Efficient Spatial Nearest Neighbor Queries Based on Multi-layer Voronoi Diagrams

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Abstract—Nearest neighbor (NN) problem is an important scientific problem. The NN query, to find the closest one to a given query point among a set of points, is widely used in applications such as density estimation, pattern classification, information retrieval and spatial analysis. A direct generalization of the NN query is the k nearest neighbors (kNN) query, where the k closest points are required to be found. Since NN and kNN problems were raised, many algorithms have been proposed to solve them. It has been indicated in literature that the only method to solve these problems exactly with sublinear time complexity, is to filter out the unnecessary spatial computation by using the pre-processing structure, commonly referred to as the spatial index.

The recently proposed spatial indexing structures which can be utilized to NN search are almost constructed through spatial partition. These indices are tree-like, and the tree-like hierarchical structure can usually significantly improve the efficiency of NN search. However, when the data are distributed extremely unevenly, it is difficult to satisfy both the balance of the tree and the non-overlap of the subspace corresponding to the nodes. Thus the acceleration performance of the tree-like indices is severely jeopardized.

In this paper, we propose a non-tree spatial index which consists of multiple layers of Voronoi diagrams (MVD). This index structure can entirely avoid the dilemma tree-like structures face, and solve the NN problems stably with logarithmic time complexity. Furthermore, it is convenient to achieve kNN search by extending NN search on MVD. In the experiments, we evaluate the efficiency of this indexing for both NN search and kNN search by comparing with VoR-tree, R-tree and kd-tree. The experiments indicate that compared to NN search and kNN search with the other three indices, these two search methods have significantly higher efficiency with MVD.

Index Terms—nearest neighbor, spatial index, Voronoi diagram, MVD

I. INTRODUCTION

Nearest neighbor (NN) is a very important problem in the field of information science and data science [1]. NN query, to find the closest point among a set of points to a given query point, is widely required in several applications such as density estimation, pattern classification, information retrieval and spatial analysis. A direct generalization of NN query is k nearest neighbors (kNN) query, where we need to find the k closest points. According to the representation of space and the measurement of distance, there are many variations of NN/kNN query. However, most problems related to NN/kNN query in the real world can be reasonably described based on Euclidean space. Hence, in this paper, we study the NN and kNN problem in Euclidean space, where the distance between points is measured by Euclidean distance.

Given two points \( A = \{a_1, a_2, ..., a_d\} \) and \( B = \{b_1, b_2, ..., b_d\} \) in \( \mathbb{R}^d \), the Euclidean distance between \( A \) and \( B \), \( \| A - B \| \), is defined as follows:

\[
\| A - B \| = \sqrt{\sum_{i=1}^{d} (a_i - b_i)^2}
\]

Mathematically, the NN/kNN in Euclidean space can be stated as follows. Given a set \( P \) of points in \( \mathbb{R}^d \) and a query point \( q \in \mathbb{R}^d \), a point \( p' \) can be called NN(\( P, q \)), the nearest neighbor of \( q \) in \( P \), if and only if it satisfies the following condition:

\[
\forall p \in P, \| p' - q \| \leq \| p - q \| \quad (2)
\]

Similarly, given a set \( P \) of points in \( \mathbb{R}^d \) and a query point \( q \in \mathbb{R}^d \), a set \( P' \) of \( k \) points can be called kNN(\( P, q \)), the \( k \) nearest neighbors of \( q \) in \( P \), if and only if it satisfies the following condition:

\[
\forall p' \in P', \forall p \in P \setminus P', \| p' - q \| \leq \| p - q \| \quad (3)
\]

Theoretically, it is not difficult to find the nearest point to a test point \( q \) among a point set \( P \). The most straightforward way for the purpose is to compute the distance between \( q \) and each point in \( P \) and then find the point with minimum distance. Since the query time of the above full search method is proportional to the size of the point set, it is often called...
Spatial partition, this structure does not have the imbalance since there is neither branching structure of the tree nor multiple layers of Voronoi diagrams, as shown in Figure 1. We propose a non-tree spatial index, MVD, which consists of completely avoid the disadvantages of tree-structured index. Their inventors hope to realize spatial query in logarithmic computational complexity by taking advantage of the multi-level feature of tree structure.

In order to realize the multi-level structure, kd-tree adopts a dichotomy strategy. The problem space is divided into a large number of subspaces and distributed to the nodes of the tree. Generally, it performs well on the NN query. However, when the spatial distribution of data is very uneven, the tree structure is easily unbalanced, that is to say, the depth of partial sub tree is much larger than that of other sub trees. Therefore, the NN query in this case is difficult to achieve the theoretical logarithmic computational complexity.

R-tree uses rectangles to divided space and builds its tree structure. It uses the node segmentation strategy to achieve the balance of the tree. However, there is often a lot of overlap between nodes. This phenomenon becomes more serious when dealing with unevenly distributed data sets. As a result, R-tree often needs to visit too many leaf nodes to get accurate results in NN query. Although some studies have reduced the overlap between nodes through some strategies, theoretically a dynamic R-tree is difficult to completely eliminate the overlap.

Later, a composite index structure, VoR-tree, was proposed. It integrates a Voronoi diagram into R-tree to improve the kNN query of R-tree. Efficient processing of nearest neighbor queries requires spatial data structures which capitalize on the proximity of the objects to focus the search of potential neighbors only [13]. Therefore, the VoR-tree utilizes the tree structure to achieve the nearest neighbor search, and then realize a series of the other nearest neighbor related search through the pointwise nearest neighbor relations in the Voronoi diagram. Compared with R-tree, VoR-tree has an effective enhancement of the performance on kNN, RkNN, kANN and SSQ integrated search.

However, since its main structure is R-tree, its efficiency of NN query is almost the same as that of R-tree. In order to completely avoid the disadvantages of tree-structured index, we propose a non-tree spatial index, MVD, which consists of multiple layers of Voronoi diagrams, as shown in Figure 1. Since there is neither branching structure of the tree nor spatial partition, this structure does not have the imbalance problem like the tree structure, and there is no node overlap problem. We also propose methods of batch creation and update maintenance of MVD, thus this index is also applicable to dynamic data. We evaluate the performance of MVD on NN and kNN through comparison experiments with kd-tree, R-tree and VoR-tree. The experiments indicate that the performance of our index is better than the other three indexes both with virtual data and real world data, when the data dimension is no more than 4.

II. Related Works

A. kd-tree

The kd-tree [2], a special case of binary space partitioning tree, is a spatial data structure for organizing points in a k-dimensional space. It is probably the simplest data structure available for nearest neighbor searches.

The average time complexity of the NN search based on kd-tree is $O(\log n)$ [5]. However, after inserting a large number of new points, kd-tree tends to lose its balance and the efficiency of the NN search based on it decreases as well in consequence. Some past studies [6], [40], [41] attempt to improve the performance of kd-tree from the perspective of spatial partition or the reconstruction of balance. It is effective to some extent, but it is still very difficult to enhance its spatial search performance when facing the extremely unevenly distributed data.

B. R-tree

The R-tree [7], proposed by Antonin Guttman in 1984, is perhaps the most widely used spatial index structure. R-tree is considered to be a generalization of B-tree [5] in multidimensional space. Contrast with kd-tree, R-tree can organize not only points, but also spatial objects of none-zero size. The key idea of R-tree is to recursively group nearby objects in $\mathbb{R}^d$ by
using $d$ dimensional minimum bounding rectangles (MBR). Similar to B-tree, R-tree maintains its balance by splitting overflow nodes.

The Depth-First (DF) algorithm \cite{12} realizes the NN search on the R-tree. The DF algorithm applies Mindist and Min-Maxdist to prune the R-tree pruning, followed by using the search distance of the recursive deep-first strategy to search the nearest point. Then the DF algorithm is improved by \cite{38}. In this improved method, the Mindist is the condition to utilize the deep-first to traverse the R-tree. A Best-First (BF) algorithm \cite{16} is also developed. Its main characteristic is to use the priority queue to save the visited nodes by the Mindist rank of nodes. It is the state-of-the-art NN/kNN algorithm of R-tree. Because R-tree is balanced, it tend not to be too deep. However, in this structure, the rectangles often overlap so much that more subtrees need to be searched during spatial queries. Therefore R-trees generally perform well, but do not guarantee good worst-case performance \cite{14}.

For the optimization of the R-tree structure, most of scholars choose to alternate the node separation strategy to deduce the overlap between nodes \cite{9}, \cite{39}. Among their proposed methods, the most effective refinement might be R*-tree \cite{10}, whereas the priority R-tree \cite{11} enhances the worst-case performance of R-tree.

C. VoR-tree

The VoR-tree \cite{13} is a state-of-the-art R-tree based spatial index. A VoR-tree is a combination of an R-tree and a Voronoi diagram. This index structure benefits from both the neighborhood exploration capability of Voronoi diagrams and the hierarchical structure of R-tree.

III. BACKGROUND

A. Voronoi diagram and its properties

The Voronoi diagram \cite{17}, proposed by Rene Descartes in 1644, is a spatial partition structure widely applied in many science domains, most notably spatial database and computational geometry. In a Voronoi diagram of $n$ points, the space is divided into $n$ regions corresponding to these points, which are called Voronoi cells. For each point of these $n$ points, the corresponding Voronoi cell consists of all locations closer to that point than to any other. In other words, each point is the NN of all the locations in its corresponding Voronoi cell. Formally, the above description can be stated as follows. Given a set $P$ of $n$ points, the Voronoi cell of a point $p \in P$, written as $V(P, p)$, is defined as \cite{4}

$$V(P, p) = \{q| \forall p' \in P, p' \neq p, \|p - q\| \leq \|p' - q\|\} \quad (4)$$

and the Voronoi diagram of $P$, written as $VD(P)$, is defined as \cite{5}.

$$VD(P) = \{V(P, p) | p \in P\} \quad (5)$$

The Voronoi diagram has the following properties:

**Property 1**: The Voronoi diagram of a certain set $P$ of points, $VD(P)$, is unique.

**Property 2**: Given the Voronoi diagram of $P$, the nearest point of $P$ to a point $q \in P$ is among the Voronoi neighbors of $q$. That is, the closest point to $q$ is one of generator points whose Voronoi cells share a Voronoi edge with $V(P, q)$.

**Property 3**: Given the Voronoi diagram of $P$ and a test point $q \notin P$, a point $p'$ is the nearest point of $P$ to $p$ if and only if $q \in V(P, p')$.

**Property 4**: Property 2 and Property 3 suggests that, given a point set $P$ and a test point $q \notin P$, the second nearest point of $P$ to $q$ is among the Voronoi neighbors of $NN(P, q)$.

**Property 5**: By generalizing Property 4, we can obtain the following relationships holds:

Let $p_1, p_2, \cdots, p_k$ be the $k \geq 1$ nearest points of $P$ to a query point $q$ (i.e., $p_i$ is the $i$-th nearest neighbor of $q$), then, $p_k$ is a Voronoi neighbor of at least one point $p_i \in \{p_1, p_2, \cdots, p_k\}$ ($p_k \in VN(p_i)$) \cite{13}.

**Property 6**: Let $n_n, n_e$, and $n_v$ be the number of generator points, Voronoi edges and Voronoi vertices of a Voronoi diagram in $\mathbb{R}^2$, respectively, and assume $n \geq 3$. Then,

$$n + n_v - n_e = 1 \quad (6)$$

Every Voronoi vertex has at least 3 Voronoi edges and each Voronoi edge belongs to two Voronoi vertices, hence the number of Voronoi edges is not less than $3(n_v + 1)/2$, i.e.,

$$n_e \geq \frac{3}{2} (n_v + 1) \quad (7)$$

According Formula (6) and Formula (7), the following relationships holds:

$$n_e \leq 3n - 6 \quad (8)$$

$$n_v \leq 2n - 5 \quad (9)$$

**Property 7**: When the number of generator points is large enough, the average number of Voronoi edges per Voronoi cell of a Voronoi diagram in $\mathbb{R}^d$ is a constant value depending only on $d$. When $d = 2$, every Voronoi edge is shared by two Voronoi Cells. Hence, the average number of Voronoi edges per Voronoi cell does not exceed 6, i.e., $2 \cdot n_v/n = 2(3n - 6)/n = 6 - 12/n \leq 6$.

B. Delaunay triangulation and its properties

Delaunay triangulation \cite{4} is a very famous triangulation proposed by Boris Delaunay in 1934. For a set $P$ of discrete points in a plane, the Delaunay triangulation $DT(P)$ is such a triangulation that no point in $P$ is inside the circumcircle
of any triangle of $DT(P)$. The Delaunay triangulation has the following properties:

**Property 8:** The Delaunay triangulation of a set of points is dual to its Voronoi diagram.

**Property 9:** A graph of Delaunay triangulation must be a connected graph, that is, any two vertices in the graph are connected.

**Property 10:** For a set of points, its nearest neighbor graph is a subgraph of its Delaunay triangulation graph.

**Property 11:** The Delaunay triangulation of $n$ points in $\mathbb{R}^d$ contains $O(n^{d/2})$ simplices, where a $d$ dimensional simplex, the generalization of triangle, consists of $d+1$ points.

### IV. Structure of MVD

In this section, we introduce the structure of MVD, a novel non-tree spatial index we proposed, and describe its construction method in detail.

![Fig. 3: a) Binary sort tree, b) Multilayer linked list](image)

As aforementioned, all the tree spatial indexing are through distributing the data points to the Multi-layer subspace. This process can achieve the NN search with logarithm time complexity. On this indexing structure, it is difficult to satisfy both the balance of the tree and the independence of the subspace corresponding to the nodes. However, the unbalance of the tree and the spatial overlap of the nodes severely affect the efficiency of the spatial search. In the past literature, the neighboring relations in the physical space are projected to the network topology structure and this network structure helps to accelerate the NN related spatial search. The VoR-tree is one of the typical examples. This combination of indexing strategy can effectively improve the $k$NN search to a certain extent, but the cause of its logarithm search efficiency of $NN$ search is still its tree main indexing structure. Thus, it cannot completely solve the weaknesses of the tree indexing structures. Hence to avoid this dilemma entirely, it is only possible to abandon the tree structure to design a new non-tree indexing structure.

The tree structure indexing can always bring the logarithm search efficiency, because it has a pyramid structure, namely, from the top root node travelling down layer by layer with a logarithm growth of the data scale. As in Figure 3(a), we demonstrate a binary search tree which manages $n$ numbers. Based on this structure, we can easily find any number by using $O(log n)$ visits to obtain any other number.

Is it only possible to achieve the logarithm complexity search by the layer-by-layer partition of the data with a certain rules? The answer is certainly no. Figure 3(b) demonstrates a 3-layer list structure where there are several connections between every two layers. At the bottom layer of this structure, there are $n$ integer values from 1 to $n$ stored in order. The second layer stores the numbers sampled from the first layer with the interval of 1/2. Evidently, this list is also ordered. Constructing the structure with the same rule, we can have this specific structure. From this specific structure, we can also find any point by traversal with $O(log n)$ times. Therefore, as long as we guarantee the list on each layer is ordered, i.e., the nearest nodes are connected in terms of the order, the search can be accomplished with the logarithm complexity.

If we extend this structure to two or higher dimensions, we can replace the sort operation with constructing the Voronoi diagram. The nearest nodes on the space can be connected. Then the data are evenly sampled from them by a certain proportion to be the upper layer. We repeat this process, until the data size of the current layer is small enough. This resulting Multi-layer Voronoi diagram structure is named as MVD. The pseudo code of the aforementioned process to create the MVD is presented in Algorithm 1, where the parameter $k$ is referred to as the construction parameter which represents the data size in the lower layer is $k$ times of what is in the upper layer across the layers. For the methods to search for the nearest neighbors based on the MVD space, we are intended to detail them in the next section.

```
Algorithm 1 MVD
Input: The point set $P$
Parameter: $k$
Output: The Multi-layer Voronoi Diagrams of $P$, $M_P$
1: $V := VD(P)$;
2: $M_P := [V]$;
3: while $Size(P) > k$ do
4:    $P := Sample(P, Size(P)/k)$;
5:    $V := VD(P)$;
6:    Append($M_P, V$);
7: end while
8: return $M_P$.
```

### V. Query Processing on MVD

In this section, we introduce the query processing on MVD from the aspects of NN and $k$NN, and elaborate on their
operation mechanism and theoretical time complexity.

A. Nearest Neighbor Query

Given a Voronoi graph, if we assume that from any generator point we can arrive at its Voronoi neighbor by moving one step only, for any two generator points, at least one connection path exists through several generator points in the neighborhood based on Property 8 and 9. This path is named as the Voronoi connection path. Certainly, there is not only one Voronoi connection path between any two nodes. If we can find one shortest path among those, namely the path through the least number of generators, we can start from any node, traverse the least intermediate nodes and visit the target node.

According to the definition of NN and Property 3, we can draw such an inference: given the Voronoi diagram of a point set \(P\) and a test point \(q \notin P\), a point \(p'\) is the closest point of \(P\) to \(q\), if and only if it satisfies the following condition:

\[
\forall p \in VN(P, p'), \|p' - q\| \leq \|p - q\| \tag{10}
\]

Conversely, we can further make the following corollary by reductio ad absurdum: given an arbitrary point \(p* \in P\) that is not the closest point to \(q\), there must exist a point in Voronoi neighbors of \(p*\) which is closer to \(q\) than \(p*\). Formally, it can be written as follows:

\[
\forall p* \in P\setminus \{NN(P, q)\}, \exists p \in VN(P, p*) : \|p - q\| < \|p* - q\| \tag{11}
\]

Based on this deduction, we develop the VD-NN search algorithm. It is an NN search algorithm based on the Voronoi diagram which finds the nearest neighbor node of the target node through the shortest Voronoi connection path. The pseudo code is presented as in Algorithm 2.

Firstly, we heuristically start from any point in the point set \(P\). If the Voronoi neighborhood of the point \(p\) contains the point that is closer to the \(P\) distance search point \(q\), then we will move to a point closest to \(q\) in \(p\)'s Voronoi neighborhood. We repeat this process until the point at the current location does not have any point which is closer to \(q\). The point where we terminate at, is the nearest neighbor point of \(q\) in the point set \(P\).

For a set \(P \in \mathbb{R}^d\) consisting of \(n\) points, the mean time complexity of VD-NN is \(O(n^{1/d})\). Since the initial point is randomly selected, this value is really uncertain. In the ideal circumstance, when starting from a very close point to the search point, the time complexity becomes extremely low and even can reach the constants. Therefore, the efficiency of VD-NN is very sensitive to the choice of the starting point.

With the MVD structure, we realize the NN search algorithm MVD-NN with logarithm time complexity, through multiple efficient executions of calls for VD-NN. Given a \(h\)-layer MVD generated by the point set \(P\) consisting of \(n\) points, the following procedure is to search for the nearest neighbor point of \(q\) from the point set \(P\) applying the MVD-NN algorithm. Firstly, the starting point is randomly selected from the top of MVD. In subsequence, VD-NN is called to find the point \(p_q\) which is closest to \(q\). Then we use \(p_1\) as

Algorithm 2 VD-NN

\begin{algorithm}
\KwIn{The Voronoi Diagrams \(V_P\), the query point \(q\) and starting point \(p_s\)}
\KwOut{The nearest neighbor point of \(q\) \(nn_q\)}
\begin{algorithmic}
1: \textbf{if} \(p_s \neq \text{Null} \) \textbf{then}
2: \hspace{1em} \(nn_q := p_s\);
3: \textbf{else}
4: \hspace{1em} \(nn_q := \text{Sample}(P)\);
5: \textbf{if} \(q \notin \text{Visited} \)
6: \hspace{1em} \(\text{Visited} := \{nn_q\}\); 
7: \hspace{1em} \(\text{found} := \text{False}\);
8: \hspace{1em} \textbf{while} \text{not} \text{found} \textbf{do}
9: \hspace{2em} \(\text{found} := \text{True}\);
10: \hspace{2em} \textbf{for all} \(n \in V_P[nn_q]\) \textbf{do}
11: \hspace{3em} \(\text{if} \ q \notin \text{Visited} \)
12: \hspace{4em} \(\text{Visited} := \text{Visited} \cup \{n\}\);
13: \hspace{4em} \textbf{if} \(\|q - n\| < \|q - nn_q\|\) \textbf{then}
14: \hspace{5em} \(nn_q := n\);
15: \hspace{5em} \(\text{found} := \text{False}\);
16: \hspace{4em} \textbf{end if}
17: \hspace{4em} \textbf{end if}
18: \hspace{3em} \textbf{end for}
19: \hspace{2em} \textbf{end while}
20: \hspace{1em} \textbf{return} \(nn_q\).
\end{algorithmic}
\end{algorithm}

the new starting point and call VD-NN to obtain the point \(p_2\) closest to \(q\). This process is executed recursively. Eventually, we can reach the last layer to attain \(p_n\). \(p_h\) is the nearest neighbor point of \(q\) in \(P\). When building MVD with \(k=10\) and 2 dimensions, it only needs approximately \(\sqrt{10} \approx 3\) nodes to find \(p_1\) from a random starting point in the first layer. The reason is that in the second layer, \(p_1\) is really close to \(p_2\). Hence \(p_2\) can also be acquired after 3 nodes starting from \(p_1\). Similarly, this procedure appears in the following layers. In each layer of MVD, the time complexity to execute VD-NN is \(O(k^{1/d})\) which is actually a constant as \(k\) is a constant. However, the number of layers of MVD is \(\log_n\). Therefore, the time complexity of MVD-NN is approximately \(O(\log n)\).

Algorithm 3 MVD-NN

\begin{algorithm}
\KwIn{The Multi-layer Voronoi Diagrams \(M_P\) and the query point \(q\)}
\KwOut{The nearest neighbor point of \(q\) \(nn_q\)}
\begin{algorithmic}
1: \(i := \text{Size}(M_P) - 1\);
2: \textbf{while} \(i > 0\) \textbf{do}
3: \hspace{1em} \(V := M_P[i]\);
4: \hspace{1em} \(nn_q := \text{VD-NN}(V, q, nn_q)\);
5: \hspace{1em} \(i := i - 1\);
6: \textbf{end while}
7: \textbf{return} \(nn_q\).
\end{algorithmic}
\end{algorithm}

B. \(k\) Nearest Neighbor Query

As with VoR-tree, MVD uses the characteristics of the Voronoi graph. It achieves the \(kNN\) query through the in-
incremental method which finds the second until the \( k \)-th nearest neighbor point by the extension of the NN search. Nevertheless, our structure still has two major differences with VoR-tree. The first difference is that the \( k \text{NN} \) search of VoR-tree is extended from BFS that is the NN search algorithm based on R-tree, whereas MVD-\( k \text{NN} \) is extended from MVD-NN. Of course, the choice of the basic NN algorithm can indirectly influence the efficiency of \( k \text{NN} \) algorithm. For the second difference, in the realization of the incremental \( k \text{NN} \) algorithm, we use the fixed length ranking array. The reason is discussed in detail in the following description of the algorithm.

![Fig. 4: \( k \text{NN} \) of \( q \)](image)

Figure 4 demonstrates the Delaunay graph a point set \( P \), and a query point \( q \). If we use \( p_i \) to represent the \( i \)-th (\( i > 1 \)) closest point to \( q \), we can present Property 5 as the following formulae.

\[
p_i \in \bigcup_{j=1}^{i-1} VN(P, p_j)
\]  

Since \( p_i \) is certainly not possible to appear in the set of the \((i-1)\)-th nearest neighbors of \( q \) and this set has to be a subset of the candidate set of Formula (12), we can further narrow down the candidate set of \( p_i \) as shown in Formula (13).

\[
p_i \in \bigcup_{j=1}^{i-1} VN(P, p_j) \setminus \{p_1, p_2, \ldots, p_{i-1}\}
\]  

Therefore, from the first nearest neighbor, by adding its Voronoi neighbor, we update the candidate set. Following that, we can find the second nearest neighbor and include the second nearest neighbor to update the candidate set. The we find the third nearest neighbor from the candidate set. We repeat this process until we obtain the \( k \)-th nearest neighbor. From this whole process, we can realize the incremental \( k \text{NN} \) algorithm based on Voronoi. If the process to update the candidate set and search the nearest neighbor from the candidate set can be seen as an atomic operation, the time complexity of the this algorithm is \( O(k) \). In order to improve the efficiency of the update and search process, in the VoR-tree, there is a minimum heap in each point of the candidate set. If the size of the candidate set is \( m \), the operation to add and pop to this candidate set is \( O(\log m) \). From Property 7, in the circumstance to obtain 2 dimensions, \( m \leq 6k \). In general, the time complexity of the \( k \text{NN} \) algorithm based on the VoR-tree is approximately \( O(\log n + k \cdot \log k) \).

In the MVD-\( k \text{NN} \) algorithm whose pseudo code is presented in Algorithm 4, we utilize the candidate set with the length of \( k \). Since we only need to acquire the \( k \)-th nearest neighbors before the search point in the \( k \text{NN} \) search, we can eliminate one point from the candidate set if there are more than \( k \) points being closer to the search point at a certain stage. With the purpose to improve the efficiency of this elimination strategy, we have to ensure the candidate set to be ordered in the whole execution process of this algorithm. For the whole operation of every inserted new point, the worst-case time complexity is \( O(k) \) and the best-case is \( O(1) \). Therefore, the time complexity of MVD-\( k \text{NN} \) is between \( O(\log n + k) \) and \( O(\log n + k^2) \). However, it is evident that if a point \( p \) is closer to \( q \) than the point \( p' \), there is an extremely high probability to have a smaller distance between a Voronoi neighbor of \( p \) and \( q \) than the distance between a Voronoi neighbor of \( p' \) and \( q \). Thus, when maintaining this ordered array, every time we insert a new point, the order of this new point is usually very close to \( k \) and this point even can be eliminated straightforwardly. It means that the time complexity of the MVD-\( k \text{NN} \) can be closer to \( O(\log n + k) \) in most cases. It is certainly not stable, but the MVD-\( k \text{NN} \) maintains a smaller temporary candidate set compared with the VoR-\( k \text{NN} \) and therefore the memory cost of execution is much smaller than the VoR-\( k \text{NN} \), especially when the dimension is high.

**Algorithm 4 MVD-\( k \text{NN} \)**

| Input: The Multi-layer Voronoi Diagrams \( M_P \), the query point \( q \) and \( k \) |
|---|
| Output: The \( k \text{NN} \) list \( K \) |

1. \( nn_q := MVD-\text{NN}(M_P, q) \);
2. \( K := [nn_q] \);
3. \( Visited := \{nn_q\} \);
4. \( V_p := M_P[i] \);
5. for \( i := 1 \) to \( k - 1 \) do
6. for all \( n \in V_p[K[i]] \) do
7. if \( n \notin Visited \) then
8. \( Visited := Visited \cup \{n\} \);
9. for \( j := i + 1 \) to Size(\( K \)) do
10. if \( ||q - n|| < ||q - K[j]\) \) then
11. Insert(\( K, j, n \))
12. if Size(\( K \)) > \( k \) then
13. Pop(\( K \))
14. end if
15. break
16. end if
17. end for
18. if Size(\( K \)) < \( k \) and \( n \notin K \) then
19. Append(\( K, n \))
20. end if
21. end if
22. end for
23. end for
24. return \( K \).
VI. MAINTENANCE OF MVD

As discussed in the sections above, we introduce how to create an MVD structure based on a given point set. However, a spatial index can still be used for dynamic data, if it contains the dynamic updating mechanism including deleting and adding the points. In this section, we describe the insert algorithm: MVD-Insert and the deleting algorithm: MVD-Delete with the MVD structure. The pseudo code is demonstrated in Algorithm 5 and Algorithm 6 respectively.

Assume that there is an MVD indexing $M_P$ which consists of the point set $P$. The process to insert a new point $p$ is as follows. Firstly, we add $p$ to the bottom layer of $M_P$ by the VD-Insert algorithm of the Voronoi diagram. The best VD-Insert algorithm has the mean time complexity as $O(log n)$. Secondly, if there is an upper layer, we move one layer up and add $p$ with the probability of $1/k$ by the VD-Inser algorithm. Thirdly, if we successfully insert $p$ in this layer, we still insert $p$ with the same probability step by step. Until $p$ cannot be inserted in a certain layer, we terminate the whole process. If we also succeed in inserting $p$ to the top layer, we can add one more layer to $M_P$ with the probability of $1/k$ and insert $p$. Obviously, as the number of layers increases, the probability of $p$ to be inserted to this layer is decreased. This strategy guarantees that after inserting a large number of new points, the number of points in each layer of $M_P$ is still $k$ times to the last layer. Similar with the MVD-Insert, after the execution of the MVD-Delete, the proportion of the number of points between the near layers should be maintained the same in $M_P$. Therefore, the execution of the MVD-Delete is as follows. We traverse all the layer of $M_P$. For every layer, if one layer contains $p$, we use the VD-Delete as the deleting algorithm in the Voronoi diagram with the time complexity $O(1)$ and eliminate $p$. Also we insert the nearest neighbor of $p$ at the lower layer with the probability $(1-1/k)$. Otherwise $p$ is eliminated in this layer with the probability $1/k$. From the above description of the algorithm, it is obvious that the time complexities of the MVD-Insert and the MVD-Delete are $O(log^2 n)$ and $O(log n)$ respectively.

VII. EXPERIMENTS

In the previous content, we discuss the theoretical advantages of the MVD. In this section, we intend to evaluate the performance of the MVD on the spatial nearest neighbor search with numerical experiments.

A. Experimental settings

In the experiments, we apply the two most common spatial indexing structures kd-tree and R-tree, and the state-of-the-art indexing as a derivative of R-tree: VoR-tree, to be the benchmarks. Thus, we can investigate the performance of MVD on the spatial nearest neighborhood in terms of the NN search and the kNN search. These four indexing methods and their related algorithms are implemented using Python. As for the parameter settings, the kd-tree has the leaf size as 100, R-tree and VoR-tree have the node capacity as 100, and MVD has $k = 100$. There are three types of our datasets used in the experiments: the simulated evenly distributed discrete data, i.e., uniform data, the simulated exponential distributed discrete data, i.e., nonuniform data, and the real-world data which are 49,603 non-repeated geographical coordinate data points from National Register of Historic Places, i.e., the US data. These data are demonstrated as in Figure 5.

The settings of our experiment environment are as follows.

| Parameter | Value |
|-----------|-------|
| CPU       | Intel Core i5-4308U 2.80GHz |
| RAM       | DDR3 8G |
| Dataset   | Simulated evenly distributed discrete data, simulated exponential distributed discrete data, real-world data |
| k         | 100 |

The algorithm is as follows:

**Algorithm 5 MVD-Insert**

**Input:** The Multi-layer Voronoi diagrams $M_P$ and the point $p$ to be inserted

**Parameter:** $k$

1. $V := M_P[0]$;
2. VD-Insert($V$, $p$);
3. for $i := 1$ to Size($M_P$)
   4. if Random$(0, 1) < 1/k$
      5. if $i <$ Size($M_P$)
         6. VD-Insert($M_P[i]$, $p$);
      7. else
         8. $V := VD\{p\}$;
         9. Append($M_P$, $V$);
        10. break;
   11. break;
4. end if
5. end if
6. end for

**Algorithm 6 MVD-Delete**

**Input:** The Multi-layer Voronoi Diagrams $M_P$ and the point $p$ to be deleted

**Parameter:** $k$

1. $V := M_P[0]$;
2. VD-Delete($V$, $p$);
3. for $i := 1$ to Size($M_P$) - 1 do
   4. $V := M_P[i]$;
   5. if $p \in V$
      6. VD-Delete($V$, $p$);
      7. if Random$(0, 1) < 1 - 1/k$
         8. $V' := M_P[i - 1]$;
         9. VD-Insert($V$, NN($V'$, $p$));
      10. end if
   11. else if Random$(0, 1) < 1/k$
      12. $p := NN(V, p)$;
      13. VD-Delete($V$, $p$);
      14. end if
   15. if Size($V$) = 0
      16. Remove($M_P$, $V$);
   17. end if
5. end for
TABLE I: Total computation time (in ns) of NN queries from data sets with various sizes.

| Size | Uniform | Nonuniform |
|------|---------|------------|
|      | MVD | VoR-tree | R-tree | kd-tree | MVD | VoR-tree | R-tree | kd-tree |
| $10^1$ | 14  | 42  | 42  | 73  | 14  | 45  | 44  | 72  |
| $10^2$ | 24  | 157 | 157 | 101 | 23  | 137 | 135 | 79  |
| $10^3$ | 47  | 158 | 156 | 159 | 36  | 129 | 134 | 156 |
| $10^4$ | 62  | 175 | 176 | 208 | 46  | 298 | 305 | 281 |
| $10^5$ | 86  | 191 | 193 | 225 | 61  | 2190 | 2331 | 1399 |

TABLE II: Total computation time (in ns) of $k$NN queries with various values of $k$.

| $k$ | Uniform | Nonuniform | US |
|-----|---------|------------|----|
|     | MVD | VoR-tree | R-tree | kd-tree | MVD | VoR-tree | R-tree | kd-tree | MVD | VoR-tree | R-tree | kd-tree |
| 2   | 82  | 185 | 227 | 72  | 356 | 361 | 117 | 195 | 199 | 258 |
| 4   | 95  | 196 | 242 | 86  | 367 | 382 | 129 | 210 | 220 | 299 |
| 8   | 114 | 215 | 287 | 105 | 402 | 453 | 157 | 226 | 232 | 352 |
| 16  | 152 | 253 | 343 | 136 | 544 | 592 | 189 | 269 | 279 | 407 |
| 32  | 228 | 328 | 489 | 199 | 714 | 778 | 276 | 348 | 353 | 562 |
| 64  | 343 | 448 | 617 | 319 | 944 | 1065 | 430 | 475 | 482 | 769 |

TABLE III: Total computation time (in ns) of NN and $k$NN queries from data sets with various dimensions.

| Dimension | Uniform | Nonuniform | $k$NN |
|-----------|---------|------------|--------|
|           | MVD | VoR-tree | R-tree | kd-tree | MVD | VoR-tree | R-tree | kd-tree |
| 2         | 62  | 175 | 173 | 205 | 158 | 252 | 259 | 368 |
| 3         | 66  | 244 | 246 | 233 | 329 | 493 | 494 | 476 |
| 4         | 105 | 351 | 342 | 306 | 746 | 994 | 821 | 705 |
| 5         | 185 | 509 | 505 | 409 | 1687 | 2018 | 1251 | 947 |
| 6         | 351 | 831 | 824 | 546 | 3803 | 4165 | 1891 | 1225 |

Fig. 5: a) Uniform data, b) Nonuniform data, c) US data

Fig. 6: NN from uniform data sets with various sizes

is mainly the total CPU computation of the algorithm. However, the total CPU computation can directly reflect the total time consumed for the execution of the algorithm. Therefore, for every spatial query method, we evaluate the performance of these algorithms based on the comparison of their time cost for one search. To decrease the error of the experiments, we repeat each experiment for $30 \times 1000$ times and calculate the average time cost.
Fig. 7: $k$NN from nonuniform data sets with various sizes

Fig. 8: $k$NN from uniform data sets with various $k$

Fig. 9: $k$NN from nonuniform data sets with various $k$

Fig. 10: $k$NN from US data set

Fig. 11: $k$NN from data sets with various dimensions

Fig. 12: $k$NN from data sets with various dimensions
B. Experimental results

For the NN search, we use the uniform data and nonuniform data simulated in 2 dimensions from two distributions, in order to evaluate the performance of these indexing methods in different scales of data. The comparison of their performance is presented in Figure 6 and 7. The detailed results are demonstrated in Table I.

For the kNN search, we investigate its performance with a set of uniform data, a set of nonuniform data and the US dataset, where the uniform dataset and the nonuniform dataset have the size as 10,000 and 2 dimensions. The comparison of their performance is demonstrated as in Figure 8, 9 and 10. The details of it are presented in Table II.

To investigate the sensitivity of these indexing methods to the dimension, we evaluate their performance on NN and kNN on 5 datasets with different dimensions. The size of these two datasets are all 10,000 and they are all evenly distributed. The comparison of their performance is demonstrated as in Figure 11 and 12. The details of it are presented in Table III.

From the experiment results above, we can observe that MVD outperforms the other 3 indexing structures no matter in NN or kNN on 5 datasets with different dimensions. The size of these two datasets are all 10,000 and they are all evenly distributed. The comparison of their performance is demonstrated as in Figure 8, 9 and 10. The details of it are presented in Table II.

The comparison of their performance is demonstrated as in Figure 11 and 12. The details of it are presented in Table III.

To investigate the sensitivity of these indexing methods to the dimension, we evaluate their performance on NN and kNN on 5 datasets with different dimensions. The size of these two datasets are all 10,000 and they are all evenly distributed. The comparison of their performance is demonstrated as in Figure 11 and 12. The details of it are presented in Table III.

From the experiment results above, we can observe that MVD outperforms the other 3 indexing structures no matter in NN or kNN for the 2 dimensional case, especially in the case of the uneven distribution. The reason is that MVD has the non-tree indexing structure. Since there is no spatial partition from the tree structure, there is no belonging relations among the nodes in MVD but only the connection relations. No node statically belongs to a certain node in an upper layer. Thus, our indexing structure does not incur the situation where there are too many layers from losing the balance. For the NN and kNN search, it is not required to evaluate too many node data from the overlap among nodes.

| Dimension | 2      | 3      | 4      | 5      | 6      |
|-----------|--------|--------|--------|--------|--------|
| Value     | 5.9942 | 15.3938| 35.6104| 76.7206| 153.8450|

In the sensitivity test to the dimensions, it can be viewed that our indexing structure is the same as the other indexing structures: the curse of dimensionality cannot be avoided. As the dimension increases, the efficiency of these four indexing methods gradually decays. Fortunately, for the NN search, as the dimension becomes larger, the time cost is already less than the other structures. Besides, for kNN, the search efficiency of MVD and VoR-tree is evidently less than R-tree and kd-tree in the case when the dimension is larger than 4. From Property 7 and 11, the topological structure of the high-dimensional Voronoi diagram. As the dimension increases, the average number of Voronoi neighbors significantly increases. We use the experiment of 10,000 discrete points to list the average number of Voronoi neighbors for every point for the dimensions between 2 to 6 as in Table IV. From this table, the number of the point-wise average number of Voronoi neighbors has the logarithm increase. The kNN search methods of MVD and VoR-tree are both through a Voronoi diagram to extend the NN search. For the high-dimensional cases, this incremental algorithm requires to evaluate more points, in order to ensure the nearest k neighbors, so the efficiency is significantly jeopardized.

VIII. Conclusions

We review the major methods for the NN/kNN search structures and methods, and analyze the weaknesses of the traditional tree indexing methods in the nearest neighbor search. Then we propose a spatial indexing structure with the Multi-layer Voronoi diagram. This indexing method abandons the tree structure, uses the neighborhood exploration and the layer-by-layer approaching abilities of the Voronoi diagram, and realizes the stable and efficient NN search and kNN search. The theoretical analysis and the experiments indicate that the efficiency of MVD is significantly higher than the tree structure indexing such as kd-tree, R-tree and VoR-tree, in terms of the real physical spatial nearest neighbor search. However, MVD also has its limitations:

- The number of realized spatial search methods based on this structure is still quite small. Nevertheless, we already begin the research for the other spatial search method based on this structure, where the range search has achieved the initial success.

- Currently, we only propose the MVD construction and nearest neighbor search methods based on the internal memory environment, and are not able to adapt to the extremely large-scale data management circumstance. Therefore, we also started the strategies on the external memory and the distributed environment.

- Because of the nature of the Voronoi diagram, MVD is very sensitive to the dimensions. Thus, when the scale of the dataset is not large enough and the dimension is high, its performance is not satisfactory enough. There is still a research gap on how to improve the search efficiency under the MVD structure in the high-dimensional circumstance.

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