three compressed cover trees $\mathcal{T}(R)$ satisfying Definition 2.1.

(2.1a) Root condition : the level of the root node r is $l(r) \ge 1 + \max_{n \in \mathbb{R} \setminus \{r\}} l(p)$.

(2.1b) Covering condition: for every non-root node $q \in R \setminus \{r\}$, we select a unique parent p and a level l(q) such that $d(q, p) \leq 2^{l(q)+1}$ and l(q) < l(p); this parent node p has a single link to its *child* node q in the tree $\mathcal{T}(R)$.

(2.1c) Separation condition : for $i \in \mathbb{Z}$, the cover set $C_i = \{p \in R \mid l(p) \geq i\}$ has $d_{\min}(C_i) = \min_{p \in C_i} \min_{q \in C_i \setminus \{p\}} d(p,q) > 2^i$.

Since there is a 1-1 correspondence between all points of R and all nodes of $\mathcal{T}(R)$, the same notation p can refer to a point in the set R or to a node of the tree $\mathcal{T}(R)$. Set $l_{\max} = 1 + \max_{p \in R \setminus \{r\}} l(p)$ and $l_{\min} = \min_{p \in R} l(p)$. For any node $p \in \mathcal{T}(R)$, Children(p) denotes the set consisting of all children of p, including p itself, which will be convenient later.

For any node $p \in \mathcal{T}(R)$, define the *node-to-root* path as a unique sequence of nodes w_0, \ldots, w_m such that $w_0 = p, w_m$ is the root and w_{j+1} is the parent of w_j for all $j = 0, \ldots, m-1$. A node $q \in \mathcal{T}(R)$ is called a *descendant* of another node p if p belongs to the node-to-root path of q. A node p is an *ancestor* of q if q belongs to the node-to-root path of p. The set of all descendants of a node p is denoted by Descendants(p) and includes p.



Figure 3 Compressed cover tree $\mathcal{T}(R)$ built on set R defined in Example 2.2 with root 16.

▶ Example 2.2 ($\mathcal{T}(R)$ in Fig. 3). Let $(\mathbb{R}, d = |x-y|)$ be the real line with euclidean metric. Let $R = \{1, 2, 3, ..., 15\}$ be its finite subset. Fig. 3 shows a compressed cover tree on the set R with the root r = 8. The cover sets of $\mathcal{T}(R)$ are $C_{-1} = \{1, 2, 3, ..., 15\}$, $C_0 = \{2, 4, 6, 8, 10, 12, 14\}$, $C_1 = \{4, 8, 12\}$ and $C_2 = \{8\}$. We check the conditions of Definition 2.1.

Root condition (2.1*a*): since $\max_{p \in R \setminus \{8\}} d(p, 8) = 7$ and $\lceil \log_2(7) \rceil - 1 = 2$, the root can have the level l(8) = 2.



Figure 4 A comparison of past cover trees and a new tree in Example 2.3. Left: an implicit cover tree contains infinite repetitions of points. Middle: an explicit cover tree. Right: a compressed cover tree from Definition 2.1 includes every point exactly once.

■ Covering condition (2.1b) : for any $i \in -1, 0, 1, 2$, let p_i be arbitrary point having $l(p_i) = i$. Then we have $d(p_{-1}, p_0) = 1 \le 2^0$, $d(p_0, p_1) = 2 \le 2^1$ and $d(p_1, p_2) = 4 \le 2^2$. ■ Separation condition (2.1c) : $d_{\min}(C_{-1}) = 1 > \frac{1}{2} = 2^{-1}$, $d_{\min}(C_0) = 2 > 1 = 2^0, d_{\min}(C_1) = 4 > 2 = 2^1$.

A cover tree was defined in [7, Section 2] as a tree version of a navigating net from [19, Section 2.1]. For any index $i \in \mathbb{Z} \cup \{\pm \infty\}$, the level *i* set of this cover tree coincides with the cover set C_i above, which can have nodes at different levels in Definition 2.1. Any point $p \in C_i$ has a single parent in the set C_{i+1} , which satisfied conditions (2.1b,c). [7, Section 2] referred to this original tree as an implicit representation of a cover tree. Such a tree in Figure 4 (left) contains infinitely many repetitions of every point $p \in R$ in long branches and will be called an *implicit cover tree*.

Since an implicit cover tree is formally infinite, for practical implementations, the authors of [7] had to use another version that they named an explicit representation of a cover tree. We call this version an *explicit cover tree*. Here is the full defining quote at the end of [7, Section 2]: "The explicit representation of the tree coalesces all nodes in which the only child is a self-child". In an explicit cover tree, if a subpath of every node-to-root path consists of all identical nodes without other children, all these identical nodes collapse to a single node, see Figure 4 (middle).

Since an explicit cover tree still contains repeated points, Definition 2.1 is well-motivated by the aim to include every point only once, which saves memory and simplifies all subsequent algorithms, see Fig. 4 (right).

▶ Example 2.3 (a short train line tree). Let G be the unoriented metric graph consisting of two vertices r, q connected by three different edges e, h, g of lengths $|e| = 2^6$, $|h| = 2^3$, |g| = 1. Let p_4 be the middle point of the edge e. Let p_3 be the middle point of the subedge (p_4, q) . Let p_2 be the middle point of the edge h. Let p_1 be the middle point of the subedge (p_2, q) . Let $R = \{p_1, p_2, p_3, p_4, r\}$. We construct a compressed cover tree $\mathcal{T}(R)$ by choosing

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the level $l(p_i) = i$ and by setting the root r to be the parent of both p_2 and p_4 , p_4 to be the parent of p_3 , and p_2 to be the parent of p_1 . Then $\mathcal{T}(R)$ satisfies all the conditions of Definition 2.1, see a comparison of the three cover trees in Fig. 4.

In any metric space X, let $\overline{B}(p,t) \subseteq X$ be the closed ball with a center p and a radius t. If this metric space is finite, $|\overline{B}(p,t)|$ denotes the number of points in $\overline{B}(p,t)$. The expansion constant c(R) below was originally defined in [7].

▶ Definition 2.4 (Expansion constants c and c_m). Let R be a finite subset of a space X with a metric d. The expansion constant c(R) is the smallest real number $c(R) \ge 2$ such that $|\bar{B}(p,2t)| \le c(R) \cdot |\bar{B}(p,t)|$ for any $p \in R$ and radius $t \ge 0$. The minimized expansion constant $c_m(R) = \inf_{R \subseteq A \subseteq X} c(A)$ is minimized over all finite sets A that cover R.

▶ Lemma 2.5 (properties of c_m). For any finite sets $R \subseteq U$ in a metric space, we have $c_m(R) \leq c_m(U), c_m(R) \leq c(R)$.

Proof. The proof easily follows from Definition 2.4.



Figure 5 Example 2.6 describes a set R with a big expansion constant c(R). Let $R \setminus \{p\}$ be a finite subset of a unit square lattice in \mathbb{R}^2 , but a point p is located far away from $R \setminus \{p\}$ at a distance larger than diam $(R \setminus \{p\})$. Definition 2.4 implies that c(R) = |R|.

Example 2.6 shows that expansion constant of a set R can be as big as |R|.

▶ **Example 2.6** (one outlier can make the expansion constant big). Let R be a finite metric space and $p \in R$ satisfy $d(p, R \setminus \{t\}) > \operatorname{diam}(R \setminus \{p\})$. Since $\overline{B}(p, 2d(p, R \setminus \{t\}) = R$ and $\overline{B}(p, d(p, R \setminus \{t\}) = \{p\})$, we get c(R) = N, see Fig. 5.

Example 2.7 shows that the minimized expansion can be significantly smaller than the original expansion constant.

▶ Example 2.7 (minimized expansion constants). Let (\mathbb{R}, d) be the Euclidean line. For an integer n > 10, consider the finite sets $R = \{2^i \mid i \in [1, n]\}$ and let $Q = \{i \mid i \in [1, 2^n]\}$. If $0 < \epsilon < 10^{-9}$, then $\overline{B}(2^n, 2^{n-1} - \epsilon) = \{2^n\}$ and $\overline{B}(2^n, 2(2^{n-1} - \epsilon)) = R$, so c(R) = n. For any $q \in Q$ and any $t \in \mathbb{R}$, we have the balls $\overline{B}(q, t) = \mathbb{Z} \cap [q-t, q+t]$ and $\overline{B}(q, 2t) = \mathbb{Z} \cap [q-2t, q+2t]$, so $c(Q) \le 4$. Lemma 2.5 implies that $c_m(R) \le c_m(Q) \le c(Q) \le 4$.

Lemma 2.8 provides an upper bound for a distance between a node and its descendants.

▶ Lemma 2.8 (a distance bound on descendants). Let R be a finite subset of an ambient space X with a metric d. In a compressed cover tree $\mathcal{T}(R)$, let q be any descendant of a node p. Let the node-to-root path S of q contain a node u satisfying $u \in \text{Children}(p) \setminus \{p\}$. Then $d(p,q) \leq 2^{l(u)+2} \leq 2^{l(p)+1}$.



Figure 6 This volume argument proves Lemma 2.9. By using an expansion constant, we can find an upper bound for the number of smaller balls of radius $\frac{\delta}{2}$ that can fit inside a larger $\bar{B}(p,t)$.

Proof. Let $(w_0, ..., w_m)$ be a subpath of the node-to-root path for $w_0 = q$, $w_{m-1} = u$, $w_m = p$. Then $d(w_i, w_{i+1}) \leq 2^{l(w_i)+1}$ for any *i*. The first required inequality follows from the triangle inequality below:

$$d(p,q) \le \sum_{j=0}^{m-1} d(w_j, w_{j+1}) \le \sum_{j=0}^{m-1} 2^{l(w_j)+1} \le \sum_{t=l_{\min}}^{l(u)+1} 2^t \le 2^{l(u)+2}$$

Finally, $l(u) \le l(p) - 1$ implies that $d(p,q) \le 2^{l(p)+1}$.

Lemma 2.9 uses the idea of [10, Lemma 1] to show that if S is a δ -sparse subset of a metric space X, then S has at most $(c_m(S))^{\mu}$ points in the ball $\overline{B}(p,r)$, where $c_m(S)$ is the minimized expansion constant of S, while μ depends on δ, r .

▶ Lemma 2.9 (packing). Let S be a finite δ -sparse set in a metric space (X, d), so $d(a, b) > \delta$ for all $a, b \in S$. Then, for any point $p \in X$ and any radius $t > \delta$, we have $|\bar{B}(p, t) \cap S| \leq (c_m(S))^{\mu}$, where $\mu = \lceil \log_2(\frac{4t}{\delta} + 1) \rceil$.

Proof. Assume that d(p,q) > t for any point $q \in S$. Then $\overline{B}(p,t) \cap S = \emptyset$ and the lemma holds trivially. Otherwise $\overline{B}(p,t) \cap S$ is non-empty. By Definition 2.4 of a minimized expansion constant, for any $\epsilon > 0$, we can always find a set A such that $S \subseteq A \subseteq X$ and

$$|B(q,2s) \cap A| \le (c_m(S) + \epsilon) \cdot |B(q,s) \cap A| \tag{1}$$

for any $q \in A$ and $s \in \mathbb{R}$. Note that for any $u \in \overline{B}(p,t) \cap S$ we have $\overline{B}(u, \frac{\delta}{2}) \subseteq \overline{B}(u, t + \frac{\delta}{2})$. Therefore, for any point $q \in \overline{B}(p,t) \cap S$, we get

$$\bigcup_{e \in \bar{B}(p,t) \cap S} \bar{B}(u,\frac{\delta}{2}) \subseteq \bar{B}(p,t+\frac{\delta}{2}) \subseteq \bar{B}(q,2t+\frac{\delta}{2})$$

Since all the points of S were separated by δ , we have

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$$|\bar{B}(p,t)\cap S|\cdot \min_{u\in\bar{B}(p,t)\cap S}|\bar{B}(u,\frac{\delta}{2})\cap A| \leq \sum_{u\in\bar{B}(p,t)\cap S}|\bar{B}(u,\frac{\delta}{2})\cap A| \leq |\bar{B}(q,2t+\frac{\delta}{2})\cap A|$$

In particular, by setting $q = \operatorname{argmin}_{a \in S \cap \overline{B}(p,t)} |\overline{B}(a, \frac{\delta}{2})|$, we get:

$$|\bar{B}(p,t) \cap S| \cdot |\bar{B}(q,\frac{\delta}{2}) \cap A| \le |\bar{B}(q,2t+\frac{\delta}{2}) \cap A|$$

$$\tag{2}$$

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Inequality (1) applied μ times for the radii $s_i = \frac{2t + \frac{\delta}{2}}{2^i}$, $i = 1, ..., \mu$, implies that:

$$|\bar{B}(q,2t+\frac{\delta}{2})\cap A| \le (c_m(S)+\epsilon)^{\mu}|\bar{B}(q,\frac{2t+\frac{\delta}{2}}{2^{\mu}})\cap A| \le (c_m(S)+\epsilon)^{\mu}|\bar{B}(q,\frac{\delta}{2})\cap A|.$$
 (3)

By combining inequalities (2) and (3), we get

$$|\bar{B}(p,t) \cap S| \le \frac{|\bar{B}(q,2t+\frac{\delta}{2}) \cap A|}{|\bar{B}(q,\frac{\delta}{2}) \cap A|} \le (c_m(S)+\epsilon)^{\mu}.$$

The required inequality is obtained by letting $\epsilon \to 0$.

[19, Section 1.1] defined dim(X) of a space (X, d) as the minimum number m such that every set $U \subseteq X$ can be covered by 2^m sets whose diameter is a half of the diameter of U. If U is finite, an easy application of Lemma 2.9 for $\delta = \frac{r}{2}$ shows that dim $(X) \leq \sup_{A \subseteq X} (c_m(A))^4 \leq \sup_{A \subseteq X} (c_m(A))^4$, where A and B are finite subsets of X.

Let T(R) be an implicit cover tree of [7] on a finite set R. [7, Lemma 4.1] showed that the number of children of any node $p \in T(R)$ has the upper bound $(c(R))^4$. Lemma 2.10 generalizes [7, Lemma 4.1] for a compressed cover tree.

▶ Lemma 2.10 (width bound). Let R be a finite subset of a metric space (X, d). For any compressed cover tree $\mathcal{T}(R)$, any node p has at most $(c_m(R))^4$ children at every level i, where $c_m(R)$ is the minimized expansion constant of the set R.

Proof. By the covering condition of $\mathcal{T}(R)$, any child q of p located on the level i has $d(q,p) \leq 2^{i+1}$. Then the number of children of the node p at level i at most $|\bar{B}(p,2^{i+1})|$. The separation condition in Definition 2.1 implies that the set C_i is a 2^i -sparse subset of X. We apply Lemma 2.9 for $t = 2^{i+1}$ and $\delta = 2^i$. Since $4 \cdot \frac{t}{\delta} + 1 \leq 4 \cdot 2 + 1 \leq 2^4$, we get $|\bar{B}(q,2^{i+1}) \cap C_i| \leq (c_m(C_i))^4$. Lemma 2.5 implies that $(c_m(C_i))^4 \leq (c_m(R))^4$, so the upper bound is proved.

In the original work [7], the *explicit depth* of a single point in a cover tree was defined in this quote: "explicit depth of any point p, defined as the number of explicit grandparent nodes on the path from the root to node p in the lowest level in which p is explicit". [7, Lemma 4.3] showed that the depth of any node p has an upper bound $O(c^2 \log |R|)$.

Example 3.1 demonstrates that, for any $m \in \mathbb{Z}_+$, there is a set R whose compressed cover tree $\mathcal{T}(R)$ has m^2 levels, but the explicit depth of any node is at most 2m + 1 by Lemma 3.3. Counterexample 3.5 and Counterexample 3.7 proves that the explicit depth cannot be used to estimate the complexities of [7, Algorithms 1 and 2], respectively. Therefore a new concept of the height $|H(\mathcal{T})|$ was needed to justify a new near linear parameterized complexity in Theorem 6.5.

▶ Definition 2.11 (the height of a compressed cover tree). For a compressed cover tree $\mathcal{T}(R)$ on a finite set R, the *height set* is $H(\mathcal{T}(R)) = \{l_{\max}, l_{\min}\} \cup \{i \mid C_{i-1} \setminus C_i \neq \emptyset\}$. The size $|H(\mathcal{T}(R))|$ of this set is called the *height* of $\mathcal{T}(R)$.

By condition (2.1b), the height $|H(\mathcal{T}(R))|$ counts the number of levels *i* whose cover sets C_i include new points that were absent on higher levels. Since any point can appear alone at its own level, $|H(\mathcal{T})| \leq |R|$ is the worst case upper bound of the height. The following parameters help prove an upper bound for the height $|H(\mathcal{T}(R))|$ in Lemma 2.13.

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▶ Definition 2.12 (diameter and aspect ratio of a reference set R). For any finite metric set R with a metric d, the diameter is diam $(R) = \max_{p \in R} \max_{q \in R} d(p,q)$. The aspect ratio [19] is $\Delta(R) = \frac{\operatorname{diam}(R)}{d_{\min}(R)}$.

▶ Lemma 2.13 (upper bound of height $|H(\mathcal{T}(R))|$). Any finite set R has the upper bound $|H(\mathcal{T}(R))| \leq 1 + \log_2(\Delta(R))$.

Proof. We have $|H(\mathcal{T}(R))| \leq l_{\max} - l_{\min} + 1$ by Definition 2.11. We estimate $l_{\max} - l_{\min}$ as follows.

Let $p \in R$ be a point such that $\operatorname{diam}(R) = \max_{q \in R} d(p, q)$. Then R is covered by the closed ball $\overline{B}(p; \operatorname{diam}(R))$. Hence the cover set C_i at the level $i = \log_2(\operatorname{diam}(R))$ consists of a single point p. The separation condition in Definition 2.1 implies that $l_{\max} \leq \log_2(d_{\max}(R))$. Since any distinct points $p, q \in R$ have $d(p, q) \geq d_{\min}(R)$, the covering condition implies that no new points can enter the cover set C_i at the level $i = [\log_2(d_{\min}(R))]$, so $l_{\min} \geq \log_2(d_{\min}(R))$. Then $|H(\mathcal{T}(R))| \leq 1 + l_{\max} - l_{\min} \leq 1 + \log_2(\frac{\operatorname{diam}(R)}{d_{\min}(R)})$.

If the aspect ratio $\Delta(R) = O(\text{Poly}(|R|))$ polynomially depends on the size |R|, then $|H(\mathcal{T}(R))| \leq O(\log(|R|))$.

3 Challenging data for implicit cover trees

In this section we show that all the main results of [7] require more justifications. Counterexample 3.5 shows a gap in the proof for the complexity of the Insert algorithm for an implicit cover tree [7, Theorem 6]. Counterexample 3.7 shows another gap in the proof of [7, Theorem 5], which gives an upper bound for the complexity of Algorithm 3.6. Both counterexamples are based on Example 3.1, which extends Example 2.3.

▶ **Example 3.1** (tall imbalanced tree). For any integer m > 10, let G be a metric graph pictured in Figure 7 that has two vertices r, q and m + 1 edges (e_i) for $i \in \{0, ..., m\}$, and the length of each edge e_i is $|e_i| = 2^{m \cdot i + 2}$ for $i \ge 1$. Finally, set $|e_0| = 1$. For every $i \in \{1, ..., m^2\}$ if i is divisible by m we set p_i be the middle point of $e_{i/m}$ and for every other i we define p_i to be the middle point of segment (p_{i+1}, q) .

Let d be the induced shortest path metric on the continuous graph G. Then d(q, r) = 1, $d(r, p_i) = 2^{i+1} + 1$, $d(q, p_i) = 2^i$ and if i > j and $\lceil \frac{i}{m} \rceil = \lceil \frac{j}{m} \rceil$ we have $d(p_j, p_i) = \sum_{t=j+1}^i 2^t$. We consider the reference set $R = \{r\} \cup \{p_i \mid i \in \{1, 2, 3, ..., m^2\}\}$ with the metric d.

Let us define a compressed cover tree $\mathcal{T}(R)$ by setting r to be the root node and $l(p_i) = i$ for all i. If i is divisible by m, we set r to be the parent of p_i . If i is not divisible by m, we set p_{i+1} to be the parent of p_i . For every i divisible by m, the point p_i is in the middle of edge $e_{i/m}$, hence $d(p_i, r) \leq 2^{i+1}$. For every i not divisible by m, by the definition p_i is middle point of (p_{i+1}, q) and therefore we have $d(p_i, p_{i+1}) \leq 2^{i+1}$. Since for any point p_i distance to its parent is at most 2^{i+1} , it follows that $\mathcal{T}(R)$ satisfies the covering condition of Definition 2.1.

For any integer t, the cover set is $C_t = \{r\} \cup \{p_i \mid i \ge t\}$. We will prove that C_t satisfies the separation condition. Let $p_i \in C_t$. If i is divisible by m, then $d(r, p_i) = 2^{i+1} \ge 2^{t+1} > 2^t$. If i is not divisible by m, then $d(r, p_i) = d(r, q) + d(q, p_i) = 1 + 2^{i+1} > 2^t$.

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Then the root r is separated from the other points by the distance 2^t . Consider arbitrary points p_i and p_j with indices $i > j \ge t$ and $\lceil \frac{i}{m} \rceil = \lceil \frac{j}{m} \rceil$. Then

$$d(p_i, p_j) = \sum_{s=j+1}^{i} 2^s \ge 2^{j+1} \ge 2^{t+1} > 2^t.$$

On the other hand, if $i > j \ge t$ and $\lceil \frac{i}{m} \rceil \neq \lceil \frac{j}{m} \rceil$, then

$$d(p_i, p_j) = d(p_i, q) + d(p_j, q) \ge 2^i + 2^j \ge 2^{j+1} \ge 2^{t+1} > 2^t.$$

For any t, we have shown that all pairwise combinations of points of C_t satisfy the separation condition in Definition 2.1. Hence this condition holds for the whole tree $\mathcal{T}(R)$.

Recall that in [7, Section 2] the explicit representation of cover tree was defined as "the explicit representation of the tree coalesces all nodes in which the only child is a self-child". Simplest way to interpret this is to consider cover sets C_i and define $p \in C_i$ to be an explicit node, if p has child at level i - 1. By [7, Lemma 4.3] depth of any node p is "defined as the number of explicit grandparent nodes on the path from the root to p in the lowest level in which p is explicit". Explicit depth of a node p in any compressed tree \mathcal{T} will be defined in Definition 3.2 using the simplest interpretation of the aforementioned quotes.

▶ Lemma 3.2 (Explicit depth for compressed cover tree). Let R be a finite subset of a metric space with a metric d. Let $\mathcal{T}(R)$ be a compressed cover tree on R. For any $p \in \mathcal{T}(R)$, let $s = (w_0, ..., w_m)$ be a node-to-root path of p. Then the explicit depth D(p) of node p belonging to compressed cover tree can be interpreted as the sum

$$D(p) = \sum_{i=0}^{m-1} |\{q \in \text{Children}(w_{i+1}) \mid l(q) \in [l(w_i), l(w_{i+1}) - 1]\}|.$$

Proof. Note that the node-to-root path of an implicit cover tree on R has $l(w_{j+1}) - l(w_j) - 1$ extra copies of w_{j+1} between every w_j and w_{j+1} for any index $j \in [0, m-1]$. Recall that a node is called explicit, if it has non-trivial children. Therefore there will be exactly

$$|\{q \in \text{Children}(w_{i+1}) \mid l(q) \in [l(w_i), l(w_{i+1}) - 1]\}|$$

explicit nodes between w_j and w_{j+1} . It remains to take the total sum.

▶ Lemma 3.3. Let $\mathcal{T}(R)$ be a compressed cover tree on the set R from Example 3.1 for some $m \in \mathbb{Z}$. For any $p \in R$, the explicit depth D(p) of Definition 3.2 has the upper bound 2m + 1.

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Proof. For any p_i , if *i* is divisible by *m*, then *r* is the parent of p_i . By definition, the explicit depth is $D(p_i) = |\{p \in \text{Children}(r) \mid l(p) \in [l(p_i), m^2]\}|$. Since *r* contains children on every level *j*, where *j* is divisible by *m*, we have $D(p_i) = m - \frac{i}{m} + 1$.

Let us now consider an index *i* that is not divisible by *m*. Note that p_{j+1} is the parent of p_j for all $j \in [i, m \cdot \lceil i/m \rceil - 1]$. Then the path consisting of all ancestors of p_i from p_i to the root node *r* has the form $(p_i, p_{i+1}, ..., p_{m \cdot \lceil i/m \rceil}, r)$. It follows that

$$D(p_i) = \sum_{j=i}^{m \cdot \lceil i/m \rceil - 1} |\{p \in \text{Children}(p_j) \mid l(p) \in [l(p_j), l(p_{j+1}) - 1]\}| + D(p_{m \cdot \lceil i/m \rceil}).$$



Figure 7 Illustration of a graph G and a point cloud R defined in Example 3.1

Since $i \ge m \cdot (\lceil i/m \rceil - 1) + 1$ and $\lceil i/m \rceil \ge 1$, we get the required upper bound:

$$D(p_i) = (m \cdot \lceil i/m \rceil - i) + (m - \lceil i/m \rceil + 1) \le m + (m + 1) = 2m + 1.$$

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- 1: **Insert**(point p, cover set Q_i , level i)
- 2: Set $Q = \{ \text{Children}(q) \mid q \in Q_i \}$
- 3: if $d(p,Q) > 2^i$ then
- 4: **return** "no parent found"
- 5: else

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- 6: Set $Q_{i-1} = \{q \in Q \mid d(p,q) \le 2^i\}$
- 7: **if** $\mathbf{Insert}(p, Q_{i-1}, i-1) =$ "no parent found" and $d(p, Q_i) \leq 2^i$ then
- 8: Pick $q \in Q_i$ satisfying $d(p,q) \le 2^i$ and insert p into Children(q), return "parent found"
- 9: **else**
- 10: **return** "no parent found"
- 11: end if
- 12: end if

Algorithm 3.4 Original Insert() algorithm for inserting point p into an implicit cover tree T [7, Algorithm 2]. This algorithm is launched with $i = l_{\text{max}}$ and $Q_i = \{r\}$, where r is the root node of T.

► **Counterexample 3.5** (Counterexample for a step in the proof of [7, Theorem 6]). First we cite a part of the proof of [7, Theorem 6].

"**Theorem 6** Any insertion or removal takes time at most $O(c^6 \log(n))$ " [In other words the run time of Algorithm 3.4 is $O(c^6 \log(n))$, where n is the number points of original dataset S on which tree T was constructed.]

[Partial proof:]: " Let $k = c^2 \log(|S|)$ be the maximum explicit depth of any point, given by Lemma 4.3. Then the total number of cover sets with explicit nodes is at most 3k + k = 4k, where the first term follows from the fact that any node that is not removed must be explicit at least once every three iterations, and the additional k accounts for a single point that may be implicit for many iterations. Thus the total amount of work in Steps 1 [Our line 2] and 2 [Our lines 3-5] is proportional to $O(k \cdot \max_i |Q_i|)$. Step 3 [Our lines 5-11] requires work no greater than step 1 [Our line 2]."



Figure 8 Illustration of the a compressed cover tree $\mathcal{T}(R)$ defined in Example 3.1

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In other words the above arguments says that the total number of times line 1 [our line 2] was called during the algorithm has the upper bound $4 \cdot \max_{p \in R} D(p)$, where D(p) is the explicit depth of a point p, see Definition 3.2. Take the reference set R, the compressed cover tree $\mathcal{T}(R)$ and the point q from Example 3.1 for any parameter m > 200. Assume that we have already constructed tree $\mathcal{T}(R)$. Let us show that $\mathcal{T}(R \cup q)$ constructed by Algorithm 3.4 from the input $q, i = m^2 + 1, Q_i = \{r\}$ runs at least $m^2 - 2$ self-recursions. This will lead to a contradiction since by Lemma 3.3 any node $p \in \mathcal{T}(R)$ has $D(p) \leq 2m + 1$.

We show by induction on m going down that, for every step $i \in [1, m^2]$, we have $Q_i = \{r, p_i\}$. The proof for the base case $i = m^2$ is similar to the induction step and thus will be omitted. Assume that Q_i has the desired form for some i. Let us show that the claim holds for i - 1. For all levels i - 1 divisible by m, the node p_{i-1} is a child of the root r. For all levels i - 1 not divisible by m, the node p_i is a child of p_i . Since $\mathcal{T}(R)$ contains exactly one node at each level, in both cases we have $Q = \{r, p_i, p_{i-1}\}$. Since d(q, r) = 1, $d(q, p_i) = 2^{i+1}$ and $d(q, p_{i-1}) = 2^i$ we have

$$Q_{i-1} = \{ p \in Q_i \mid d(p,q) \le 2^i \} = \{r, p_i\}.$$

The actual implementation of algorithm 3.4 iterates over all levels *i* for which there exists a node in Q_i that contains at least one non-trivial child on level i - 1 and for which the condition in line 7 is satisfied. Since for every index $i \in [2, m^2 + 1]$ we have $Q_i = \{r, p_i\}$ and since either *r* or p_i has a child at level i - 1 and the condition in line 7 is always satisfied, it follows that $m^2 - 2$ is a low bound for the number ξ of self-recursions. Therefore the contradiction follows from the inequality:

$$m^2 - 2 \le \xi \le 4 \cdot \max_{p \in R} D(p) \le 8 \cdot (2m+1) \le 16 \cdot m + 8$$

where m > 20.

- 1: **Input** : implicit cover tree T, a query point p
- 2: Set $Q_{\infty} = C_{\infty}$ where C_{∞} is the root level of T
- 3: for *i* from ∞ down to $-\infty$ do
- 4: Set $Q = \{ \text{Children}(q) \mid q \in Q_i \}.$
- 5: Form cover set $Q_{i-1} = \{q \in Q \mid d(p,q) \le d(p,Q) + 2^i\}$
- 6: end for
- 7: return $\operatorname{argmin}_{q \in Q_{-\infty}} d(p,q)$

■ Algorithm 3.6 Original [7, Algorithm 1] based on an implicit cover tree T [7, Section 2] for nearest neighborhood search, which is used in Counterexample 3.7. The children of a node q of an implicit cover tree are defined as the nodes at one level below q that have q as their parent. In the actual implementationm the loop in lines 3-6 runs only for the levels containing nodes with non-trivial children (not coinciding with their parents). The level $+\infty$ can be replaced by $l_{\max}(T)$ and $-\infty$ can be replaced by $l_{\min}(T)$ in the code.

▶ **Counterexample 3.7** (Counterexample for a step in the proof of [7, Theorem 5]). We cite a part of the proof of [7, Theorem 5].

"Theorem 5 If the dataset $S \cup \{p\}$ has expansion constant c, the nearest neighbor of p can be found in time $O(c^{12}\log(n))$." [Partial proof:] "Let Q^* be the last Q considered by the Algorithm 3.6 (so Q^* consists only of lead nodes with scale $-\infty$). Lemma 4.3 bounds the explicit depth of any node in the tree (and in particular any node in Q^*) by $k = O(c^2 \log(N))$. Consequently the number of iterations is at most $k|Q^*| \leq k \max_i |Q_i|$."

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In other words, the above argument claims that the total number ξ of times when Algorithm 3.6 runs lines 3-6 has an upper bound

$$\xi \le \max_{p \in R} D(p) \cdot \max_i |Q_i|.$$

Take $R, \mathcal{T}(R)$ and q from Example 3.1. We will apply Algorithm 3.6 to the tree $\mathcal{T}(R)$ and query point q. By Lemma 3.3 the cover tree $\mathcal{T}(R)$ having parameter m has $D(p) \leq 2m + 1$ for all $p \in R$. A contradiction to the original argument will follow after showing that max $|Q_i| \leq 2$ and $\xi \geq m^2 - 2$.

Let us first estimate $\max_i |Q_i|$. Similarly to Counterexample 3.5 we will show that, for every iteration (lines 3-5) $i \in [1, m^2]$ of Algorithm 3.6, we have $Q_i = \{r, p_i\}$. The proof for the basecase $i = m^2$ is similar to the induction step and thus will be omitted. Assume that Q_i has the desired form for some *i*. Let us show that the claim holds for i - 1. For all levels i - 1 divisible by *m*, the node p_{i-1} is a child of the root *r*. For all levels i - 1 not divisible by *m*, the node p_{i-1} is a child of p_i . Since $\mathcal{T}(R)$ contains exactly one node at each level, in both cases we have $Q = \{r, p_i.p_{i-1}\}$. Since d(q, r) = 1, $d(q, p_i) = 2^{i+1}$ and $d(q, p_{i-1}) = 2^i$, we have

$$Q_{i-1} = \{ p \in Q_t \mid d(p,q) \le 2^i + 1 \} = \{ r, p_i \}$$

Therefore it follows that $|Q_i| \leq 2$ for all $i \in [1, m^2]$.

The actual implementation of algorithm 3.6 iterates over all levels i for which there exists a node in Q_i containing at least one non-trivial child at level i - 1. Since $Q_i = \{r, p_i\}$ and for every index $i \in [2, m^2 + 1]$, either r or p_i has a child on level i - 1, it follows that $m^2 - 2$ is a low bound for the number ξ of iterations. A contradiction follows from

$$m^2 - 2 \le \xi \le \max_{p \in R} D(p) \cdot \max_i |Q_i| \le (2m+1) \cdot 2 \le 4m+2$$
 for any $m > 20$.

4 Building a compressed cover tree with a near linear parameterized complexity

In this section main Theorem 4.5 will correct the complexity in [7, Theorem 6] whose proof discussed in Counterexample 3.5.

▶ Definition 4.1 (Children(p, i) and Next $(p, i, \mathcal{T}(R))$ for a compressed cover tree). In a compressed cover tree $\mathcal{T}(R)$ on a set R, for any level i and a node $p \in R$, set Children $(p, i) = \{a \in \text{Children}(p) \mid l(a) = i\}$. Let Next $(p, i, \mathcal{T}(R))$ be the maximal level j satisfying j < i and Children $(p, i) \neq \emptyset$. If such level does not exist we set $j = l_{\min}(\mathcal{T}(R)) - 1$. For every node p, we store its set of children in a linked hash map so that

- (1) any key *i* gives access to Children(p, i),
- (2) every Children(p, i) has access to Children $(p, Next(p, i, \mathcal{T}(R)))$,
- (3) we can directly access $\max\{j \mid \text{Children}(p, j) \neq \emptyset\}$.

Let R be a finite subset of a metric space (X, d). A compressed cover tree $\mathcal{T}(R)$ will be incrementally constructed by adding points one by one as summarized in Algorithm 4.2. First we select a root node $r \in R$ and form a tree $\mathcal{T}(\{r\})$ of a single node r at the level $l_{\max} = l_{\min} = +\infty$. Assume that we have a compressed cover tree $\mathcal{T}(W)$ for a subset $W \subset R$. For any point $p \in R \setminus W$, Algorithm 4.3 builds a larger compressed cover tree $\mathcal{T}(W \cup \{p\})$ from $\mathcal{T}(W)$.

- 1: **Input** : a finite subset R of a metric space (X, d)
- 2: **Output** : a compressed cover tree $\mathcal{T}(R)$.
- 3: Choose a random point $r \in R$ to be a root of $\mathcal{T}(R)$
- 4: Build the initial compressed cover tree $\mathcal{T} = \mathcal{T}(\{r\})$ by making $l(r) = +\infty$.
- 5: for $p \in R \setminus \{r\}$ do
- 6: $\mathcal{T} \leftarrow \text{run AddPoint}(\mathcal{T}, p)$ described in Algorithm 4.3.
- 7: end for
- 8: For root r of \mathcal{T} set $l(r) = 1 + \max_{p \in R \setminus \{r\}} l(p)$
- 9: **Return** a compressed cover tree \mathcal{T} built on the set R.

Algorithm 4.2 Building a compressed cover tree $\mathcal{T}(R)$ from Definition 2.1 for a finite metric space (R, d).

- 1: Function AddPoint(a compressed cover tree $\mathcal{T}(W)$ with a root r for a finite subset $W \subseteq X$, a point $p \in X$)
- 2: **Output** : compressed cover tree $\mathcal{T}(W \cup \{p\})$.
- 3: Set $i \leftarrow l_{\max}(\mathcal{T}(R))$ {If the root r has no children l_{\max} is undefined, then $i \leftarrow -\infty$ }
- 4: Set $m \leftarrow \max_{j \le i} \{ j \mid d(p, R_i) > 2^j \}$
- 5: Set $R_i \leftarrow \{r\}, i' \leftarrow +\infty$
- 6: while $m \leq i \operatorname{do}$
- 7: Set $C(R_i) \leftarrow \{a \in \text{Children}(p) \text{ for some } p \in R_i \mid l(a) \ge i 1\}$ {Recall that Children(p) contains node p }
- 8: Set $R_{i-1} = \{a \in \mathcal{C}(R_i) \mid d(p,a) \le 2^i\}$
- 9: $t = \max_{a \in R_{i-1}} \operatorname{Next}(a, i 1, \mathcal{T}(W))$ {If R_{i-1} is empty or it has no children we set $t = -\infty$ }
- 10: Set $m = \max_{j \le i-1} \{ j \mid d(p, R_{i-1}) > 2^j \}$
- 11: Set $R_{t+1} \leftarrow R_i$, $i' \leftarrow i$ and $i \leftarrow t+1$ {if $t = -\infty$, then $t+1 = -\infty$ }
- 12: end while

13: Set
$$j \leftarrow \begin{cases} i & \text{if } R_i \neq \emptyset \\ i' & \text{else} \end{cases}$$

- 14: Pick $a \in R_j$ minimizing d(p, a).
- 15: Set l(p) = m and define a to be the parent of p

Algorithm 4.3 This algorithm building $\mathcal{T}(W \cup \{p\})$ from $\mathcal{T}(W)$ runs in the main loop (lines 3-5) of Algorithm 4.2.

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Note that during construction of the compressed cover tree in Algorithm 4.3 we write down additional information for every node p, which includes number of descendants of node p and the maximal level of nodes in set Children(p).

► Theorem 4.4 (correctness of Algorithm 4.2). Algorithm 4.2 builds a compressed cover tree satisfying Definition 2.1.

Proof. It suffices to prove that Algorithm 4.3 correctly extends a compressed cover tree $\mathcal{T}(W)$ for any finite subset $W \subseteq X$ by adding a point p. Let C_i be the *i*-th cover set of $\mathcal{T}(W)$. Since d(p, W) > 0, the integer m from line 10 is always well-defined. Since $\mathcal{T}(W)$ is a finite tree, it will run out of children at a finite level l_{\min} . Thus the condition $m \leq i$ of the while loop (lines 6 - 12) will be satisfied at some point of the iteration and the algorithm will terminate.

It remains to prove that $\mathcal{T}(W \cup \{p\})$ satisfies Definition 2.1. The parent of p is selected at the end (lines 13 - 15) reached only when u > t. By definition of m in line 10 we have $d(p, R_{i-1}) \leq 2^{m+1}$. Therefore a node $v \in R_i$ that minimizes the distance $d(v, R_{i-1})$ satisfies $d(p, v) \leq 2^{m+1}$. Since the rest of tree is unchanged, condition (2.1b) holds.

To check (2.1c), let $r \in C_h$ be any other node for $h \leq l(p)$. Let q be a node that has the lowest index j over all ancestor of r that is contained in some set R_j . If j = i - 1 in the last iteration (lines 6 - 12) of input p, then the separation condition is satisfies trivially by definition of u on line 10. Otherwise $q \in R_j \setminus R_{j-1}$ and thus $d(p,q) > 2^j$. Since q is an ancestor of r there is a chain of nodes (a_t) satisfying $a_0 = r$ and $a_m = q$ so that for all $s \in [0, m - 1]$ node a_{s+1} is parent of a_s . Since $l(r) \geq h$ we know that $l(a_1) \geq h + 1$, generally $l(a_s) \geq h + s$ for any $s \in [0, m - 1]$. Then $d(q, r) \leq \sum_{s=0}^{m-1} d(a_s, a_{s+1}) \leq \sum_{s=0}^{m-1} 2^{h+s} \leq \sum_{s=h+1}^{j-1} 2^x = (2^j - 2^{h+1})$. The triangle inequality gives $d(p, r) \geq d(p, q) - d(q, r) > 2^j - (2^j - 2^{h+1}) \geq 2^{h+1}$, then $d(p, r) > 2^h$. Since r was arbitrarily, we get $d(C_h, p) > 2^h$, therefore (2.1c) holds.

To correct [7, Theorem 6] in Theorem 4.5, the depth estimate $O(c^2 \log n)$ is replaced by the concept of the height $|H(\mathcal{T}(R))|$, which has the upper bound $O(\log_2(\Delta(R)))$ in Lemma 2.13, where $\Delta(R)$ is the aspect ratio of a set R.

Additionally, another step in the past proof of [7, Theorem 6] estimated the complexity of line 1 of [7, Algorithm 2], corresponding to line 7 of Algorithm 4.3 as $c(R)^4$. However, since $C(R_i)$ is children set of R_i we should have $|C(R_i)| \leq c_m(R)^4 \max_i |R_i|$. In the proof of Theorem 4.5 it is shown that $\max_i |R_i| \leq c_m(R)^4$, therefore our new estimate shows that $|C(R_i)| \leq c_m(R)^8$, instead of original estimate $c(R)^4$.

▶ Theorem 4.5 (complexity of a compressed cover tree). Let R be a finite subset of a metric space (X, d). Algorithm 4.2 builds a compressed cover tree $\mathcal{T}(R)$ with a height $|H(\mathcal{T}(R))|$ from Definition 2.11 in time $O((c_m(R))^8 \cdot |H(\mathcal{T}(R))| \cdot |R|)$, where $c_m(R)$ is the minimized expansion constant from Definition 2.4.

Proof. The complexity of Algorithm 4.2 is dominated by lines 3-5 which call Algorithm 4.3 O(|R|) times.

Assume that we have already constructed a cover tree on set $\mathcal{T}(W)$, the goal Algorithm 4.3 is to construct tree $\mathcal{T}(W \cup \{p\})$ for some $p \in R \setminus W$. Since $\mathcal{T}(R)$ can have a chain-like structure, in worst case loop determined by lines 6-12 is performed $|H(\mathcal{T}(R))|$ times. By Lemma 2.10 since $W \subseteq R \subseteq X$ we have $|\mathcal{C}(R_i)| \leq c_m(W)^4 |R_i| \leq c_m(R)^4 |R_i|$ nodes, where $\mathcal{C}(R_i)$ is defined in line 7. Therefore both, lines 8 and 7 take at most $c^4 |R_i|$ time. In line 9 we



Figure 9 Consider a compressed cover tree $\mathcal{T}(R)$ that was built on set $R = \{1, 2, 3, 4, 5, 7, 8\}$. Let $\mathcal{S}_i(p, \mathcal{T}(R))$ be a distinctive descendant set of Definition 5.1. Then $V_2(1) = \emptyset, V_1(1) = \{5\}$ and $V_0(1) = \{3, 5, 7\}$. And also $\mathcal{S}_2(1, \mathcal{T}(R)) = \{1, 2, 3, 4, 5, 7, 8\}$, $\mathcal{S}_1(1, \mathcal{T}(R)) = \{1, 2, 3, 4\}$ and $\mathcal{S}_0(1, \mathcal{T}(R)) = \{1\}$.

handle $|R_{i-1}|$ elements, for each of them we can retrieve index Next $(a, i-1, \mathcal{T}(W))$ in O(1) time, since for every $a \in \mathcal{T}(R)$ we can update the last index j, when a had children on level j in line 7. Therefore line 9 takes at most $O(|R_i|)$ time. Line 10 can be computed in time $O(|R_i|)$. Let us now bound the maximal size of R_i during whole run-time of the algorithm.

Note that $R_{i-1} \subseteq B(p, 2^i) \cap C_{i-1}$ where C_{i-1} is a i-1th cover set of $\mathcal{T}(R)$. Since C_{i-1} is 2^{i-1} -spares subset of R we can apply packing Lemma 2.9 with $r = 2^i$ and $\delta = 2^{i-1}$ to obtain $|B(p, 2^i) \cap C_{i-1}| \leq (c_m(W))^4$. Lemma 2.5 implies $(c_m(W))^4 \leq (c_m(R))^4$, therefore $|B(p, 2^i) \cap C_{i-1}| \leq (c_m(R))^4$.

The complexity of Algorithm 4.3 is dominated by line 7 that has time $O(|C(R_i)|) \leq O((c_m(R))^4 \max_i |R_i|) \leq O((c_m(R))^8)$. Then the whole Algorithm 4.2 has time $O((c_m(R))^8 \cdot |H(\mathcal{T}(R))| \cdot |R|)$ as desired.

5 Distinctive descendant set

In this section we introduce auxiliary concepts for the future. The main concept of this Section is distinctive descendant set of Definition 5.1. Distinctive descendant set at a level iof a node $p \in \mathcal{T}(R)$ in a compressed cover tree corresponds to set of descendants of a copy of node p at level i in the original implicit cover tree T(R).

Other important concepts are λ -point of Definition 5.7 that is used in Algorithm 6.1 as an approximation for k-nearest neighboring point. Its β -point property of Lemma 5.15 that play a major role in the proof of the main time complexity result Theorem 6.5.

▶ Definition 5.1 (Distinctive descendant sets). Let $R \subseteq X$ be a finite reference set with a cover tree $\mathcal{T}(R)$. For any node $p \in \mathcal{T}(R)$ in a compressed cove tree on a finite set Rand $i \leq l(p) - 1$, set $V_i(p) = \{u \in \text{Descendants}(p) \mid i \leq l(u) \leq l(p) - 1\}$. If $i \geq l(p)$, then set $V_i(p) = \emptyset$. For any level $i \leq l(p)$, the distinctive descendant set is $\mathcal{S}_i(p, \mathcal{T}(R)) =$ Descendants $(p) \setminus \bigcup_{u \in V_i(p)} \text{Descendants}(u)$ and has the size $|\mathcal{S}_i(p, \mathcal{T}(R))|$.

▶ Lemma 5.2 (Distinctive descendant set inclusion property). In conditions of Definition 5.1 let $p \in R$ and let i, j be integers satisfying $l_{\min}(\mathcal{T}(R)) \leq i \leq j \leq l(p) - 1$. Then $S_i(p, \mathcal{T}(R)) \subseteq S_j(p, \mathcal{T}(R))$.

Essential levels of a node $p \in \mathcal{T}(R)$ has 1-1 correspondence to the set consisting of all nodes containing p in the explicit representation of cover tree in [7], see Figure 4 middle.

▶ Definition 5.3 (Essential levels of a node). Let $R \subseteq X$ be a finite reference set with a cover tree $\mathcal{T}(R)$. Let $q \in \mathcal{T}(R)$ be a node. Let (t_i) for $i \in \{0, 1, ..., n\}$ be a sequence of $H(\mathcal{T}(R))$ in such a way that $t_0 = l(q), t_n = l_{\min}(\mathcal{T}(R))$ and for all i we have $t_{i+1} = \operatorname{Next}(q, t_i, \mathcal{T}(R))$. Define the set of essential indices $\mathcal{E}(q, \mathcal{T}(R)) = \{t_i + 1 \mid i \in \{0, ..., n\}\}$.

▶ Lemma 5.4 (Number of essential levels). Let $R \subseteq X$ be a finite reference set with a cover tree $\mathcal{T}(R)$. Then $\sum_{p \in R} |\mathcal{E}(p, \mathcal{T}(R))| \le 2 \cdot |R|$, where $\mathcal{E}(p, \mathcal{T}(R))$ appears in Definition 5.3.

Proof. Let us prove this claim by induction on size |R|. In basecase $R = \{r\}$ and therefore $|\mathcal{E}(r, \mathcal{T}(R))| = 1$. Assume now that the claim holds for any tree $\mathcal{T}(R)$, where |R| = m and let us prove that if we add any node $v \in X \setminus R$ to tree $\mathcal{T}(R)$, then $\sum_{p \in R} |\mathcal{E}(p, \mathcal{T}(R \cup \{v\}))| \leq 2 \cdot |R| + 2$. Assume that we have added u to $\mathcal{T}(R)$, in such a way that v is its new parent. Then $|\mathcal{E}(p, \mathcal{T}(R \cup \{v\}))| = |\mathcal{E}(p, \mathcal{T}(R))| + 1$ and $|\mathcal{E}(v, \mathcal{T}(R \cup \{v\}))| = 1$. We have:

$$\sum_{p \in R \cup \{u\}} |\mathcal{E}(p, \mathcal{T}(R))| = \sum_{p \in R} |\mathcal{E}(p, \mathcal{T}(R))| + 1 + |\mathcal{E}(v, \mathcal{T}(R \cup \{v\}))| \le 2 \cdot |R| + 2 \le 2(|R \cup \{v\}|)$$

which completes the induction step.

- 1: Function : CountDistinctiveDescendants(Node p, a level i of $\mathcal{T}(R)$)
- 2: **Output** : an integer 3: **if** $i > l_{\min}(\mathcal{T}(Q))$ **then** 4: **for** $q \in \text{Children}(p)$ having l(p) = i - 1 or q = p **do** 5: Set s = 06: $j \leftarrow 1 + \text{Next}(q, i - 1, \mathcal{T}(R))$ 7: $s \leftarrow s + \text{CountDistinctiveDescendants}(q, j)$ 8: **end for** 9: **else** 10: Set s = 1
- 11: end if
- 12: Set $|S_i(p)| = s$ and **return** s

Algorithm 5.5 This algorithm returns sizes of distinctive descendant set $S_i(p, \mathcal{T}(R))$ for all essential levels $i \in \mathcal{E}(p, \mathcal{T}(R))$

▶ Lemma 5.6. Let R be a finite subset of a metric space. Let $\mathcal{T}(R)$ be a compressed cover tree on R. Then, Algorithm 5.5 computes the sizes $|\mathcal{S}_i(p, \mathcal{T}(R))|$ for all $p \in R$ and essential levels $i \in \mathcal{E}(p, \mathcal{T}(R))$ in time O(|R|).

Proof. By Lemma 5.4 we have $\sum_{p \in R} |\mathcal{E}(p, \mathcal{T}(R))| \leq 2 \cdot |R|$. Since CountDistinctiveDescendants is called once for every any combination $p \in R$ and $i \in \mathcal{E}(p, \mathcal{T}(R))$ it follows that the time complexity of Algorithm 5.5 is O(R).

Let *i* be an arbitrary level and let $j = \text{Next}(p, i, \mathcal{T}(R))$. By definition of Next it follows that $l(q) \notin [j + 1, i - 1]$ for all $q \in \text{Descendants}(p)$. Therefore we have $V_i(p) = V_j(p)$ and $\mathcal{S}_i(p, \mathcal{T}(R)) = \mathcal{S}_j(p, \mathcal{T}(R))$. It follows that $|\mathcal{S}_i(p, \mathcal{T}(R))|$ can change only at indices $i \in H(\mathcal{T}(R))$. Therefore Lemma 5.6 shows that all the essential distinctive descendants sets of compressed cover tree $\mathcal{T}(R)$ can be precomputed in $O((c_m(R))^4 \cdot |R|)$ time.

Recall that the neighborhood $N(q;r) = \{p \in C \mid d(q,p) \leq d(q,r)\}$ was introduced in Definition 1.1.

◀

▶ Definition 5.7 (λ -point). Fix a query point q in a metric space (X, d) and fix any level $i \in \mathbb{Z}$. Let $\mathcal{T}(R)$ be its compressed cover tree on a finite reference set $R \subseteq X$. Let C be a subset of a cover set C_i from Definition 2.1 satisfying $\sum_{p \in C} |\mathcal{S}_i(p, \mathcal{T}(R))| \ge k$, where $\mathcal{S}_i(p, \mathcal{T}(R))$ is the distinctive descendant set from Definition 5.1. For any $k \ge 1$, define $\lambda_k(q, C)$ as a point $\lambda \in C$ that minimizes $d(q, \lambda)$ subject to $\sum_{p \in N(q;\lambda)} |\mathcal{S}_i(p, \mathcal{T}(R))| \ge k$.

- 1: **Input:** A point $q \in X$, a subset C of level set C_i of a compressed cover tree $\mathcal{T}(R)$, an integer $k \in \mathbb{Z}$
- 2: Initialize an empty max-binary heap B and an empty array D.
- 3: for $p \in C$ do
- 4: add p to B with priority d(q, p)
- 5: **if** $|H| \ge k$ then
- 6: remove the point with a maximal value from B
- 7: end if
- 8: end for
- 9: Transfer points from the binary heap B to the array D in reverse order.
- 10: Find the smallest index j such that $\sum_{t=0}^{j} S_i(D[t], \mathcal{T}(R)) \ge k$.
- 11: return $\lambda = D[j]$.
- **Algorithm 5.8** Computation of a λ -point of Definition 5.7 in line 6 of Algorithm 6.1

▶ Lemma 5.9 (Time complexity of λ -point). In the conditions of Definition 5.7, the time complexity of Algorithm 5.8 is $O(C \cdot \max_i |R_i| \cdot \log(k))$.

Proof. To compute $\lambda = \lambda_k(q, R)$ in Algorithm 5.8, we need to select k elements by using an ordering from the set C. This selection takes takes at most $|C| \cdot \log(k)$ time by using a binary heap data structure [8, section 6.5].

▶ Lemma 5.10 (Separation lemma). In the conditions of Definition 5.1, let $p \neq q$ be nodes of $\mathcal{T}(R)$ with $l(p) \geq i$, $l(q) \geq i$. Then $\mathcal{S}_i(p, \mathcal{T}(R)) \cap \mathcal{S}_i(q, \mathcal{T}(R)) = \emptyset$.

Proof. Without loss of generality assume that $l(p) \ge l(q)$. If q is not a descendant of p, the lemma holds trivially due to $\text{Descendants}(q) \cap \text{Descendants}(p) = \emptyset$. If q is a descendant of p, then $l(q) \le l(p) - 1$ and therefore $q \in V_i(p)$. It follows that $S_i(p, \mathcal{T}(R)) \cap \text{Descendants}(q) = \emptyset$ and therefore

$$\mathcal{S}_i(p,\mathcal{T}(R)) \cap \mathcal{S}_i(q,\mathcal{T}(R)) \subseteq \mathcal{S}_i(p,\mathcal{T}(R)) \cap \text{Descendants}(q) = \emptyset.$$

▶ Lemma 5.11 (Sum lemma). In the notations of Definition 5.1 assume that *i* is arbitrarily index and a subset $V \subseteq R$ satisfies $l(p) \ge i$ for all $p \in V$. Then

$$|\bigcup_{p \in V} \mathcal{S}_i(p, \mathcal{T}(R))| = \sum_{p \in V} |\mathcal{S}_i(p, \mathcal{T}(R))|.$$

Proof. Proof follows from Lemma 5.10.

By Lemma 5.11 in Definition 5.7 it is enough to assume that $|\bigcup_{p \in C} S_i(p, \mathcal{T}(R))| \ge k$.

▶ Lemma 5.12. In the notations of Definition 5.1, let $p \in \mathcal{T}(R)$ be any node. If $w \in S_i(p, \mathcal{T}(R))$ then either w = p or there exists $a \in \text{Children}(p) \setminus \{p\}$ such that l(a) < i and $w \in \text{Descendants}(a)$.

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Proof. Let $w \in S_i(p)$ be an arbitrary node satisfying $w \neq p$. Let s be the node-to-root path of w. The inclusion $S_i(p) \subseteq \text{Descendants}(p)$ implies that $w \in \text{Descendants}(p)$.

Let $a \in \text{Children}(p) \setminus \{p\}$ be a child on the path s. If $l(a) \geq i$ then $a \in V_i(p)$. Note that $w \in \text{Descendants}(a)$. Therefore $w \notin \mathcal{S}_i(p)$, which is a contradiction. Hence l(a) < i.

▶ Lemma 5.13. In the notations of Definition 5.1, let $p \in \mathcal{T}(R)$ be any node. If $w \in S_i(p, \mathcal{T}(R))$ then $d(w, p) \leq 2^{i+1}$.

Proof. By Lemma 5.12 either $w = \gamma$ or $w \in \text{Descendants}(a)$ for some $a \in \text{Children}(\gamma) \setminus \{\gamma\}$ for which l(a) < i. If $w = \gamma$, then trivially $d(\gamma, w) \le 2^i$. Else w is a descendant of a, which is a child of node γ on level i - 1 or below, therefore by Lemma 2.8 we have $d(\gamma, w) \le 2^i$ anyway.

▶ Lemma 5.14. Let R be a finite subset of a metric pace. Let $\mathcal{T}(R)$ be a compressed cover tree on R. Let $R_i \subseteq C_i$, where C_i is the *i*th cover set of $\mathcal{T}(R)$. Set $\mathcal{C}(R_i) = \{a \in Children(p) \text{ for some } p \in R_i \mid l(a) \geq i-1\}$. Then

$$\bigcup_{p \in \mathcal{C}(R_i)} \mathcal{S}_{i-1}(p, \mathcal{T}(R)) = \bigcup_{p \in R_i} \mathcal{S}_i(p, \mathcal{T}(R)).$$

Proof. Let $a \in \bigcup_{p \in C} S_{i-1}(p, \mathcal{T}(R))$ be an arbitrary node. Then there is $v \in C$ having $a \in S_{i-1}(v, \mathcal{T}(R))$. Let $w \in R_i$ be an ancestor of v that has the lowest level among all ancestors from in R_i . The node v has always an ancestor in R_i . Indeed, by the choice of $v \in C$, either $v \in R_i$ or v has a parent in R_i . Hence $a \in \text{Descendants}(w)$. Since w has a minimal level among all ancestors of v, we conclude that $a \notin \bigcup_{u \in V_i(w)} \text{Descendants}(u)$. Then

$$a \in \mathcal{S}_i(w, \mathcal{T}(R)) \subseteq \bigcup_{p \in R_i} \mathcal{S}_i(p, \mathcal{T}(R)).$$

Assume now that $a \in \bigcup_{p \in R_i} S_i(p, \mathcal{T}(R))$. Then $a \in S_i(v, \mathcal{T}(R))$ for some $w \in R_i$. Let w have no children at the level i - 1. Then $V_i(w) = V_{i-1}(w)$ and

$$a \in \mathcal{S}_{i-1}(w, \mathcal{T}(R)) \subseteq \bigcup_{p \in \mathcal{C}(R_i)} \mathcal{S}_{i-1}(p, \mathcal{T}(R)).$$

Assume now that w has children at the level i-1. If there exists $b \in \text{Children}(w)$ for which $a \in \text{Descendants}(b)$. Since $V_{i-1}(b) = \emptyset$, we conclude that

$$a \in \mathcal{S}_{i-1}(b, \mathcal{T}(R)) \subseteq \bigcup_{p \in C} \mathcal{S}_{i-1}(p, \mathcal{T}(R)).$$

To prove the converse inclusion assume that $a \notin \text{Descendants}(b)$ for all $b \in \text{Children}(w)$ with l(b) = i - 1. Then $a \in \text{Descendants}(w)$ and $a \notin \text{Descendants}(b')$ for any $b' \in V_i(w)$. Then $a \in S_{i-1}(w, \mathcal{T}(R))$ and the proof finishes:

$$\bigcup_{p \in R_i} \mathcal{S}_i(p, \mathcal{T}(R)) \subseteq \bigcup_{p \in \mathcal{C}(R_i)} \mathcal{S}_{i-1}(p, \mathcal{T}(R)).$$

▶ Lemma 5.15 (β -point). In the notations of Definition 5.7, let $C \subseteq C_i$ so that $\cup_{p \in C} S_i(p, \mathcal{T}(R))$ contains all k-nearest neighbors of q. Set $\lambda = \lambda_k(q, C)$. Then R has a point β among the first k nearest neighbors of q such that $d(q, \lambda) \leq d(q, \beta) + 2^{i+1}$.

4

Proof. We show that R has a point β among the first k nearest neighbors of q such that

$$\beta \in \bigcup_{p \in C} \mathcal{S}_i(p, \mathcal{T}(R)) \setminus \bigcup_{p \in N(q, \lambda) \setminus \{\lambda\}} \mathcal{S}_i(p, \mathcal{T}(R))$$

Lemma 5.11 and Definition 5.7 imply that

$$|\bigcup_{p \in N(q,\lambda) \setminus \{\lambda\}} S_i(p, \mathcal{T}(R))| = \sum_{p \in N(q,\lambda) \setminus \{\lambda\}} |S_i(p, \mathcal{T}(R))| < k.$$

Since $\bigcup_{p \in C} s_i(p, \mathcal{T}(R))$ contains all k-nearest neighbors of q, a required point $\beta \in R$ exists.

Let us now show that β satisfies $d(q, \lambda) \leq d(q, \beta) + 2^{i+1}$. Let $\gamma \in C \setminus N(q, \lambda) \cup \{\lambda\}$ be an ancestor of β . Since $\gamma \notin N(q, \lambda) \setminus \{\lambda\}$, we get $d(\gamma, q) \geq d(q, \lambda)$. The triangle inequality says that $d(q, \gamma) \leq d(q, \beta) + d(\gamma, \beta)$. Finally, Lemma 2.8 implies that $d(\gamma, \beta) \leq 2^{i+1}$. Then

$$d(q,\lambda) \le d(q,\gamma) \le d(q,\beta) + d(\gamma,\beta) \le d(q,\beta) + 2^{i+1}$$

So β is a desired k-nearest neighbor satisfying the condition $d(q, \lambda) \leq d(q, \beta) + 2^{i+1}$.

6 Corrected parameterized complexity for exact all *k*-nearest neighbor search

In Counterexample 3.7 it was shown that the proof of [7, Theorem 5] contained mistakes. New results, Theorem 6.4 and Theorem 6.5 will not only correct, but also extend the run time bound for k-nearest neighbor search [7, Theorem 5] from k = 1 to any $k \ge 1$. Note that Algorithm 6.1 uses different pruning rule in line 7 than Algorithm 3.6 in line 5. Distance bound $d(p, Q) + 2^i$ is replaced by $d(q, \lambda) + 2^{i+1}$, so any k-nearest neighbors of point q are not removed during the traversal of the algorithm.

By lemma 5.6 we can precompute the sizes of distinctive descendants $|S_i(p, \mathcal{T}(R))|$ in a linear time O(|R|). Hence we can retrieve sizes of $|S_i(p, \mathcal{T}(R))|$ in time O(1) for any $p \in R$ and $i \in H(\mathcal{T}(R))$.

- 1: Input : compressed cover tree $\mathcal{T}(R)$, a query point $q \in X$, positive integer $k \in \mathbb{Z}_+$
- 2: Set $i \leftarrow l_{\max}(\mathcal{T}(R))$
- 3: Let r be the root node of $\mathcal{T}(R)$. Set $R_i = \{r\}$.
- 4: while $i > l_{\min} \operatorname{do}$
- 5: Assign $C(R_i) \leftarrow \{a \in \text{Children}(p) \text{ for some } p \in R_i \mid l(a) \ge i 1\}$ {Recall that Children(p) contains node p }
- 6: Compute $\lambda = \lambda_k(q, \mathcal{C}(R_i))$ from Definition 5.7, run Algorithm 5.8 to compute.
- 7: Find $R_{i-1} = \{r \in \mathcal{C}(R_i) \mid d(q, r) \le d(q, \lambda) + 2^{i+1}\}$
- 8: Set $j \leftarrow \max_{a \in R_{i-1}} \operatorname{Next}(a, i-1, \mathcal{T}(R))$ {If such j is undefined, we set $j = l_{\min}$ }
- 9: Set $R_j = R_{i-1}$ and i = j
- 10: end while
- 11: Compute k-nearest neighbors of query point q from set $R_{l_{\min}}$ and **output** them as array.

Algorithm 6.1 Updated *k*-nearest neighbor search by using a compressed cover tree, see Theorems 6.4 and 6.5.

Example 6.2 (Simulated run of Algorithm 6.1). Let R and $\mathcal{T}(R)$ be as in Example 2.2. Let q = 0 and k = 5. Figures 10, 11, 12 and 13 illustrate simulated run of Algorithm 6.1 on

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input $(\mathcal{T}(R), q, k)$. Recall that $l_{\max} = 2$ and $l_{\min} = -1$. During the iteration *i* of Algorithm 6.1 we maintain the following coloring: Points in R_i are colored orange. Points $\mathcal{C}(R_i)$ (of line 5) that are not contained in R_i are colored yellow. The λ -point of line 6 is denoted by using purple color. All the nodes that were present in R_{i-1} , but are no longer included in R_i will be colored red. Finally all the points that are selected as *k*-nearest neighbors of *q* are colored green in the final iteration. Nodes that haven't been yet visited or that will never be visited are colored white. Consider the following steps:

Iteration i = 2: Figure 10 illustrates iteration i = 2 of the Algorithm 6.1. In line 5 we find $C(R_2) = \{4, 8, 12\}$. Since node 4 minimizes distance $d(C(R_2), 0)$ and distinctive descendant set $S_2(4, \mathcal{T}(R))$ consists of 7 elements we get $\lambda = 4$. In line 7 we find $R_1 = \{r \in C \mid d(0, r) \leq d(q, \lambda) + 2^3 = 12\} = \{4, 8, 12\}.$

Iteration i = 1: Figure 11 illustrates iteration i = 1 of the Algorithm 6.1. In line 5 we find $C(R_1) = \{2, 4, 6, 8, 10, 12, 14\}$. Since $|S_1(2, \mathcal{T}(R))| = 3$, $|S_1(4, \mathcal{T}(R))| = 1$ and $|\mathcal{T}_1(6)| = 3$ and 6 is the node with smallest to distance 0 satisfying $\sum_{p \in N(0,6) = \{2,4,6\}} |S_1(p, \mathcal{T}(R))| \ge 5 = k$. It follows that $\lambda = 6$. In line 7 we find $R_0 = \{r \in C(R_1) \mid d(0,r) \le d(q,\lambda) + 2^2 = 10\} = \{2,4,6,8,10\}$.

Iteration i = 0: Figure 12 illustrates iteration i = 0 of the Algorithm 6.1. In line 5 $C(R_0) = \{1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11\}$. We note that $|s_0(p, \mathcal{T}(R))| = 1$ for all $p \in C(R_0)$. Thus 5 is the first number to satisfy $\sum_{p \in N(0,5) = \{1,2,3,4,5\}} |S_0(p, \mathcal{T}(R))| \ge 5 = k$. It follows that $\lambda = 5$. In line 7 : $R_{-1} = \{r \in C(R_0) \mid d(0,r) \le d(q,\lambda) + 2^1 = 7\} = \{1,2,3,4,5,6,7\}$.

Final selection: Figure 13 illustrates the final iteration of Algorithm 6.1. We simply select k-shortest distances d(q, p) for $p \in R_{-1}$ to obtain the final output $\{1, 2, 3, 4, 5\}$.



Figure 10 Iteration i = 2 of simulation in Example 6.2 of Algorithm 6.1



Figure 11 Iteration i = 1 of simulation in Example 6.2 of Algorithm 6.1



Figure 12 Iteration i = 0 of simulation in Example 6.2 of Algorithm 6.1



Figure 13 Final iteration i = -1 of simulation in Example 6.2 of Algorithm 6.1

Note that $\bigcup_{p \in R_l} S_i(p, \mathcal{T}(R))$ is decreasing set for which $\bigcup_{p \in R_{l_{\max}}} S_{l_{\max}}(p, \mathcal{T}(R)) = R$ and $\bigcup_{p \in R_{l_{\min}}} S_{l_{\min}}(p, \mathcal{T}(R)) = R_{l_{\min}}$.

▶ Lemma 6.3 (Real k-nearest neighbors are contained in candidate set for all i). Let R be a finite subset of an ambient metric space (X, d) and let $k \in \mathbb{Z} \cap [1, \infty)$ be a parameter. Let $\mathcal{T}(R)$ be a compressed cover tree of R. Assume that $|R| \ge k$. Then for any iteration $i \in H(\mathcal{T}(R))$ of lines 4-10 of Algorithm 6.1 the candidate set $\bigcup_{p \in R_i} S_i(p, \mathcal{T}(R))$ contains all k-nearest neighbors of q.

Proof. Since $R_{l_{\max}} = \{r\}$, where r is the root $\mathcal{T}(R)$ we have $S_{l_{\max}}(r, \mathcal{T}(R)) = R$ and therefore any point among k-nearest neighbor of q is contained in $R_{l_{\max}}$. Let i be the largest index for which there exists a point among k-nearest neighbor of q that doesn't belong to $\bigcup_{p \in R_{i-1}} S_i(p, \mathcal{T}(R))$. Let us denote such point by β , then:

$$\beta \in \bigcup_{p \in R_i} S_i(p, \mathcal{T}(R)) \setminus \bigcup_{p \in R_{i-1}} S_{i-1}(p, \mathcal{T}(R)).$$

By Lemma 5.14 we have

$$\bigcup_{p \in \mathcal{C}(R_i)} \mathcal{S}_{i-1}(p, \mathcal{T}(R)) = \bigcup_{p \in R_i} \mathcal{S}_i(p, \mathcal{T}(R))$$
(4)

Let λ be as in line 6 of Algorithm 6.1. By Equation (4) we have $|\bigcup_{p \in \mathcal{C}(R_i)} \mathcal{S}_{i-1}(p, \mathcal{T}(R))| \geq k$, therefore by Definition 5.7 such λ exists. Since $\beta \in \bigcup_{p \in \mathcal{C}(R_i)} \mathcal{S}_{i-1}(p, \mathcal{T}(R))$, there exists $\alpha \in \mathcal{C}(R_i)$ satisfying $\beta \in \mathcal{S}_{i-1}(\alpha, \mathcal{T}(R))$. By assumption it follows $\alpha \notin R_{i-1}$. By line 7 of the algorithm we have

$$d(\alpha, q) > d(q, \lambda) + 2^{i+1}.$$
(5)

Let w be arbitrary point in set $\bigcup_{p \in N(q;\lambda)} S_{i-1}(p,\mathcal{T}(R))$. Therefore $w \in S_{i-1}(\gamma,\mathcal{T}(R))$ for some $\gamma \in N(q;\lambda)$. By Lemma 5.13 applied on i-1 we have $d(\gamma,w) \leq 2^i$. By Definition 5.7 since $\gamma \in N(q; \lambda)$ we have $d(q, \gamma) \leq d(q, \lambda)$. By (5) and the triangle inequality we obtain:

$$d(q,w) \le d(q,\gamma) + d(\gamma,w) \le d(q,\lambda) + 2^i < d(\alpha,q) - 2^i \tag{6}$$

On the other hand β is a descendant of α thus we can estimate:

$$d(q,\beta) \ge d(q,\alpha) - d(\alpha,\beta) \ge d(\alpha,q) - 2^i \tag{7}$$

By combining Inequality (6) with Inequality (7) we obtain $d(q, w) < d(q, \beta)$. Since w was arbitrary point from $\bigcup_{p \in N(q;\lambda)} S_{i-1}(p, \mathcal{T}(R))$, that contains at least k points, β cannot be any k-nearest neighbor of q, which is a contradiction.

▶ Theorem 6.4 (correctness of Algorithm 6.1). Algorithm 6.1 correctly finds all k nearest neighbors of query point q within reference set R.

Proof. Claim follows directly from Lemma 6.3 by noting that since $i = l_{\min}$ all the nodes $p \in R_{l_{\min}}$ do not have any children. Therefore it follows $\bigcup_{p \in R_{l_{\min}}} S_i(p, \mathcal{T}(R)) = R_{l_{\min}}$. Thus all the k-nearest neighbors of q are contained in the set $R_{l_{\min}}$.

Theorem 6.5 estimates the complexity as the number of iterations multiplied by the maximal size of the reference subsets $R_i \subseteq R$ in Algorithm 6.1. Example 6.2 shows how R_i varies in size during the main iteration phase (lines 4-10) of Algorithm 6.1. The size of R_i depends on a distance $d(q, \lambda)$ for λ in Definition 5.7. If $d(q, \lambda) \ge 2^i$ then we use the expansion constant $c(R \cup \{q\})$ to estimate size of R_i . Since $\overline{B}(q, \frac{d(q,\lambda)}{2})$ contains at most k points, the definition of the expansion constant will implies that $|R_i| \le (c(R \cup \{q\}))^3 \cdot k$. If $d(q, \lambda)$ is small, Lemma 2.9 implies that $|R| \le (c_m(R))^6$.

▶ Theorem 6.5 (complexity for exact all k-nearest neighbors). Let R be a finite reference set in a metric space (X, d). Let $q \in X$ be a query point, $c(R \cup \{q\})$ be the expansion constant of $R \cup \{q\}$ and $c_m(R)$ be the minimized expansion constant from Definition 2.4. Given a compressed cover tree $\mathcal{T}(R)$ with a height $|H(\mathcal{T}(R))|$ from Definition 2.11, Algorithm 6.1 finds all k nearest neighbors of q in time $O((c_m(R))^4 \cdot \max\{(c(R \cup \{q\}))^3 \cdot k, (c_m(R))^6\} \cdot$

 $\log(k) \cdot |H(\mathcal{T}(R))|$).

Proof. We note that the number of iterations (lines 4-10) are bounded by height $|H(\mathcal{T}(R))|$. The total number of children encountered in line 5 during single iteration (lines 4-10) is at most $(c_m(R))^4 \cdot \max_i |R_i|$ by Lemma 2.10. From Lemma 5.9 we obtain that line 6, which launches Algorithm 5.8 takes at most $|\mathcal{C}(R_i)|\log(k) = (c_m(R))^4 \cdot \max_i |R_i| \cdot \log(k)$ time. Line 7 never does more work than line 5, because in the worst case scenario R_i is copied to R_{i-1} in its current form. Line 8 handles $|R_{i-1}|$ nodes, since we can keep track of value of Next $(a, i, \mathcal{T}(R))$ by updating it when necessary in line 5 we can retrieve its value in O(1) time. Therefore maximal run-time of line 8 is $O(\max |R_i|)$. Final line 11 picks k-elements from ordered set $R_{l_{\min}}$, which can be done using binary heap data structure similarly to Algorithm 5.8, which gives time-complexity of $O(\log(k) \cdot \max_i |R_i|)$. Consequently, the running time is bounded by

$$O((c_m(R))^4 \cdot \log(k) \cdot \max |R_i| \cdot D(\mathcal{T})).$$
(8)

To finish the proof we will show that $\max_i |R_i| \le \max\{(c_m(R))^6, k \cdot (c(R \cup q))^3\}$.

Consider any R_{i-1} constructed during the *i*-th iteration and let $d = d(p, \lambda)$. We have

$$R_{i-1} = \{ r \in \mathcal{C}(R_i) \mid d(p,q) \le d + 2^{i+1} \}$$
(9)

$$= B(q, d+2^{i+1}) \cap \mathcal{C}(R_i) \tag{10}$$

$$\subseteq B(q, d+2^{i+1}) \cap C_{i-1} \tag{11}$$

We assume first that $d > 2^{i+1}$. Note first that by Lemma 6.3 set $\cup_{p \in R_i} S_i(p, \mathcal{T}(R))$ contains all k-nearest neighbors of q and by Lemma 5.14 $\cup_{p \in C} S_{i-1}(p, \mathcal{T}(R)) = \cup_{p \in R_i} S_i(p, \mathcal{T}(R))$. Therefore $\cup_{p \in C} S_{i-1}(p, \mathcal{T}(R))$ contains all k-nearest neighbors of q. Using Lemma 5.15 we find β among k-nearest neighbors of q satisfying $d \leq d(q, \beta) + 2^i$. From assumption It follows $2^i \leq d(q, \beta)$. Combining this with Equation 9 and Definition 2.4, we obtain:

$$|R_{i-1}| \le |B(q, 2d(q, \beta) + 2^{i+1})| \le |B(q, 4d(q, \beta))| \le (c(R \cup \{q\}))^3 \cdot |B(q, \frac{d(q, \beta)}{2})|$$
(12)

We note that β is among k-nearest neighbors of q. It follows that $|R_{i-1}| \leq c^3 \cdot k$. Assume now that $d \leq 2^{i+1}$. By using (11) we obtain:

$$R_{i-1} \subseteq B(q, 2^{i+2}) \cap C_{i-1}$$

From cover-tree condition we know that all the points in C_{i-1} are separated by 2^{i-1} . We will now apply Lemma 2.9 with $t = 2^{i+2}$ and $\delta = 2^{i-1}$. Since $4\frac{t}{\delta} + 1 = 2^5 + 1 \le 2^6$ we obtain $|R_{i-1}| \le |B(q, 2^{i+2}) \cap C_{i-1}| \le c_m(R)^6$. By combining both cases we obtain $|R_{i-1}| \le \max\{c_m(R)^6, (c(R \cup \{q\}))^3 \cdot k\}$. By substituting the relevant information in (8) we obtain the final bound.

Theorem 6.5 shows that we can find k-nearest neighbors of single point q in a near-linear time that depends on expansion constant $c(R \cup \{q\})$ and minimized expansion constant $c_m(R)$. If the ambient space $X = \mathbb{R}^d$ is euclidean, it can be shown that $c_m(R) \leq 2^d$. However, no such bound exists for $c(R \cup \{q\})$, since $c(R \cup \{q\})$ depends only on distribution of points in set $R \cup q$. In case point $d(q, R) > \operatorname{diam}(R)$ then $c(R \cup \{q\}) = N$ leading to worse-time complexity, than we would have if we had simply used linear-search. In general than further point q is from set R, than less benefit is obtained from compressed cover tree datastructure.

▶ Corollary 6.6 (solution to Problem 1.2). In the notations of Theorem 6.5, set $c = \max_{q \in Q} c(R \cup \{q\})$. Let $\Delta(R)$ be the aspect ratio from Definition 2.12. Algorithms 4.2 and 6.1 solve Problem 1.2 in time $O(c^{10}k \log(k) \cdot \log_2(\Delta(R)) \cdot (|Q| + |R|))$.

Proof. We estimate the complexity from Theorem 6.5 by using the upper bounds $c_m(R) \leq c(R \cup \{q\}) \leq c$ and $|H(\mathcal{T}(R))| \leq \log_2(\Delta(R))$ by Lemmas 2.5 and 2.13, respectively. Then we multiply the result by the size |Q| of the query set and add the complexity $O(c^8 \cdot \Delta(R) \cdot |R|)$ to build a compressed cover tree $\mathcal{T}(R)$ by Theorem 4.5.

7 Approximate k-nearest neighbor search by a compressed cover tree

The original navigating nets and cover trees were used in [19, Theorem 2.2] and [7, Section 3.2] to solve the $(1 + \epsilon)$ -approximate nearest neighbor problem for k = 1. Theorem 7.4 justifies a near linear parameterized complexity to find approximate a k-nearest neighbor set \mathcal{P} formalized in Definition 7.1.

▶ **Definition 7.1** (approximate k-nearest neighbor set \mathcal{P}). Let R be a finite reference set and let Q be a finite query set of a metric space (X, d). Let $q \in Q \subseteq X$ be a query point, $k \ge 1$ be an integer and $\epsilon > 0$ be a real number. Let $\mathcal{N}_k = \bigcup_{i=1}^k \mathrm{NN}_i(q)$ be the union of neighbor sets from Definition 1.1. A set $\mathcal{P} \subseteq R$ is called an *approximate k-nearest neighbors set*, if $|\mathcal{P}| = k$ and there is an injection $f : \mathcal{P} \to \mathcal{N}_k$ satisfying $d(q, p) \le (1 + \epsilon) \cdot d(q, f(p))$ for all $p \in \mathcal{P}$.

- Input : Compressed cover tree *T*(*R*), a query point *q* ∈ *X*, positive integer *k* ∈ Z₊, index *i* ∈ Z, Subset *C*(*R_i*) of cover set *C_{i-1}* of *T*(*R*), λ-point of line 6 of Algorithm 6.1.
 if ^{2ⁱ⁺¹}/_ε + 2ⁱ ≤ d(q, λ) then
- 3: Let $\mathcal{P} = \emptyset$.
- 4: for $p \in \mathcal{C}(R_i)$ do
- 5: **if** $d(p,q) < d(q,\lambda)$ **then**
- 6: $\mathcal{P} = \mathcal{P} \cup \mathcal{S}_{i-1}(p, \mathcal{T}(R))$
- 7: end if
- 8: end for
- 9: Fill \mathcal{P} until it has k points by adding any points from sets $\mathcal{S}_{i-1}(p, \mathcal{T}(R))$, where $d(p,q) = d(q,\lambda)$.
- 10: return \mathcal{P} .

11: end if

Algorithm 7.2 Expansion for Algorithm 6.1 that can be inserted between lines 6 and 7 to find approximate *k*-nearest neighbor of Definition 7.1

We can modify Algorithm 6.1 , in such a way that the algorithm would terminate once $\frac{2^{i+1}}{\epsilon} + 2^i \leq d(q,\lambda)$ is satisfied between lines 6 and 7. This extra method is illustrated in Algorithm 7.2.

Lemma 7.3 shows that Algorithm 7.2 correctly returns Approximate k-nearest neighbor set of Definition 7.1.

▶ Lemma 7.3 (correctness of Algorithm 7.2). In the notations of Definition 7.1, Algorithm 6.1 modified by inserting Algorithm 7.2 between lines 6 and 7 finds an approximate k-nearest neighbors set of any query point $q \in X$.

Proof. Note first that by Lemma 6.3 set $\bigcup_{p \in R_i} S_i(p, \mathcal{T}(R))$ contains all k-nearest neighbors of q and by Lemma 5.14 $\bigcup_{p \in \mathcal{C}(R_i)} S_{i-1}(p, \mathcal{T}(R)) = \bigcup_{p \in R_i} S_i(p, \mathcal{T}(R))$. Therefore $\bigcup_{p \in \mathcal{C}(R_i)} S_{i-1}(p, \mathcal{T}(R))$ contains all k-nearest neighbors of q.

Assume first that condition on line 2 of Algorithm 7.2 is satisfied during some iteration $i \in H(\mathcal{T}(R))$ of Algorithm 7.2. Let us denote

$$\mathcal{A} = \bigcup_{p \in \mathcal{C}(R_i)} \{ \mathcal{S}_{i-1}(p) \mid d(p,q) < d(q,\lambda) \} \text{ and } \mathcal{B} = \bigcup_{p \in \mathcal{C}(R_i)} \{ \mathcal{S}_{i-1}(p) \mid d(p,q) = d(q,\lambda) \}.$$

By Algorithm 7.2 set \mathcal{P} contains all points of \mathcal{A} and rest of the points are filled form \mathcal{B} .

We will now form $f: \mathcal{P} \to \mathcal{N}_k$ by mapping every point $p \in \mathcal{A} \cap \mathcal{P}$ into itself and then by extending f to be injective map on whole set \mathcal{P} . The claim holds trivially for all points $p \in \mathcal{A} \cap \mathcal{P}$. Let us now consider points $p \in \mathcal{P} \setminus \mathcal{A}$. Let $\gamma \in \mathcal{C}(R_i)$ be such that $p \in \mathcal{S}(\gamma, \mathcal{T}(R))$ and let $\psi \in C$ be such that $f(p) \in \mathcal{S}(\psi, \mathcal{T}(R))$. By using triangle inequality, Lemma 2.8 and the fact that $p \in \mathcal{A} \cup \mathcal{B}$ we obtain:

$$d(q,p) \le d(q,\gamma) + d(\gamma,p) \le d(q,\lambda) + 2^i \tag{13}$$

On the other hand since $f(p) \notin \mathcal{A}$ we have

$$(1+\epsilon) \cdot d(q, f(p)) \ge (1+\epsilon) \cdot (d(q, \psi) - d(\psi, f(p))) \ge (1+\epsilon) \cdot (d(q, \lambda) - 2^i)$$
(14)

Note that by line 2 we have $\frac{2^{i+1}}{\epsilon} \leq d(q, \lambda)$, therefore

$$d(q,\lambda) + 2^{i} \le d(q,\lambda) + 2^{i+1} - 2^{i} \le \epsilon(d(q,\lambda) - 2^{i}) - 2^{i} \le (1+\epsilon) \cdot (d(q,\lambda) - 2^{i})$$
(15)

By combining Equations (13) - (15) we obtain $d(q, p) \leq (1 + \epsilon) \cdot d(q, f(p))$.

If condition on line 2 of Algorithm 7.2 is never satisfied, then the Algorithm finds real k-nearest neighbors of point q in the end of the algorithm and therefore the claim holds.

► Theorem 7.4 (correctness of modified Algorithm 6.1). In the notations of Definition 7.1, the complexity of modified Algorithm 6.1 after inserting Algorithm 7.2 between lines 6 and 7 is $O((c_m(R))^{8+\lceil \log(2+\frac{1}{\epsilon}) \rceil} \cdot \log(k) \cdot \log_2(\Delta(R)) + k)$.

Proof. Note first that the time complexity of Algorithm 7.2 is k. Then similarly to Theorem 6.5 it can be shown that the Algorithm is bounded

$$O((c_m(R))^4 \cdot \log(k) \cdot \max|R_i| \cdot |H(\mathcal{T}(R))| + k)$$
(16)

Let us now bound the size of R_i . By line 2 of Algorithm 7.2 either Algorithm 7.2 is launched that terminates the program or $\frac{2^{i+1}}{\epsilon} + 2^i > d(q, \lambda)$. To bound $|R_i|$ we can assume the latter. Similarly to Theorem 6.5 we have:

$$R_{i-1} = \{ r \in C \mid d(p,q) \le d(q,\lambda) + 2^{i+1} \}$$
(17)

$$= \bar{B}(q, d(q, \lambda) + 2^{i+1}) \cap \mathcal{C}(R_i)$$
(18)

$$\subseteq \bar{B}(q, d(q, \lambda) + 2^{i+1}) \cap C_{i-1} \tag{19}$$

$$\subseteq \bar{B}(q, 2^{i+1}(\frac{3}{2} + \frac{1}{\epsilon})) \cap C_{i-1}$$
(20)

Since the cover set C_{i-1} is a 2^{i-1} -sparse subset of the ambient metric space X, we can apply Lemma 2.9 with $t = 2^{i+1}(\frac{3}{2} + \frac{1}{\epsilon})$ and $\delta = 2^{i-1}$. Since $4\frac{t}{\delta} + 1 = 2^4(\frac{3}{2} + \frac{1}{\epsilon}) + 1 \leq 2^4(2 + \frac{1}{\epsilon})$, we get $\max |R_i| \leq (c_m(R))^{4+\lceil \log_2(2+\frac{1}{\epsilon}) \rceil}$. The final complexity is obtained by plugging the upper bound of $|R_i|$ above into 16.

► Corollary 7.5 (complexity for approximate k-nearest neighbors set \mathcal{P}). In the notations of Definition 7.1, an approximate k-nearest neighbors set is found for all $q \in Q$ in time $O\left(|Q| \cdot (c_m(R))^{8+\lceil \log(2+\frac{1}{\epsilon}) \rceil} \cdot \log(k) \cdot \log_2(\Delta(R)) + |Q| \cdot k\right)$.

Proof. This corollary follows directly from Theorem 7.4.

8 Conclusions

This paper resolved the complexity problems for the k-nearest neighbor search, which is used in many areas of Computer Science. The motivations were the past challenges in the proofs of time complexities in [19, Theorem 2.7], [7, Theorem 5] and in other related problems [29, Theorem 3.1], [23, Theorem 5.1]. Though [12, Section 5.3] pointed out some difficulties, no corrections were published. The main results (Theorem 6.5 and Corollary 6.6) fill the above gaps in the literature.

First, Definition 1.1 and Problem 1.2 rigorously deal with a potential ambiguity of knearest neighbors at equal distances, which wasn't discussed in the past work. The main new data structure of a compressed cover tree in Definition 2.1 substantially simplifies the navigating nets [19] and original cover trees [7] by avoiding any repetitions of given data points. This compression has substantially clarified the construction and search Algorithms 4.2 and 6.1.

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Second, the past approaches missed broad classes of challenging data, which are constructed in Counterexamples 3.5 and 3.7. To estimate the worst-case time complexity for any reference set, Definition 2.11 introduced the height of a compressed cover tree, which has become a novel parameter in the proved complexities. If the height, expansion constants and aspect ratio of a reference set R are fixed, all time complexities are linear in the maximum size of R and a query set Q and near linear $O(k \log k)$ in the number k of neighbors. Third, the proofs for all k-nearest neighbor search are generic enough to hold in any metric space and were extended to the approximate k-nearest search in section 7.

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