Index-based Solutions for Efficient Density Peaks Clustering

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ABSTRACT

Density Peaks Clustering (DPC), a novel density-based clustering approach, has received considerable attention of the research community primarily due to its simplicity and less parameter requirement. However, the resultant clusters obtained using DPC are influenced by its sensitive parameter \(d_c\) which depends upon data distribution and requirements of different users. Besides, the original DPC algorithm requires visiting a large number of objects making it slow.

To this end, this paper investigates index-based solutions for DPC. Specifically, we propose two list-based index methods viz. (i) a simple List Index and (ii) an advanced Cumulative Histogram Index. Efficient query algorithms are proposed for these indices which significantly avoids irrelevant comparisons at the cost of space. To remedy this for memory-constrained systems, we further introduce an approximate solution to the above indices which allows substantial reduction in the space cost provided slight inaccuracies are admissible. Furthermore, owing to considerably lower memory requirements of existing tree-based index structures, we also present effective pruning techniques and efficient query algorithms to support DPC using the popular Quadtree Index and R-tree Index. Finally, we practically evaluate all the above indices and present the findings and results, obtained from a set of extensive experiments on six synthetic and real datasets. The experimental insights obtained help to guide in selecting the befitting index.

1. INTRODUCTION

Clusters reflect a potential relationship among different entities of data. This data can be sourced from a wide-ranging domains like market research, social network analysis, spatial data analysis, pattern recognition, etc. Many clustering algorithms have been developed in last few decades in response to the proliferating demands across industries and organizations which helps them to make operational and strategic decisions. Among them, the density-based clustering algorithms are popular as they can identify arbitrary shaped clusters. The basic idea of these algorithms is to find subsets of objects in “dense regions” separated by not-so dense region where each subset represents a cluster.

In this paper, our focal point will be Density Peaks Clustering (DPC), a novel approach towards obtaining density-based clusters, proposed by Rodrigues and Laio [19]. The key aspects of DPC apart from its simplicity are (i) it does not require prespecifying the number of cluster centers, (ii) it finds arbitrary shaped clusters, (iii) it requires minimum parameters, (iv) it gives users the flexibility to select the number of cluster centers intuitively from its unique decision graph. In recent years, DPC has been studied and employed by researchers to solve problems in various domains, such as time-series data mining problems [4], neuroscience [14], geoscience [21], biology [25], computer vision [7], etc.

DPC aims to identify the cluster centers among the set of objects for which it defines two metrics (i) local density \(\rho\) and (ii) dependent distance \(\delta\). Given a set of objects \(P\) and parameter \(d_c\), local density \(\rho\) of an object \(p \in P\) denotes the the number of objects within distance \(d_c\) from \(p\). The dependent distance \(\delta\) for an object \(p \in P\) is the distance to its nearest higher density neighbor. Based on this, cluster centers are selected as objects having high \(\rho\) and large \(\delta\). Once cluster centers have been determined, rest of the objects are assigned to clusters containing their nearest higher density neighbor. However, there are two major challenges.

- **Parameter Selection.** DPC suffers from the parameter setting problem and its clustering results are heavily influenced by \(d_c\). The selection of parameter \(d_c\) is dependent on data distribution. Moreover, a user can have various requirements for clustering and wants to test several \(d_c\) to obtain a desired clustering. Besides, different users may want different clustering results for different \(d_c\). Figure 1 illustrates that setting different \(d_c\) will produce different clustering results based on the real-world dataset Gowalla containing user check-ins for the area around US and Caribbean.

- **Query cost.** Given a \(d_c\), DPC algorithm needs to determine the pair-wise distances and compute the two metrics \(\rho\) and \(\delta\) for each object which requires visiting a large number of irrelevant objects. As this has prohibitive time cost for large datasets, running the DPC algorithm for different values of \(d_c\) further exacerbates the problem.

Motivated by the above challenges, this paper aims to investigate employing index to speed up DPC for a given \(d_c\). As such, the whole clustering process which probably
involve trying many $d_c$ can be substantially shortened. The importance of such a solution is impelled more by the fact that there are two expensive queries for each object.

To this end, we propose two list-based index structures namely List Index and Cumulative Histogram (CH) Index. The List Index efficaciously captures the neighborhood of an object which facilitates fast access to close neighbors and allows bypassing the need to compare most objects for finding clusters. Based on List Index, efficient query algorithms are proposed to compute DPC metrics for any clusters. However, for large datasets, the computation of $\rho$ using List Index is still expensive. Therefore, the advanced CH Index is proposed which enables fast computation of $\rho$. Both of these indices require large memory cost which may not be suitable for memory-constrained systems. To this end, we present an approximate solution which significantly reduce the space cost with slight loss in accuracy.

Furthermore, we also study the tree-based index structures capable of providing fast data access and substantially lower memory requirements. Moreover, they have efficient support to several queries such as range and nearest neighbor (NN) search. Range search can be easily adapted to compute $\rho$, however, large number of search operations are still needed. Moreover, the computation of $\delta$ is different to NN search query and requires developing algorithm for it. In this context, we provide enhanced $\rho$ and $\delta$ queries based on effective pruning techniques using the popular Quadtree and R-tree Index to make them competitive for DPC.

We summarize the key contributions of this paper as follows.

- **The first work to study index-based approaches for density peaks clustering.** This paper presents effective index-based methods for DPC. To the best of our knowledge, this is the first work to support DPC using index-based approaches.

- **List-based index.** We propose two list-based index structures namely List Index and CH Index along with efficient query algorithms. An approximate solution is also suggested for the memory-constrained systems to reduce the space cost.

- **Tree-based index.** We revisit the popular tree-based index structure having lower space cost and present efficient algorithms based on effective pruning techniques using the Quadtree Index and R-tree Index.

- **Extensive experimental evaluation.** Finally, we conduct extensive experiments to evaluate the proposed and existing index structures on six datasets.

The rest of the paper is organized as follows. Section 2 revisits the DP method. In Section 3, we introduce our proposed list-based indices and their respective query algorithms followed by the tree-based index structures in Section 4. The comprehensive evaluation of the proposed index structures is done in Section 5. Section 6 deals with the related work. Lastly, Section 7 concludes the paper.

## 2. PRELIMINARY

In this section, we first discuss the original Density Peaks clustering method and then discuss our index-based approach.

### Density Peaks Clustering (DPC):

DPC [19] is based on the observation that cluster centers are characterized by (i) locally higher density, i.e., densities of cluster centers are higher than the neighboring objects, and (ii) relatively large separation, i.e., they are at a relatively large distances from other objects with higher local densities. On the basis of this observation, DPC distinguishes the cluster centers from rest of the objects. Let $P$ be a set of objects, then the clustering procedure of DPC involves mainly four steps as follows:

1. **Compute local density $\rho_p$.** The local density $\rho_p$ of an object $p \in P$ is computed as

   $$\rho_p = \sum_{q \in P} \chi(dist(p,q) - d_c)$$

   where $dist(p,q)$ is the distance between $p$ and $q$, $\chi(x) = 1$ if $x < 0$, otherwise $\chi(x) = 0$, and $d_c$ is the threshold distance. Basically, $p$ of an object $p$ is the number of objects that lie within distance $d_c$ from $p$.

2. **Compute dependent distance $\delta_p$.** The dependent distance ($\delta_p$) is the minimum distance between object $p \in P$ and any other object $q \in P$ with higher density. It is computed as

   $$\delta_p = \min_{q \in P \land \rho_q > \rho_p} \{dist(p,q)\}$$

   We denote the corresponding higher density neighbor by $\mu_p$. For the highest density object (global peak) $p$, its $\delta_p = \max_{q=1}^{n} \{dist(p,q)\}$.

3. **Finding cluster centers.** Next, DPC distinguishes the cluster centers (peaks) from the set of objects based on their computed $\rho$ and $\delta$. An object with locally high density has their nearest neighbor of higher density relatively far and therefore have large $\delta$. Based on this, cluster centers are recognized as objects with high $\rho$ and anomalously large $\delta$. DPC employs a decision graph to determine the cluster centers. Figure 2a shows a data distribution of objects numeroed according to the rank of their local density. A decision graph of $\rho$ vs $\delta$ is shown in Figure 2b, which determines cluster centers (1,10) found on top right side of graph while the outliers (26,27,28) are on the left.
4. Clustering. After the cluster centers have been determined, the rest of the objects are directly assigned to the cluster containing their nearest neighbor of higher density.

The time complexity of the original DPC algorithm is $\Theta(n^2)$ dominated by the computation of pair-wise distance of objects. Then, computing $\rho$ and $\delta$ metrics for each object requires comparing a large number of objects which is expensive. The third step of finding cluster centers requires manual input from user after which the object to cluster assignment in the fourth step is done in $O(n)$ time. Thus, the first two steps of computing $\rho$ and $\delta$ metrics apart from computing the pair-wise distances are most expensive. As DPC algorithm is sensitive to $\rho$, it entails that solutions be found where, for any $d_e$, redundant computations are not made and metric queries are significantly fast to produce the decision graph from which users can recognize the cluster centers and eventually obtain the clusters. Based on this, we introduce our index-based approach for DPC.

Index-based Approach: Our approach for DPC consists of an index and efficient queries to compute $\rho$ and $\delta$ (the first and second steps of the original algorithm) correctly based on the designed index. As the third and fourth steps are inexpensive and require user input, they can be used as they are in the original algorithm. Based on this approach, we propose two list-based indices namely List Index and Cumulative Histogram Index along with efficient queries to compute $\rho$ and $\delta$ for each object. We also enable the popular tree-based indices Quadtree and R-tree for handling the large datasets by developing enhanced queries based on effective pruning techniques for computing the two metrics. Once these metrics are obtained, cluster centers are determined using the decision graph and finally the object to cluster assignment is done by following the the third and fourth steps of the original algorithm.

3. LIST-BASED INDEX STRUCTURES

In this section, we present our proposed List Index and Cumulative Histogram (CH) Index as part of list-based indices for DPC. The general idea behind list-based index is that the computation of $\rho$ and $\delta$ for an object requires neighboring objects to be retrieved and matched. However, in this process the query visits a large number of unnecessary objects. Knowing the object’s neighborhood beforehand can help to reduce the irrelevant comparisons significantly. List Index is based on the above idea and utilizes ordering technique to maintain neighbors of each object in order of their proximity. Using the List Index, efficient query algorithms for $\rho$ and $\delta$ metrics are developed which find DPC clusters in $O(n\log n)$ expected time. We propose an advanced CH Index which utilizes aggregation technique for enhancing the query processing of List Index. The CH Index integrates the merits of both cumulative histograms and list into their structure and achieves DPC clustering in just $O(n)$ expected time. We first provide an overview of the List Index and give the general idea of the query algorithms. Later we discuss the CH Index.

3.1 List Index

The List Index maintains a list known as Neighbor List (NList) for each object, such that for an object $p$, its NList($p$) stores other objects in non-decreasing order of their distance to $p$. This is useful in the sense that given a $d_e$, the portion of list containing distance $\geq d_e$ is irrelevant. Then, $\rho_p$ can be simply determined by just finding the location of farthest object with distance $\leq d_e$ in NList for which a binary search is efficient. The computation of $\delta$ is based on the observation that for peaks and outliers, $\delta$ is relatively large. This means that for most non-peak objects $p$, their $\delta_p$ is small, i.e., their $\mu_p$ lies very close to them. The NList($p$), which stores the nearest neighbor objects in the starting locations, needs to visit only few objects to retrieve the corresponding $\delta_p$. We explain the computation of these metrics using an example as follows:

Example 1. Figure 3 shows NList for the objects 10, 13, 15, 19, 22 of distribution in Figure 2 containing other objects in non-decreasing order of their distances. Suppose $d_e = 0.25$, to find $\rho_{10}$ for object 10, the number of objects in NList(10) up to the the farthest object with distance $< 0.25$ is the required $\rho_{10}$. Thus, we only need to find the location of the farthest object in NList(10) which can be efficiently performed by a binary search. Therefore, for object 10, the farthest object is 22 and its corresponding location gives the required $\rho_{10} = 4$. Similarly, we obtain $\rho_{13} = 3$, $\rho_{22} = 1$, $\rho_{15} = 3$ and $\rho_{19} = 3$. Next we explain how to compute $\delta$. For object 13, the first object in its NList(i.e., object 10 is of higher density (Remember the object ID is actually the ranking according to its density $\rho$) and is also the nearest. Thus, $\mu_{13} = 10$ and its corresponding distance gives $\delta_{13} = 0.12$ obtained in just one search. Similarly, for object 15, 19 and 22, $\delta$ can be obtained in $1$-$2$ search operations. For object 10, relatively large search operation is performed as there is no near object with smaller $\rho$. Therefore, it has relatively higher $\delta$.

3.1.1 Construction

The pseudo-code of construction of List-Index is shown in Algorithm 1. Line 1 initializes a List Index which stores the list of distances for each object. The algorithm first picks
an object \( p \), computes the distances to all other objects and stores the objects (along with their distances \( \text{dist}(p,q) \)) in a temporary list as shown in lines 3-6. This list is then sorted using an efficient sorting technique in non-decreasing order in line 6 and finally stored in List Index in line 8. This is repeated for all the objects and finally List Index is returned containing \( N\text{List} \) for each object. The time complexity of Algorithm 1 is \( O(n^2 \log n) \).

### 3.1.2 Query Algorithm

The general idea of query algorithm to compute \( \rho \) and \( \delta \) using List Index has been discussed earlier. The pseudo-code for both \( \rho \) (lines 2-5) and \( \delta \) (lines 7-12) query is given in Algorithm 2. The algorithm initializes \( \rho\text{-set}, \delta\text{-set}, \mu\text{-set} \) in line 1 as list which stores the set of \( \rho_p, \delta_p \) and \( \mu_p \) values of each object \( p \). To compute \( \rho_p \), it employs the efficient binary search technique over the \( N\text{List}(p) \) in line 5 to find the required location of object which is its corresponding \( \rho \). The computed \( \rho \) is stored in \( \rho\text{-set} \) in line 6.

The query for computing \( \delta \) is given in Lines 7-13. The algorithm iteratively picks an object \( p \) and performs a sequential search over its \( N\text{List}(p) \) each time comparing if the current object has higher density in line 9. The search terminates when the first object \( i \) satisfying the condition is met which is the required \( \mu \) and its distance \( \text{dist}(p,i) \) is the corresponding \( \delta \). The obtained values are stored in their corresponding set in line 13 after which the algorithm terminates returning the final \( \rho\text{-set}, \delta\text{-set}, \mu\text{-set} \).

**Theorem 1.** The expected time complexity of the Algorithm 2 is \( O(n \log n) \).

**Proof.** Let \( P \) be a set of \( n \) objects. The time complexity for computing \( \rho \) in lines 3-6 is \( O(n \log n) \). This is because, for each object \( q \in P \), binary search performs \( O(\log n) \) comparisons. Therefore, for \( n \) objects the overall time complexity of computing \( \rho \) is \( O(n \log n) \).

Next, the expected time complexity for computing \( \delta \) in lines 6-11 is \( O(1) \). To prove this, we assume that in a cluster, density increases while moving toward local peaks. To compute \( \delta \) for an object \( q \), the query probes each object from near to far in its \( N\text{List} \) until it finds the first object \( p \) with higher density. Suppose query object \( q,p \) are located at points \( D \) and \( A \) in Figure 35. For the non-peak object \( q \), the area defined by circular region centered at \( D \) and radius \( \text{dist}(D,A) \) is the total area that the query needs to explore to find \( \delta \) defined as \( \text{area}(\text{near})+\text{area}(\text{far}) \). Area(\text{near}) is the dense area in between \( q \) and \( p \) while area(\text{far}) is the rest area which is sparse. The ratio of area(\text{far})/area(\text{near}) is equal to a constant \( f = \frac{\pi/3 + \sqrt{3}/4}{2\pi/3 - \sqrt{3}/4} \). Therefore, the total number of objects probed for an object is expected to be a constant number. For peak objects, since the higher density neighbors are not near, in the worst case, the number of probes is \( n \). Assuming the number of peaks as constant \( c \), the total number of probes is bounded by \( cn \). Thus, finding \( \delta \) for all the objects requires total \( fn + cn \) probes which costs \( O(n) \) expected time. Hence, the overall expected time complexity of Algorithm 2 is \( O(n \log n) \).

### 3.2 Cumulative Histogram

List Index significantly enhances the DPC \( \rho \) and \( \delta \) queries, however, the computation of \( \rho \) is affected by the size of \( N\text{List} \). With increase in dataset size, the size \( N\text{List} \) grows larger which requires more comparisons and, hence, makes queries slow. In other words, the \( O(n \log n) \) time to compute \( \rho \) is expensive for large datasets because of large search space in an \( N\text{List} \). To this end, we introduce a Cumulative Histogram (CH) Index for DPC which takes \( O(1) \) running time to compute \( \rho \) for an object. CH Index merges the merits of both List Index and cumulative histogram which helps to tremendously reduce the search space of List Index. The basic idea behind CH Index is to divide the \( N\text{List} \) of an object into smaller subsets. This means that the subset corresponding to \( d_e \) contains fewer objects in non-decreasing order.

The CH Index contains a cumulative histogram for each object consisting of several bins where each bin represents a disjoint range of distance w.r.t. \( p \). For an object \( p \), the first bin indicates the number of objects \( (n_b) \) in \( N\text{List} \) within distance \( w \) from \( p \) where \( w \) is the bin width and is user defined. The second bin indicates the same within distance \( 2w \) from \( p \) and so on until the bins cover all the objects of \( N\text{List} \). Here, the distances \( w \) and \( 2w \) denote the upper limit of first and second bin. In this way, a number of bins are constructed for each object. Since the number of objects within distance denoted by upper limit from \( p \) in \( N\text{List} \) is equal to the location of last object \( q \) with \( \text{dist}(p,q) < w \), each bin stores the location of such object as \( n_b \) such that two consecutive \( n_b \) represents a section of \( N\text{List} \). To compute \( \rho \) for each object, the query just needs to locate the bin (say \( \text{targetBin} \)) containing the farthest object \( q \) with \( \text{dist}(p,q) < d_e \) and uses binary search on the section of \( N\text{List} \) from \( n_b-1 \) and \( n_b \). A smaller \( w \) represent a smaller section of \( N\text{List} \) and results in faster query time at the cost of additional space as there will be large number of bins. Thus, for a particular dataset,
Figure 4: Cumulative Histogram for Object 10 in Figure 2 selecting an appropriate \( w \) is of paramount importance to both the running time and space cost and depends solely on the choice of user.

**Example 2.** Figure 4 represents a cumulative histogram for object 10 along with its NList. It is constructed by counting the number of objects in NList with distance less than upper limit of each bin shown at the abscissa \( (0.16, 0.32, 0.48, 0.64, 0.96) \) and the count \( n_b \) obtained for each bin is stored at each bin. The last bin contains the total number of objects in NList. Given \( d_{\text{c}} = 0.25 \), first find the targetBin \( T \) by calculating \( d_{\text{c}}/w = 1 \). In the figure, the green bin is the targetBin as \( d_{\text{c}} \) lies within \( (0.16, 0.32) \). Here, \( n_{b,1} = 4 \) and \( n_{b,1} = 2 \) (previous bin) determines the section of NList which needs to be explored to find \( p \) of object 10. Perform binary search operation on this section of NList containing only 2 objects \( (19, 22) \) which returns the location of object 22 which is the corresponding \( p \). Notice List Index has to search among 28 objects while the CH Index just needed 2 objects in this case.

### 3.2.1 Construction

The pseudo-code for construction of CH Index is given in Algorithm 3. The algorithm uses the List Index to construct cumulative histograms for each object in lines 2-13. For each object \( p \), first it initializes upper limit of first bin with \( w \), \( i \) to iterate over NList and a list \( c_{\text{histogram}} \) to store \( n_b \) for each bin in lines 3-5. The while loop in line 6 helps to iterate over the NList\( (p) \). To find \( n_b \) of first bin, the algorithm starts from the first object of NList\( (p) \) and examines if its distance to object \( i \) \( \text{dist}(p, i) < \text{upper limit} \) as shown in line 7-8. If it falls within the first bin, it increments \( i \) in line 9 and moves to next object of NList. This is repeated until the first object at location \( i \) with \( \text{dist}(p, i) > \text{upper limit} \) is met. The location \( i \), which at this instance gives the number of objects corresponding to first bin, is stored as \( n_b \) of the same in \( c_{\text{histogram}} \) as shown in line 11. Line 12 increments upper limit by \( w \), to indicate the upper limit of second bin. The algorithm again starts to examine the objects from the last location \( i \) and repeats the same procedure to store the \( n_b \) of second bin. In this way, the loop executes until all the objects of NList\( (p) \) have been visited. Finally, line 13 stores the \( n_b \) of last bin. The list containing the \( n_b \) values (i.e., \( c_{\text{histogram}} \)) of object \( p \) is stored in CH Index in line 14. The same procedure is repeated for all the objects after which the algorithm terminates. The total time complexity to construct CH Index based on Algorithm 1 and Algorithm 3 is \( O(n^2 \log n) \).

### 3.2.2 Query Algorithm

In this section, we describe the query algorithm to compute \( \rho \) using CH Index. Basically, for an object \( p \), the algorithm finds the targetBin to determine which section of the NList is to be searched. Then the algorithm performs a binary search on the determined section and finds the location of farthest object \( q \) with \( \text{dist}(p, q) < d_c \) which is the required \( \rho \).

The pseudo-code for computing \( \rho \) is shown in Algorithm 4. For each object, the algorithm first finds the targetBin as shown in line 1-2. Next, the algorithm proceeds to compute \( \rho \) for that object in lines 5-14. If \( d_c \) is equal to the upper limit of targetBin, all the objects up to that bin are within distance \( d_c \). Thus, the \( n_b \) of targetBin is directly assigned to \( \rho_p \) as shown in line 5-6. Otherwise, in lines 8-14, the algorithm performs a binary search on the section of NList corresponding to targetBin which gives corresponding \( \rho_p \). Since each bin contains the location of object in NList, first and last are retrieved from the previous and current bin respectively as in lines 12-13. If the targetBin is greater than total number of bins, all the objects are within \( d_c \) and \( n_b \) of last bin is assigned to \( \rho \) as shown in line 17. The \( \rho_p \) obtained is stored in \( \rho \) set in line 18. The same procedure is repeated to compute \( \rho \) for all the objects which are stored in \( \rho \) set after which the algorithm terminates.

**Theorem 2.** The time complexity of Algorithm 4 is \( O(n) \).

**Proof.** The algorithm takes \( O(1) \) time to locate the targetBin in lines 1-2. Then, if say, there are \( b \) objects of
NList to be explored between first and last location, binary search takes \( O(\log b) \) time to compute \( \rho \) of an object. Assuming \( b \) to be constant, the time complexity is \( O(1) \). Therefore, the overall time complexity of Algorithm 1 is \( O(n) \).

**Theorem 3.** Given any \( d_c \), Algorithm 2 and Algorithm 4 compute correctly the set of all clusters \( C \) in \( D \).

**Proof.** Let’s assume that our algorithm returned a set of clusters \( C \). We will show its correctness w.r.t. the original DPC algorithm. The correctness depends upon the set of cluster centers obtained which depends on the computed \( \rho \) and \( \delta \), provided the user selects the same cluster centers from decision graph. We show that the algorithms obtain correct \( \rho \) and \( \delta \) for any given \( d_c \). As an object’s NList stores objects in the non-decreasing order of their distances, binary search finds the location that stores \( d_c \) in the object’s list. As the objects are in sorted order, the list guarantees that all the objects stored before \( d_c \) lies within the range \( d_c \) and thus correspond to local density \( \rho \) of that object. Thus, Algorithm 2 successfully obtains correct values of \( \rho \) for all objects. Similarly, histogramming provides a subset of list containing \( d_c \). Binary search is applied as above which returns the required location. Therefore, Algorithms 1 also obtains correct \( \rho \) for all objects.

To compute \( \delta \), the algorithm performs a linear search which returns the first object with higher \( \rho \) in its list. As \( \rho \) has been computed correctly, performing a sequential search guarantees to find correct \( \mu \). Based on these values, correct cluster centers are determined and hence the correct clustering results.

### 3.3 Approximate Solution

We present an approximate solution to adapt these indices to work with low memory systems while still providing fast queries for larger datasets. The approximate solution significantly reduces the memory requirement of indices at the cost of slight inaccuracies in the clustering results.

The idea behind this solution is that the DP metrics \( \rho \) and \( \delta \) mainly requires visiting neighboring objects. An NList contains a large number of near and far object where the far objects with distance \( d \) do not contribute to \( \rho \). Similarly, for most objects, their \( \mu \) is near and are easily found in the starting locations of NList. This implies that the far neighbors are not meaningful and storing them costs unnecessary space for most objects. Therefore, if the maximum relevant neighborhood region of the objects is known, only the objects of these regions needs to be stored.

Based on the above idea, we introduce a Reduced Neighbor List (RNList) with a neighborhood threshold parameter \( \tau \). Using the NList, the RNList of an object retrieves and stores only those neighbors with distance \( d \) \(<\tau \) where \( \tau \) determines the radius of maximum relevant neighborhood region and the queries are executed using the RNList instead of NList. Usually \( \tau \) should be set to a large value greater than any possible value of \( d_c \) to be tested by user. This helps to obtain correct \( \rho \) for any \( d_c \). Given correct \( \rho \) and large \( \tau \), correct \( \delta \) can be obtained for non-peak objects as they have smaller \( \delta \). For peak objects with \( \delta > \tau \), their \( \delta \) is set to a large value. This simple setting helps to find cluster centers with high \( \rho \) and anomalously large \( \delta \). Note that, a very small \( \tau \) may change most objects to cluster centers/outliers. Thus, it is important that a sufficiently large \( \tau \) is selected to obtain near accurate results. Interestingly, it was observed that for some datasets, less than 1% of the total number of objects were probed using List Index during the computation of \( \rho \) and \( \delta \).

However, the storage cost may be still high and may not ensure quality for very large datasets as the size of RNList gets very small for such datasets. In addition, it is also difficult to provide approximation ratios due to different data distribution of different datasets. This motivates the use of tree-based index to be introduced in the subsequent section.

### 4. TREE-BASED INDEX STRUCTURES

The list-based indices significantly accelerate the query time of DPC but requires storing neighbors for each object which has high space cost. For low memory systems, it may not be possible to store the list-based index for large datasets and therefore such users cannot exploit its advantages to find DPC clusters for different \( d_c \) efficiently. It would be perfect if the index structures could support efficient queries along with minimum space requirement. Moreover, the preprocessing cost of the list-based index structures is also high especially for large datasets. Although such index are constructed once, this high cost may be undesirable where a user wants fast construction of index for any set of objects and obtain DPC clusters for different \( d_c \) efficiently.

To this end, we study tree-based index structures which have low memory requirements and efficient neighborhood search queries owing to their ability to focus on the most important region. As discussed earlier, we focus on the popular and commonly used Quadtree and R-tree Index. These indices are well suited to the problem of DPC as they can easily eliminate large irrelevant regions from consideration and mainly focus on the neighboring objects. This focusing can improve the execution time of queries like \( \rho \) and \( \delta \) intending to seek information about the neighborhood. Thus, DPC clusters can be obtained using tree-based indices based on the solution framework.

The popular range search and nearest neighbor search are efficient algorithms for their purpose. Nevertheless, they cannot be directly adapted for the computation of DPC metrics particularly \( \delta \). The range search can answer the \( \rho \) query, however, it requires substantial number of search operations even for a moderately large \( d_c \). The computation of \( \delta \) metric is different to the nearest neighbor search where the nearest object is retrieved. We are interested in finding the higher density nearest neighbor which may be different from the nearest neighbor. This is true especially for the peak objects for which the normal query will end up searching a large search space. Thus, these queries are slow in finding DPC clusters which motivates developing efficient algorithms for the same. Next, we first discuss the Quadtree index and present efficient query algorithms to compute DPC metrics based on effective pruning techniques.

### 4.1 Quadtree

A Quadtree involves hierarchical decomposition of the space in a regular manner. The root of the tree is congruous to the whole space in consideration and rest of the levels below root depicts a refinement of space. In a quadtree, each non-leaf node has four children and the leaf node contains the actual data objects. These children are obtained by recursively subdividing the space into four regions. The division of node occurs when the number of objects increases...
4.1 Pruning Techniques

We first give some common terminologies that will be used to explain the pruning techniques and algorithms. Let $P$ be a set of objects such that $p, q \in P$ then $nc$ denotes number of objects within a node, $d_{\text{min}}(p,n)$, $d_{\text{max}}(p,n)$ denote the minimum and maximum distance between object $p$ and node $n$ respectively, $\text{maxrho}$ denotes the maximum $\rho$ of an object inside a node, and $\text{dist}(p,q)$ denotes distance between objects $p$ and $q$.

The first observation helps to improve the computation cost of $\rho$ by pruning several nodes. It is as follows:

**Observation 1.** Given an object $p \in P$, a query, defined by circular region $Q$, centered at $p$ and radius $d_c$, determine whether a node representing region $R$ is fully contained, if $R \subset Q$; discarded, if $R \cap Q = \emptyset$; or explored otherwise.

This is very straightforward because if $R$ is entirely within $Q$ i.e., $R \subset Q$, all the objects in $R$ are guaranteed to be in $Q$ and can be directly added to $p$. This can be found by checking if $d_{\text{max}}(p, node) < d_c$. If it is completely outside $Q$, i.e., $R \cap Q = \emptyset$, no object of $R$ lies in $Q$. This can be found by checking if $d_{\text{min}}(p, node) \geq d_c$. In both the cases, there is no need to explore these nodes. However, if $Q$ intersects the node, the number of objects in $R$ also within $Q$ needs to be determined and thus only these nodes need to be explored at each level.

Next, we present two lemmas which help to prune the irrelevant nodes during the computation of $\rho$ metric.

**Lemma 1.** (Density Pruning) Given an object $p \in P$ with local density $\rho_p$, its $\mu$ does not lie in a node of Quadtree which satisfy $\text{maxrho}(node) < \rho_p$ where $\text{maxrho}(node)$ is the maximum local density of an object inside that node.

Clearly, for an object $p$, its $\mu$ cannot be found in nodes that bounds no object $q$ such that $\rho_q > \rho_p$. Therefore, such nodes can be density pruned. This is highly effective in case of peak objects where many unnecessary nodes as well as objects of lower density are visited.

**Lemma 2.** (Distance Pruning) Given an object $p \in P$, its $\mu$ does not lie in a node of Quadtree which satisfy $d_{\text{min}} > \text{candidate}(\delta)$, where $\text{candidate}(\delta)$ is the best $\delta$ obtained before visiting this node.

Once a candidate $\delta$ has been obtained, the next nodes that have $d_{\text{min}}(p, node) > \text{candidate}(\delta)$ are guaranteed to not give any better $\delta$. Such nodes can be distance pruned. Based on these pruning techniques, efficient query algorithms are designed to compute the two metrics. To summarize, we store $nc$ and $\text{maxrho}$ at the nodes where the former helps in computing $\rho$ metric while the latter helps to compute $\delta$ metric by using the above pruning.

4.1.2 Construction

The construction of Quadtree is simple and follows hierarchical decomposition of the space into four children at each level as discussed earlier. For insertions, query performs comparisons at each level of quadtree and decides the relevant subtree to be followed. The object is inserted finally at the leaf node of the corresponding subtree. Once the objects have been inserted, at each node, we store the $nc$ value based on Observation 1. This can be simply done by performing a depth first traversal over the tree.

The time complexity for construction of Quadtree highly depends upon the resulting Quadtree. For random insertions, the average time spent is proportional to $O(n \log_4 n)$. However, the worst-case where the objects are inserted only in the deepest node can cost $O(n^2)$ time. Maintaining $nc$ at each node requires traversing the complete tree once which is proportional to number of nodes.

4.1.3 Query Algorithm

We first present a general idea of both the query algorithms for the DPC metrics and then explain it in detail using their pseudo codes. To compute $\rho$ of an object, the query visits the root and performs filtering of candidate nodes at each level by categorizing them as fully contained, intersected or discarded by query based on Observation 4. The fully contained node is pruned and its $nc$ is directly added to $\rho$. Similarly, a discarded node is also pruned. Only the intersected nodes at each level are explored. At the leaf nodes of intersected nodes, the query counts the number of objects $q$ with $\text{dist}(p,q) < d_c$ and adds count to $\rho$. The final $\rho$ obtained is the required answer.

To compute $\delta$ for an object, we employ the best-first search heuristic which visits that candidate node first which has higher chances of finding $\mu$. This node apart from not satisfying Lemma 1 should also be the nearest one among all candidate nodes. This helps to find the first candidate $\delta$ very fast based on which the candidate nodes with $d_{\text{min}}(p, node) > \delta$ are pruned. If a better $\delta$ is obtained using the unpruned candidate nodes, the candidate $\delta$ is updated. This is repeated until all candidate nodes have either been explored or pruned and the final candidate $\delta$ obtained is the required answer.

Now we discuss these algorithms in detail. Below, $d_{\text{min}}$ and $d_{\text{max}}$ for an object $p$ are calculated by simple functions

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**Algorithm 5:** Query Algorithm for $\rho$

| Input: | Object $p$, distance $d_c$, current node, $\rho_p$ |
| Output: | $\rho_p$ |
| 1 Function | $\text{computeRho}(p, d_c, \rho_p)$ |
| 2 if node is leaf then |
| 3 foreach object $q \in$ node do |
| 4 if $\text{dist}(q,p) < d_c$ then |
| 5 count = count + 1; |
| 6 return count; |
| 7 else |
| 8 if $d_{\text{min}}(p, node) \geq d_c$ then |
| 9 return 0; // discard |
| 10 else if $d_{\text{max}}(p, node) < d_c$ then |
| 11 return nc; // fully contained |
| 12 else |
| 13 foreach children $c$ of node do |
| 14 $p^+ = \text{computeRho}(p, d_c, c, \rho_p)$; |
| 15 return $\rho_p$; |
Algorithm 6: Query Algorithm for δ

Input: Object p, Tree node, δ_p
Output: δ_q, µ_p
1 stack < Tree.Node > nodes;
2 root.dmin ← 0;
3 nodes.push(root, root.dmin);
4 while nodes is not empty do
5 tp ← nodes.pop;
6 // Distance Pruning
7 if tp.dmin < δ_p then
8 if node is Leaf then
9 foreach object q at Leaf do
10 if δ_p > dist(p, q) then
11 δ_p ← dist; µ_p ← p;
12 else
13 temp.dmin ← inf; temp.node ← null;
14 foreach child c of tp.node do
15 // Density Pruning
16 if c.maxrho > δ_p then
17 if temp.dmin ≤ dmin(p, c) then
18 nodes.push(c, c.dmin);
19 else
20 if temp.dmin != inf then
21 nodes.push(temp.node, temp.dmin);
22 temp.dmin ← c.dmin;
23 temp.node ← c;
24 if temp.node != null then
25 nodes.push(temp.node, temp.dmin);
26 return δ_p, µ_p;

minDistToNode(p, node) and maxDistToNode(p, node) which compute the minimum and maximum distances of the node from the object respectively.

Algorithm for ρ. The pseudo-code for computing ρ of object p is shown in Algorithm 5 and uses function computeRho() which is called with parameters p, d_c, current node (initially root), and ρ_p (initially zero) shown in line 1 which performs a depth first traversal over the nodes of Quadtree. The query starts from the root node and examines whether it is discarded, fully contained or intersected in lines 8,10,12 respectively. If the root node is fully contained, its nc is returned as required ρ and the algorithm terminates. Since query object p is within root i.e., dmin(p, node) = 0, it is not discarded. The root node is explored only if it is intersected by the query and its children are visited by recursively calling the function computeRho() as shown in line 14. The current child node of root is again examined for the three conditions and is explored only if it is intersected by the query. This continues until the leaf node is reached. If the current node is leaf, the query visits each object q of leaf and counts the number of objects within distance d_c from p i.e., dist(p, q) < d_c as shown in lines 3-5 and returns the count to calling function in line 14. The algorithm repeats the procedure until all the intersected nodes are explored and terminates after returning the required ρ_p in line 15.

Algorithm for δ. To compute δ, firstly a simple depth first traversal algorithm is required which maintains the pruning information based on Lemmas 2, 3, i.e., for each node store its maxrho. For the leaf nodes, the query finds the object with highest local density bounded by it, stores its value at that node as maxrho. For the internal nodes, it finds its maxrho by finding the maximum maxrho of each of its children. Based on this information, the next algorithm computes δ for each object.

The pseudo code to compute δ is shown in Algorithm 6. The inputs are object p, node of tree (initially root) and δ_p (initially set to Infinity). We call it a candidate δ_p. Line 1 initializes a stack, nodes, of TreeNode’s which contains nodes along with their minimum distance dmin from object q. The algorithm first starts from root node, assigns zero to its dmin as the query object q is within root and then pushes it into stack. The query enters the while loop as shown in Lines 4-24 which the algorithm executes until the stack is empty. The top element of stack (now root) is popped out in line 5 and is examined for distance pruning i.e., if its dmin < δ_p in line 6. Since, δ_p at this instance is infinity, the node is not pruned and the algorithm proceeds to check if it is a leaf or non-leaf node in line 7. Since node is not leaf, lines 13-24 are executed. In line 13, a temporary node temp node is initialized with node as null and dmin as infinity. The purpose of this temp node is to find the best node from the candidate nodes i.e., root’s children as shown in lines 14-24. Density pruning is performed to filter those nodes that have higher maxrho as shown in line 15. Then dmin is computed for all such filtered nodes using dmin(p, c) for all c and the algorithm pushes the node with smallest dmin to the top and rest after it without any preference. This is shown in lines 16-24.

The best node is explored further and its children are again filtered using density pruning and a best node is selected. This is repeated until it reaches the leaf node where each object is examined to find the one with higher ρ shown in line 9. The distance to first object with higher ρ is computed and tested if it is better than the current candidate δ. If it is better, the query updates the candidate δ and µ. Remember at this instance the top element in stack is one of the last candidate nodes which was filtered from the density pruning step in line 15. This node of stack is popped and examined if its dmin is smaller than candidate δ in line 6, i.e., has chance of finding a better candidate δ. If it is true, the algorithm performs the same procedure shown in lines 7-24. Otherwise, the algorithm moves to next element of stack and examines it. In this way, the algorithm pops and examines all the nodes of stack and once the stack is empty it comes out of loop and finally returns the last candidate δ and µ which are the required results.

4.2 R-tree

Although Quadtree is a simple and powerful index structure, its height is sensitive to the order of insertion of objects and the resulting tree can be unbalanced. This results in declining query performance for the neighborhood search queries. Even the pruning strategies may be ineffective in such scenarios. This requires a need to explore other index structures with better structure guarantees. One such structure is R-tree proposed by Guttman [12].

R-tree is an extension of B-tree for multidimensional objects. It is a balanced tree structure and is also based on hierarchical decomposition of data. In an R-tree, a node contains multiple entries of the form (rect, ptr). rect basically describes the region of space occupied by the child nodes. At the leaf node, rect is the minimum bounding rectangle (mbr) of the close objects in space and ptr is the pointer to
it. At internal node, \textit{rect} is the \textit{mbr} of child nodes and \textit{ptr} is pointer to it. The root of R-tree must contain at least 2 children unless it is a leaf. Thus, the height of an R-tree indexing \( n \) objects is bounded by \( O(\log_M n) \) where \( M \) is the maximum entry of each node.

However, the nodes of an R-tree may suffer from node \textit{overlap} and \textit{region coverage} by \textit{mbr}. Overlapping increases chances of unnecessary path search while a large region coverage by an \textit{mbr} reduces the performance of pruning. To this end, several variants of R-tree \cite{3,13,16,11} were proposed to improve the query performance of R-tree by reducing the overlap and the region coverage. These variants basically differ in the method of constructing the R-tree but the traversal and search queries are the same as original R-tree. Among the variants, the packing algorithm \cite{16,11} often results in better structure with typically less overlap and better storage utilization as compared to other variants which results in improved query performances. Therefore, our implementation is based on the packing algorithm \cite{16} for efficiently computing the DPC metrics.

4.2.1 Construction

We describe the basic idea of the construction using packing algorithm \cite{16} which is based on bulk-loading of objects. The packing algorithm requires data to be preprocessed first before loading. Suppose, \( n \) objects of data space is to be inserted. The overall strategy is to recursively split the data space into small partitions, where each partition is stored at leaf node. These leaf nodes are further grouped together to form the non-leaf or internal nodes of the tree. Lastly, the grouping stops when the root node is created.

The partitioning strategy is explained as follows. If \( M \) is the maximum capacity of nodes and \( L \) is the number of leaf nodes where \( L = \left\lceil \frac{n}{M} \right\rceil \), the partitioning strategy for the first split is to sort the objects by first dimension \( x \) and divide them into \( \sqrt{L} \) partitions where each partition contains \( M \times \left\lceil \sqrt{L} \right\rceil \) objects. Similarly, these partitions are recursively split by sorting the objects of each partition using the other dimension \( y \) until each partition contains maximum \( M \) objects.

4.2.2 Query Algorithm

Since both the Quadtree and R-tree nodes represent a region of space bounding a set of objects, the pruning technique is still valid for R-tree and the nodes can be examined for pruning if they are not relevant. The pruning technique and query algorithms for DPC metrics can be easily adapted for the above constructed R-tree. Therefore, we do not discuss the algorithms in this section. The time complexities of both the queries are summarized using following lemma.

\textbf{Theorem 4}. The average time complexity of DPC algorithm using R-tree is \( O(n \log_M n) \).

A range query with R-tree takes \( O(\log_M n) \) average time. For \( n \) objects, the average time complexity for computing \( \rho \) which performs \( n \) range queries in Algorithm \cite{5} is bounded by \( O(n \log_M n) \). Similarly, our modified query for \( \delta \) in Algorithm \cite{5} which explores nodes in a way similar to nearest neighbor search but with additional pruning also takes \( O(n \log_M n) \) time for \( n \) objects. Therefore, the overall average time complexity for DPC algorithm is \( O(n \log_M n) \).

5. EXPERIMENTAL STUDY

We conduct a comprehensive set of experiments to evaluate the performance of all the indices (List, CH Index, Quadtree, R-tree) discussed in this paper. The evaluation of these indices and their algorithms comprise of following tasks: (i) Query performance on different datasets with varying size. (ii) Preprocessing and storage cost of index. (iii) Query performance under influence of different parameters \( d_c, \text{binwidth } w, \text{neighbor threshold } \tau \). (iv) Clustering quality. Based on these tasks, experiments were conducted on a machine equipped with core i5 2.40 GHz processor, 16 GB of RAM and Windows 10 Operating system. All algorithms including the original DPC algorithm have been programmed in C++ and compiled using g++ and optimization level set to O3.

\textbf{Datasets}. We used both synthetic and real datasets to evaluate the indices. The datasets, shown in Table 1 with varying size were deployed to test the algorithms. S1 and Birch are benchmark dataset obtained from \cite{9} where S1 dataset contains 5000 objects and 15 clusters while the Birch dataset contains 100000 objects and 100 clusters. The Query and Range datasets consists of 50,000 and 200,000 objects respectively with spatial attributes. These have been obtained from UCI machine learning archive \cite{8}. Blob dataset with 100,000 objects has been used in popular work like \cite{17} for comparing the clustering accuracy of algorithms. Gowalla (available at SNAP \cite{15}) is a real data set of users check-ins collected from the Gowalla social networking website. We used 1.25 million check-ins for the experiments.

\textbf{Parameters}. For each dataset, we inspected the query performance of algorithms for different \( d_c \). For the list-based indices, different values of \( \tau \) were chosen in large intervals to find the influence on running time, memory as well as clustering quality. The large intervals were needed to demonstrate the substantial effect on memory as well as running time. The influence of bin width \( w \) was also analysed on the performance of CH Index.

\textbf{Evaluation Metric}. In order to analyse the clustering quality of our approximate solution, we use the well known measures Precision, Recall and F1 Score.

5.1 Running Time

We test the running time of all the algorithms on various datasets including the original DPC algorithm. Figure 5

| Data set   | Objects | Types    |
|------------|---------|----------|
| S1 \cite{10} | 5000    | Synthetic|
| Query \cite{12} | 100000  | Synthetic|
| Birch \cite{20} | 100000  | Synthetic|
| Range \cite{20} | 200000  | Synthetic|
| Gowalla \cite{6} | 1250000 | Real     |

Table 1: Datasets
Table 2: Memory Usage by different Indices (in MB)

| Dataset | List Index | CH Index | R-Tree | Quadtree |
|---------|------------|----------|--------|----------|
| S1      | 0.01       | 0.09     | 0.2    | 0.6      |
| Query   | 9.51       | 9.64     | 8.8    | 14.2     |
| Blob    | 108.00*    | 112.40*  | 17.6   | 34.8     |
| Birch   | 8004.1*    | 7806.8*  | 15.4   | 29.2     |
| Range   | 8469.3*    | 8728.4*  | 28.6   | 55.9     |
| Gowalla | 7805.8*    | 7475.2*  | 140.2  | 214.8    |

Table 3: Construction Time of different Indices (in Sec)

| Dataset | List | CH Index | R-Tree | Quadtree |
|---------|------|----------|--------|----------|
| S1      | 15.29 | 22.09    | 101.59 | 0.001    |
| Query   | 158.59 | 96.14    | 0.290  | 0.040    |
| Blob    | 2260.08* | 140.120* | 0.330  | 0.074    |
| Birch   | 1282.690* | 52.570*  | 0.250  | 0.046    |
| Range   | 2078.060* | 68.460*  | 0.440  | 0.124    |
| Gowalla | 290700.83* | 69.150*  | 0.925  | 1.946    |

5.2 Memory Usage and Construction Time

Table 2 and Table 3 show the memory requirement and construction time of different indices for various datasets. The ‘*’ indicates the memory and construction time of the List and CH Index for the largest τ used. For Blob, Birch, Range and Gowalla datasets, τ is 1, 0, 250000, 2500 and 0.05 respectively. Selection of this τ range has been done to fully utilize the memory. For CH Index, a medium size w is selected for each of the above dataset whose values are 0.10, 8000, 600 and 0.015 respectively.

List-based indices clearly require significantly large storage space compared to the tree-based indices. However, experiments show that using a smaller RNList, the memory requirement can be controlled. For example, although Blob, Birch, Range and Gowalla have different sizes, the index constructed have nearly the same size. Further, R-tree needed slightly lower memory than Quadtree (owing to its balanced structure).

The index construction time is considerably less for the tree-based indices as compared to list-based indices as shown in Table 3. For CH Index, we only report the extra time taken to build histograms on top of List Index. The table shows a bar graph where datasets are shown on the x-axis in order of their non-decreasing size while the running time is shown on y-axis. For each dataset, comparisons were made for the same value of dc.

For the smaller datasets, S1 and Query, the list-based index outperforms the tree-based indices in providing set of ρ and δ values while the CH Index performs the best. However, DPC took much higher time for the same. The running time of two datasets clearly show that with increase in size, DPC requires higher time. For the larger datasets, both DPC and list-based indices need large memory and thus could not be tested. Therefore, the list-based indices with approximation were used to handle larger datasets, the results of which will be shown in Section 5.3.

In general, with increase in size, the running time of all the algorithms increased. R-tree performed better than the Quadtree on most datasets as shown in the figure. For S1, the results were almost the same for both the indices. Since Blob and Birch have the same size, the running time are almost similar. Faster query time of R-tree on large datasets is a result of its balanced structure as compared to Quadtree.

5.3 Effect of Parameter Variation

This section examines the effect of different parameters on the behaviour of different query algorithms.

5.3.1 Effect of dc

Figure 6 shows the influence of dc on the running time of algorithms on different datasets. The values of dc depend on the underlying space of each dataset. The results of list-based indices shows no significant difference in running time behaviour for all datasets with varying dc. However, if dc is found at the initial or ending locations of RNList, the running time is slightly higher as a result of additional searches involved. Moreover, if dc > τ, the running time has further improvement but at the cost of loss of accuracy.

The running time of tree-based indices generally increases with increasing dc as more nodes are explored during p computation and more distance computations are performed. However, for large dc, the general trend does not hold and the running time significantly drops from the expected behaviour. This is because of the pruning we developed which avoids exploring most of the tree nodes as they are within dc from the queried object. For the largest dc, ρ for an object is equal to the total number of objects which is obtained in constant time as the root’s nc is directly assigned to ρ. As all the indices do not perform any search operation for largest dc and directly obtain ρ, their running time are very close as shown in the figure.

5.3.2 Effect of Bin Width

We also analysed the influence of bin width(w) on running time of CH Index for Blob, Birch, Range and Gowalla
For this purpose, the clustering results of DPC is taken to obtained for different values have been selected to give better running time at the cost of space and vice-versa. This is because binary search performs the query on smaller objects. Similarly, for smaller w, a large number of bins are required which requires more memory. Thus, a CH Index with smaller w provides better running time at the cost of space and vice-versa.

5.4 Approximate Index Evaluation

This section analyses the effect of approximation on the running time, memory and clustering quality of list-based indices for the the medium and large datasets Blob, Birch, Range and Gowalla where parameter d_c is fixed at 0.1, 100000, 1500, 0.001 respectively.

Figure 7 shows the variation of running time with varying \( \tau \). We selected three different values of \( \tau \) greater than selected \( d_c \) for each dataset. The results clearly show that, for both the List and CH Index, the running time is directly proportional to \( \tau \) or the size of RNList. The shorter the RNList, the lower the running time of the algorithm and vice-versa. This is because binary search performs the query on smaller number of objects. When \( \tau \) is very small, their performance is comparable because of nearly same search space. Moreover, the running time variation with \( \tau \) is smaller for the CH Index than for List Index. This is because, for any \( \tau \), CH Index takes almost the same time in computing \( \rho \) as \( w \) is fixed and the computation of \( \delta \) is same for both the index. Figure 8 shows the influence of \( \tau \) on memory of List Index for the different datasets. Clearly, larger the \( \tau \), higher will be the space cost and vice-versa.

Finally, we examine the quality of the clustering results obtained for different \( \tau \) w.r.t. the results of original DPC algorithm. Additional \( \tau \) values have been selected to give better idea about the results. As mentioned earlier, we use Precision, Recall and F1 Score metrics for this purpose. These measures try to evaluate cluster membership of object pairs in the reference clustering \( G \) and the obtained clustering \( C \). For this purpose, the clustering results of DPC is taken to be the reference clustering \( G \). Precision tries to find the pro-
portion of pairs correctly identified in $C$ to the total number of pairs in $C$, while Recall reflects the proportion of correct pairs identified in $C$ to the total number of pairs in $G$. These are defined as follows:

$$\text{Precision} = \frac{TP}{TP + FP}$$

(3)

$$\text{Recall} = \frac{TP}{TP + FN}$$

(4)

Here, $TP$ denotes True Positive which states the number of cases when a pair of objects found in $C$ is also found in $G$. $FP$ denotes False Positive which states the number of cases when a pair of objects found in $C$ is not found in $G$. $FN$ denotes False Negative which states the number of cases when a pair of objects in $G$ which does not appear in $C$.

$F1$ Score tries to seek the balance between the two metrics Precision and Recall and is defined as the harmonic mean of both.

$$F1 \text{ Score} = \frac{2 \times \text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}}$$

(5)

If $\tau$ is reduced, many objects may be assigned a large $\delta$ which either makes them clusters or outliers. Thus, many true positives will be lost and many false positives and false negatives occur which will result in decrease of both precision and recall and consequently affect the $F1$ Score. Therefore, higher the values of these metrics obtained, better the clustering quality.

Figure 10 represents the three metric values of the clustering obtained using the list-based indices for different values of $\tau$. Note that the RNList of list-based index using the selected largest $\tau$ in the figure is still smaller than the complete NList. For each dataset $d_c$ is fixed, and we determine the metric values while reducing $\tau$. In each of the figure, $d_c$ is the the value from where the curve attains the maximum value. For the datasets in Figure 10a, Figure 10b and Figure 10c, the results clearly indicate that correct clustering results were obtained when $d_c \leq \tau$. All the three metric values are $> 0.99$ which signifies the list-based indices found approximately the same clusters as original DP algorithm. If $\tau$ is further slightly reduced below $d_c$, the metrics notice a small drop in their values which indicates slight difference with the original clustering results. However, when $\tau$ is reduced to very small value, the metrics fall dramatically to a very low value indicating large difference in the clustering results.

Interestingly, for the selected $d_c$ and largest $\tau$, for which correct results were obtained, we found only 1% of the index for Blob and Range dataset and only 3% of the index for the Birch dataset were probed by the queries which signifies the strength of the approximate solution.

However, for the largest dataset, Gowalla, only a very small RNList could be loaded into memory which resulted in incorrect $\delta$ values for most objects. As such, the metric values dropped significantly with Precision and $F1$ Score went below 0.01 and Recall went below 0.05 as shown in Figure 10d. This shows that the approximate solution can support only the medium size datasets but does not lend well to large datasets if enough memory is not available.

5.5 Discussion

In this section, we present a discussion of the indices and their suitability under different scenarios for users.

List-based indices are fast methods to find density peaks clusters for any given $d_c$ and outperform the tree-based indices w.r.t. running time. The List Index is simple and has faster running time. However, with slight additional space CH Index outperforms the List Index achieving 20-30% improved running time. Therefore, for smaller datasets we would recommend list-based indices especially CH Index. For medium datasets, if a user desires fast running time but allows slight approximation, list-based indices could be still a good choice. When dealing with large datasets such as Gowalla, tree-based indices are recommended since the sufficient part of list-based indices cannot be uploaded to memory even though the quality of results could be reasonably compromised. Among the tree-based indices, R-tree is more preferred which overall has the better running time than Quadtree. Moreover, tree-based indices also dominate list-based indices in terms of index construction phase by large difference and can be preferred for such requirements.

6. RELATED WORKS

Several research works have focussed on improving the efficiency and scalability of the Density Peaks method. Wu et al. [23] proposed a density and grid-based clustering method which avoids unnecessary pairwise distance computations. A k-means based strategy was presented in [2] for enhancing the scalability of density peaks clustering method. However, this method has high time complexity for large datasets. So, another approximate method was proposed to improve the speed. Xu et al. [24] proposed grid-based strategy to select dense grid cells and find the local density using the objects of those cells. To address the sparsity of grid cells, a circle division strategy was proposed. Zhang et al. [27] proposed a distributed algorithm for DPC using MapReduce and employed locality sensitive hashing to obtain clustering results.

Few recent works have discussed the robustness of the density metric with respect to the parameter $d_c$. These works have proposed alternative density metrics to handle the high density variation in clusters. Wang et al. [22] proposed a new clustering algorithm which uses a density metric based on k-nearest neighbor. The idea is that the dense objects will have k-nearest neighbors (kNN) very close as compared to the sparse objects. The $\rho$ metric was redefined using kNN. Chen et al. [6] proposed Neighbourhood Contrast (NC) as an alternative to density for detecting cluster centers which can admit all local density maxima. According to this, all local density maxima have similar NC values, irrespective of the density values. Zhu et al. [28] proposed a multi-dimensional scaling method for identifying clusters with varied densities. Instead of scaling each attribute it rescales the pairwise distance between points.

7. CONCLUSION

In this paper, we have studied index-based methods for density peaks clustering. We propose two list-based indices namely List Index and CH Index for DPC. For the List Index, efficient algorithms are proposed to compute the two DPC metrics for each object for any $d_c$. CH Index further improves upon the List Index with faster running time. These indices have higher space requirement and so
for memory-constrained systems, approximate solution has been suggested to reduce space cost if marginal variation in clustering results are allowed. Moreover, two popular tree-based indices Quadtree and R-tree have also been studied for DPC as a solution to address the high space cost of the list-based indices. Effective pruning techniques and efficient algorithms have been designed to enable these indices for efficiently computing DPC metrics. The experimental results demonstrate that i) CH Index outperforms other indices w.r.t. query time but suffers from high preprocessing and space cost, ii) approximate solution supports list-based indices to handle medium size datasets with near accurate clustering results, iii) R-tree is faster than Quadtree for DPC queries and suitable to handle medium to large datasets.

8. REFERENCES

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