

PECANN: Parallel Efficient Clustering with Graph-Based Approximate Nearest Neighbor Search

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Abstract

This paper studies density-based clustering of point sets. These methods use dense regions of points to detect clusters of arbitrary shapes. In particular, we study variants of density peaks clustering, a popular type of algorithm that has been shown to work well in practice. Our goal is to cluster *large high-dimensional* datasets, which are prevalent in practice. Prior solutions are either sequential, and cannot scale to large data, or are specialized for low-dimensional data (they use spatial trees, which suffer from the curse of dimensionality).

This paper unifies the different variants of density peaks clustering into a single framework, PECANN (Parallel Efficient Clustering with Approximate Nearest Neighbors), by abstracting out several key steps common to this class of algorithms. One such key step is to find nearest neighbors that satisfy a predicate function, and one of the main contributions of this paper is an efficient way to do this predicate search using graph-based approximate nearest neighbor search (ANNS). To provide ample parallelism, we propose a doubling search technique that enables points to find an approximate nearest neighbor satisfying the predicate in a small number of rounds. Our technique can be applied to many existing graph-based ANNS algorithms, which can all be plugged into PECANN.

We implement five clustering algorithms with PECANN and evaluate them on synthetic and real-world datasets with up to 1.28 million points and up to 1024 dimensions on a 30-core machine with two-way hyper-threading. Compared to the state-of-the-art FASTDP algorithm for high-dimensional density peaks clustering, which is sequential, our best algorithm is 45x–734x faster while achieving competitive ARI scores. Compared to the state-of-the-art parallel DPC-based algorithm, which is optimized for low dimensions, we show that PECANN is two orders of magnitude faster. As far as we know, our work is the first to evaluate DPC variants on large high-dimensional real-world image and text embedding datasets.

PVLDB Reference Format:

Shangdi Yu, Joshua Engels, Yihao Huang*, and Julian Shun. PECANN: Parallel Efficient Clustering with Graph-Based Approximate Nearest Neighbor Search. PVLDB, 17(1): XXX-XXX, 2024.
doi:XX.XX/XXX.XX

PVLDB Artifact Availability:

The source code, data, and/or other artifacts have been made available at <https://github.com/yushangdi/PECANN-DPC>.

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Proceedings of the VLDB Endowment, Vol. 17, No. 1 ISSN 2150-8097.
doi:XX.XX/XXX.XX

1 Introduction

Clustering is the task of grouping similar objects into clusters and is a fundamental task in data analysis and unsupervised machine learning [2, 9, 51]. For example, clustering algorithms can be used to identify different types of tissues in medical imaging [100], analyze social networks [70], and identify weather regimes in climatology [19]. They are also widely used as a data processing subroutine in other machine learning tasks [21, 63, 68, 97]. One popular type of clustering is density-based clustering, where clusters are defined as dense regions of points in space. Recently, density-based clustering algorithms have received a lot of attention [3, 7, 34, 45, 46, 53, 77, 81, 93] because they can discover clusters of arbitrary shapes and detect outliers (unlike popular algorithms such as k -means, which can only detect spherical clusters).

Density peaks clustering (DPC) [77] is a popular density-based clustering technique for spatial data (i.e., point sets) that has proven very effective at clustering challenging datasets with non-spherical clusters. Due to DPC’s success, many DPC variants have been proposed in the literature (e.g., [16, 29, 35, 38, 47, 83, 86, 87, 98, 102, 103]). However, existing DPC variants are sequential and/or tailored to low-dimensional data, and so cannot scale to the large, high-dimensional datasets that are common in practice.

This paper addresses this gap by proposing a novel framework called PECANN: Parallel Efficient Clustering with Approximate Nearest Neighbors. PECANN contains implementations for a variety of different DPC density techniques that both scale to large datasets (via efficient parallel implementations) and run on high dimensional data (via approximate nearest neighbor search). Before going into more details on our contributions, we review the main steps of DPC variants and discuss existing bottlenecks.

The three key steps of DPC variants are as follows:

- (1) Compute the density of each point x .
- (2) Construct a tree by connecting each point x to its closest neighbor with higher density than x .
- (3) Remove edges in the tree according to a pruning heuristic. Each resulting connected component is a separate cluster.

Step (1) is computed differently based on the variant, but all variants use a function that depends on either the k -nearest neighbors of x or the points within a given distance from x . Efficient implementations of this step rely on nearest neighbor queries or range queries. In low dimensions, these queries can be answered efficiently using spatial trees, such as kd -trees. However, kd -trees are inefficient in high dimensions due to the curse of dimensionality [96]. Step (2) again requires finding nearest neighbors, but with the constraint that only

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neighbors with higher density are considered. Step (3) can easily be computed using any connected components algorithm. Steps (1) and (2) form the bottleneck of the computation, and take quadratic work in the worst case, while Step (3) can be done in (near) linear work. Note that different clusterings can be generated by reusing the tree from Step (2) and simply re-running Step (3) using different pruning heuristics. The tree from Step (2) can be viewed as a cluster hierarchy (or dendrogram) that contains clusterings at different resolutions.

Existing papers on DPC variants mainly focus on their own proposed variant, and as far as we know, there is no unified framework for implementing and comparing DPC variants and evaluating them on the same datasets. Furthermore, most DPC papers focus on clustering low-dimensional data, but many datasets in practice are high dimensional ($d > 100$). The PECANN framework unifies a broad class of DPC variants by abstracting out these three steps and providing efficient parallel implementations for different variants of each step. For Step (1), we leverage graph-based approximate nearest neighbor search (ANNS) algorithms, which are fast and accurate in high dimensions [26, 92]. For Step (2), we adapt graph-based ANNS algorithms to find higher density neighbors by iteratively doubling the number of nearest neighbors returned until finding one that has higher density. The doubling search guarantees that the algorithm finishes in a logarithmic number of rounds, making it highly parallel. For Steps (1) and (2), PECANN supports the following graph-based ANNS algorithms: VAMANA [55], PYNDESCENT [69], and HCNNG [72]. For Step (3), we use a concurrent union-find algorithm [54] to achieve high parallelism. Prior work [83] has explored using graph-based ANNS for high-dimensional clustering, but their algorithm is not parallel and they only consider one DPC variant and one underlying ANNS algorithm. In addition, we provide theoretical work and span bounds¹ of PECANN that depend on the complexity of the underlying ANNS algorithm. PECANN is implemented in C++, using the ParlayLib [10] and ParlayANN [26] libraries, and provides Python bindings as well.

We use PECANN to implement five DPC variants and evaluate them on a variety of synthetic and real-world data sets with up to 1.28 million points and up to 1024 dimensions. We find that using a density function that is the inverse of the distance to the k^{th} nearest neighbor, combined with the VAMANA algorithm for ANNS, gives the best overall performance. On a 30-core machine with two-way hyper-threading, this best algorithm in PECANN achieves 37.7–854.3x speedup over a parallel brute force approach, and 45–734x speedup over FASTDP [83], the state-of-the-art DPC-based algorithm for high dimensions, while achieving similar accuracy in terms of ARI score. FASTDP is sequential, but even if we assume that it achieves a perfect speedup of 60x, PECANN still achieves a speedup of 0.76–12.24x. Compared to the state-of-the-art parallel density peaks clustering algorithm by Huang et al. [48], which is optimized for low dimensions, our best algorithm achieves 320x speedup while achieving a higher ARI score on the MNIST dataset (in high dimensions, this algorithm is slower than brute force and failed to run on larger datasets).

Our contributions are summarized below.

¹The *work* is the number of operations and the *span* (or parallel time) is the length of the longest sequential dependence of a computation.

Notation	Meaning
P	input set of points
n, d	size and dimensionality of P
x_i	i^{th} point in P
G	a similarity search index
$D(x_i, x_j)$	distance (dissimilarity) between x_i and x_j
ρ_i, λ_i	density and dependent point of x_i
δ_i	dependent distance of x_i (i.e., $D(x_i, \lambda_i)$)
k	the number of neighbors used for computing densities
\mathcal{N}_i	(approximate) k -nearest neighbors of x_i
$\mathcal{W}_c, \mathcal{S}_c$	the work and span of constructing G
$\mathcal{W}_{nn}, \mathcal{S}_{nn}$	the work and span of finding nearest neighbors using G

Table 1: Notation

1. We introduce the PECANN framework that unifies existing k -nearest neighbor-based DPC variants and supports parallel implementations of them that scale to large high-dimensional datasets.
2. We extend graph-based ANNS algorithms with a parallel doubling-search method for finding higher density neighbors.
3. We provide fast parallel implementations for five DPC variants.
4. We perform comprehensive experiments on a 30-core machine with two-way hyper-threading showing that PECANN outperforms the state-of-the-art DPC-based algorithm for high dimensions by 45–734x. As far as we know, we are the first to compare different variants of DPC on large high-dimensional real-world image and text embedding datasets.

2 Preliminaries

2.1 Definitions and Notation

A summary of the notation is provided in Table 1. Let $P = \{x_1, \dots, x_n\}$ represent a set of n points in d -dimensional coordinate space to be clustered. We use x_i to represent the i^{th} point in P . Let G be a search index that supports searching for the exact or approximate nearest neighbors of a query point. Let $D(x_i, x_j)$ denote the distance (dissimilarity) between points x_i and x_j , where a larger distance value means the two points are less similar. D can be any distance measure the search index G supports.

Let the **neighbors** (\mathcal{N}_i) of a point x_i be either its exact or approximate k -nearest neighbors. Let ρ_i be the **density** of point x_i , representing how dense the local region around x_i is. A larger ρ_i value indicates a denser local region. For example, in the original DPC algorithm [77], the density of a point x is the number of points within a given radius of x , and in the SD-DP (sparse dual of density peaks) algorithm [35], the density of a point is the inverse of its distance to its k^{th} nearest neighbor. In this paper, we consider the densities that can be computed from the k -nearest neighbors of x .

DEFINITION 1. Let $P_i = \{x_j \mid x_j \in P \wedge \rho_j > \rho_i\}$. For x_i , the exact **dependent point** is a point $\lambda_i \in P_i$ such that, $D(x_i, \lambda_i) \leq D(x_i, x_j) \forall x_j \in P_i$ (i.e., it is the closest point with higher density than x_i). The **dependent distance** (δ_i) of x_i is $D(x_i, \lambda_i)$, i.e., the distance to its dependent point (or ∞ if it does not have one).

Definition 1 defines the dependent point to be the *closest* point with higher density, which is expensive to compute in high dimensions. For high-dimensional data, we relax the constraint to allow reporting an *approximate* nearest neighbor with higher density (i.e., considering just the points with higher density, choose approximately

the closest one). Roughly speaking, an *approximate nearest neighbor* of a point x is one whose distance from x is not too far from the distance of the true nearest neighbor from x . In our experiments, we use the Euclidean distance function, which is one of the most commonly used distance functions for clustering.

Points that are outliers and do not belong to any cluster are classified as *noise points*. A noise point is in its own singleton cluster. For example, some algorithms require a density cutoff parameter ρ_{\min} , and points that have $\rho_i < \rho_{\min}$ are considered noise points. A *cluster center* is a point whose density is a local maximum within a cluster. Each cluster center corresponds to a separate cluster. One way to pick cluster centers is using a parameter δ_{\min} , where a point x_i is considered a cluster center if $\delta_i \geq \delta_{\min}$. We consider and describe other ways of determining cluster centers in Section 4.

We use the *work-span model* [22, 52], a standard model of computation for analyzing shared-memory parallel algorithms. The *work* \mathcal{W} of an algorithm is the total number of operations executed by the algorithm, and the *span* \mathcal{S} is the length of the longest sequential dependence of the algorithm (it is also the parallel time complexity when there are an infinite number of processors). We can bound the expected running time of an algorithm on \mathcal{P} processors by $\mathcal{W}/\mathcal{P} + O(\mathcal{S})$ using a randomized work-stealing scheduler [11].

2.2 Relevant Techniques

Graph-based Approximate Nearest Neighbor Search. We use approximate nearest neighbor search (ANNS) algorithms in PECANN. Graph-based ANNS algorithms can find approximate nearest neighbors in high dimensions efficiently and accurately compared to alternatives such as locality-sensitive hashing, inverted indices, and tree-based indices [26, 92, 95]. These algorithms first construct a graph index on the input points, and later answer nearest neighbor queries by traversing the graph using a greedy search. Some popular methods include Vamana [55], HNSW [67], HCNNG [72], and PyN-NDescent [69]. Dobson et al. [26] provides parallel implementations for constructing these indices using a prefix-doubling approach, as well as a sequential implementation for answering a single query. Multiple queries can be processed in parallel. We describe more graph-based ANNS methods in Section 7. Graph-based indices usually support any distance measure, while some indices [55, 69] use heuristics that assume the triangle inequality holds.

ANNS on a Graph Index. We use the function $G.\text{FIND-KNN}(x, k)$ to perform an ANNS on a graph G for the point x , which returns the approximate k -nearest neighbors of x . Most graph-based ANNS methods use a variant of a *greedy (beam) search* (Algorithm 1) to answer a k -nearest neighbor query [26]. For a query point x , the algorithm maintains a *beam* \mathcal{L} with size at most L (the *width* of the beam) as a set of candidates for the nearest neighbors of x .

Let $G.E_{\text{out}}(x)$ be the vertices incident to the edges going out from x in G . We call these the *out-neighbors* of x . On each step, the algorithm pops the closest vertex to x from \mathcal{L} (Line 4), and processes it by adding all its out-neighbors to the beam (Line 5). A set \mathcal{V} is used to maintain all points that have been processed (Line 6). If $|\mathcal{L}|$ exceeds L , only the L closest points to x will be kept (Line 7). The algorithm stops when all vertices in the beam have been visited, as no new vertices can be explored (Line 3). The algorithm returns the k closest points to x from \mathcal{L} and the visited point set \mathcal{V} (Line 8).

Algorithm 1 Greedy Beam Search, modified from [55]

Input: Query point x , starting point set S , graph index G , beam width L , dissimilarity measure D , and integer k .

```

1:  $\mathcal{V} \leftarrow \emptyset$  ▷ visited points
2:  $\mathcal{L} \leftarrow S$  ▷ points in the beam
3: while  $\mathcal{L} \setminus \mathcal{V} \neq \emptyset$  do
4:    $p^* \leftarrow \text{argmin}_{(q \in \mathcal{L} \setminus \mathcal{V})} D(x, q)$ 
5:    $\mathcal{L} \leftarrow \mathcal{L} \cup G.E_{\text{out}}(p^*)$ 
6:    $\mathcal{V} \leftarrow \mathcal{V} \cup \{p^*\}$ 
7:   if  $|\mathcal{L}| > L$  then keep only the  $L$  closest points to  $x$  in  $\mathcal{L}$ 
8: return  $k$  closest points to  $x$  in  $\mathcal{L} \cup \mathcal{V}$ 
```

In some circumstances (e.g. when parts of the dataset contain many near duplicates), it is possible that the algorithm will traverse fewer than k points for a query, and thus return fewer than k points. To solve this problem, options include resorting to a brute force search or repeating the search from other starting points.

Parallel Primitives. $\text{PAR-FILTER}(A, f)$ takes as input a sequence of elements A and a predicate f , and returns all elements $a \in A$ such that $f(a)$ is true. $\text{PAR-ARGMIN}(A, f)$ takes as input a sequence of elements A and a function $f : A \rightarrow \mathbb{R}$, and returns the element $a \in A$ that has the minimum $f(a)$. $\text{PAR-SUM}(A)$ takes as input a sequence of numbers A , and returns the sum of the numbers in A . PAR-FILTER , PAR-ARGMIN , and PAR-SUM all take $O(n)$ work and $O(\log n)$ span. $\text{PAR-SELECT}(A, k)$ takes as input a sequence of elements A and an integer $0 < k \leq |A|$, and returns the k^{th} largest element in A . It takes $O(n)$ work and $O(\log n \log \log n)$ span [52]. We use the implementations of these primitives from ParlayLib [10].

A *union-find* data structure maintains the set membership of elements and allows the sets to merge. Initially, each element is in its own singleton set. A $\text{UNION}(a, b)$ operation merges the sets containing a and b into the same set. A $\text{FIND}(a)$ operation returns the membership of element a . We use a concurrent union-find data structure [54], which supports unions and finds operations in parallel. Performing m unions on a union-find data structure with n elements takes $O(m(\log(\frac{n}{m} + 1) + \alpha(n, n)))$ work and $O(\log n)$ span (α denotes the inverse Ackermann function) [54].

3 PECANN Framework

We present the PECANN framework in Algorithm 2. To make our description of the framework more concrete, we will give an example of instantiating the framework in this section. Section 4 will provide more examples and Section 5 will provide the work and span analysis of PECANN.

The input to PECANN is a point set P , a positive integer k , a distance measure D , and three functions F_{density} , F_{noise} , and F_{center} that indicate how the density, noise points, and center points are computed, respectively. In the pseudocode, ρ is an array of densities of all points in P and \mathcal{N} is an array containing k -nearest neighbors for all points. λ is an array containing dependent points. c is an array containing the cluster IDs of all points and c_i is the cluster ID of x_i . The framework has the following six steps.

1. Construct Index. On Line 1, we construct an index G , which can be any index that supports k -nearest neighbor search. For example, it can be a kd -tree, which is suitable for low-dimensional exact k -nearest neighbor search [37], or a graph-based index for ANNS on high-dimensional data [26, 55, 67, 69, 72]. It can also be an

Algorithm 2 PECANN Framework

Input: Point set P , integer $k > 0$, distance measure D , F_{density} , F_{noise} , F_{center}

```

1:  $G = \text{BUILDINDEX}(P)$ 
2: parfor  $i \in 1 \dots n$  do
3:    $N_i \leftarrow G.\text{FIND-KNN}(x_i, k)$  ▷ find  $k$ -nearest neighbors
4: parfor  $i \in 1 \dots n$  do
5:    $\rho_i \leftarrow F_{\text{density}}(x_i, N_i)$  ▷ compute densities
6:  $\lambda \leftarrow \text{COMPUTEDPTPTS}(G, P, \rho, N, D)$ 
7:  $P_{\text{noise}} \leftarrow F_{\text{noise}}(P, \rho, \lambda, N)$  ▷ compute noise points
8:  $P_{\text{center}} \leftarrow F_{\text{center}}(P \setminus P_{\text{noise}}, \rho, \lambda, N)$  ▷ compute center points
9: Initialize a union-find data structure  $UF$  with size  $n = |P|$ 
10: parfor  $x_i \in P \setminus (P_{\text{noise}} \cup P_{\text{center}})$  do
11:    $UF.\text{UNION}(i, \lambda_i)$ 
12: parfor  $i \in 1 \dots n$  do
13:    $c_i \leftarrow UF.\text{FIND}(i)$ 
14: Return  $c$ 

```

Algorithm 3 Dependent Point Computation

```

1: function DPBRUTEFORCE( $x_i, N_{\text{candidates}}, \rho, D$ )
2:    $N_{\text{candidates}} \leftarrow \text{PAR-FILTER}(N_{\text{candidates}}, j : \rho_j > \rho_i)$ 
3:   if  $N_{\text{candidates}} = \emptyset$  then return  $\emptyset$ 
4:    $\lambda_i \leftarrow \text{PAR-ARGMIN}(N_{\text{candidates}}, j : D(x_i, x_j))$ 
5:   return  $\lambda_i$ 
6: function COMPUTEDPTPTS( $G, P, \rho, N, D$ )
7:   parfor  $x_i \in P$  do
8:      $\lambda_i \leftarrow \text{DPBRUTEFORCE}(x_i, N_i, \rho, D)$ 
9:    $P_{\text{unfinished}} \leftarrow \text{PAR-FILTER}(P, x_i : \lambda_i = \emptyset)$ 
10:   $k^{\text{dep}} \leftarrow L_d$  ▷  $L_d$  is an integer parameter  $> k$ 
11:  while  $|P_{\text{unfinished}}| > \text{threshold}$  do
12:    parfor  $x_i \in P_{\text{unfinished}}$  do
13:       $N_{\text{candidates}} \leftarrow G.\text{FINDKNN}(i, k^{\text{dep}})$ 
14:       $\lambda_i \leftarrow \text{DPBRUTEFORCE}(x_i, N_{\text{candidates}}, \rho, D)$ 
15:       $k^{\text{dep}} \leftarrow 2 \cdot k^{\text{dep}}$ 
16:       $P_{\text{unfinished}} \leftarrow \text{PAR-FILTER}(P_{\text{unfinished}}, x_i : \lambda_i = \emptyset)$ 
17:  parfor  $x_i \in P_{\text{unfinished}}$  do
18:     $\lambda_i \leftarrow \text{DPBRUTEFORCE}(x_i, P, \rho, D)$ 
19:  return  $\lambda$ 

```

empty data structure, which would lead to doing brute force searches to find the exact k -nearest neighbors. An example of a graph index corresponding to a point set is shown in Figure 1.

2. Compute k -nearest Neighbors. On Lines 2–3, we compute the k -nearest neighbors of all points in parallel, using the index G . If we run the greedy search (Algorithm 1) on the example in Figure 1 with $k = 1, L = 1$, and S containing only the query point, we would find that the nearest neighbors of a, b, c, d, e , and f are c, c, b, f, d , and d , respectively (in this example, we assume that the graph index returns exact nearest neighbors).

3. Compute Densities. On Lines 4–5, we compute the density for each point in parallel using F_{density} . An example density function is $\frac{1}{D(x_i, x_j)}$, where x_j is the furthest neighbor from x_i in N_i [35]. For this density function, the densities of the points in Figure 1 are $\rho_a = \frac{1}{\sqrt{2}}, \rho_b = 1, \rho_c = 1, \rho_d = \frac{1}{\sqrt{2}}, \rho_e = \frac{1}{2}$, and $\rho_f = \frac{1}{\sqrt{2}}$. The ranking of the densities from high to low (breaking ties by node ID) is b, c, a, d, f, e .

4. Compute Dependent Points. On Line 6, we compute the dependent point of all points in parallel. The dependent points in our example are shown in Figure 2. We explain the details of how we

compute the dependent points in Section 3.1. As mentioned in Section 1, the resulting tree from this step is a hierarchy of clusters (dendrogram), which can be returned if desired. To compute a specific clustering, the following two steps are needed.

5. Compute Noise and Center Points. On Lines 7–8, we compute the noise points and center points using the input functions F_{noise} and F_{center} . An example of F_{noise} is $\text{par-filter}(P, x_i : \rho_i > \rho_{\min})$, where ρ_{\min} is a user-defined parameter. Points whose densities are at most ρ_{\min} are classified as noise points. An example of F_{center} is $\text{par-filter}(P, x_i : D(x_i, \lambda_i) \geq \delta_{\min})$, where δ_{\min} is a user-defined parameter. Non-noise points whose distance are at least δ_{\min} from their dependent point are classified as center points. In our example (Figure 3), if we let $\rho_{\min} = \frac{1}{\sqrt{2}}$, then e is a noise point. If we let $\delta_{\min} = 2.5$, then b and d are center points.

6. Compute Clusters. On Lines 9–13, we compute the clusters using a concurrent union-find data structure [54]. In parallel, for all points that are not noise points or center points, we merge them into the same cluster as their dependent point. This ensures that points (except noise points and center points) are in the same cluster as their dependent point. Figure 3 shows the clustering obtained on our example. Since e is a noise point and b and d are center points, we skip processing their outgoing edge during the union step (Line 11 of Algorithm 2).

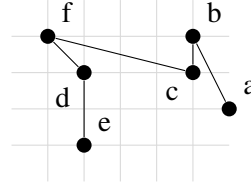


Figure 1: Example point set and a corresponding graph index.

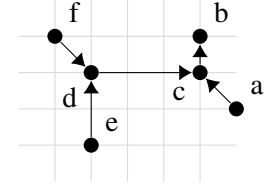


Figure 2: Each point has an edge pointing to its dependent point.

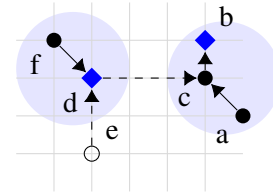


Figure 3: Clustering result with e as a noise point (white circle), and b and d as center points (blue diamond shaped). The dashed edges are ignored during the union step (Line 11 of Algorithm 2). The two blue circles are the two clusters found.

3.1 Dependent Point Computation

Our parallel algorithm for computing the dependent points (Algorithm 3) takes as input the index G , the point set P , the array of densities ρ , the array of (approximate) k -nearest neighbors N , and the distance measure D .

DPBRUTEFORCE is a helper function (Lines 1–5) that searches for the nearest neighbor of x_i with density higher than ρ_i among $N_{\text{candidates}}$ using brute force. It returns \emptyset if no points in $N_{\text{candidates}}$ have a higher density than ρ_i .

On Lines 7–8, we first search within the k -nearest neighbors of each point to find its dependent point. This optimization is also used in several other works [16, 35, 87]. On Line 9, we obtain the set of points $P_{\text{unfinished}}$ that have not found their dependent points. Line 10 initializes k^{dep} to L_d .

L_d and `threshold` are parameters used for our performance optimizations. We defer a discussion of these parameters to Section 3.2, and ignore their effect here by setting L_d to be $2k$ and `threshold` to be 0 (this causes Lines 17–18 to have no effect, since $P_{\text{unfinished}}$ will be empty at that point).

The while-loop on Line 11 terminates when all points have found their dependent point. On Lines 12–14, we compute the dependent point for points in $P_{\text{unfinished}}$. If the index is designed for approximate k -nearest neighbor search, we guarantee that the dependent point has a higher density, but it might not be the closest among points with higher densities. Note that on Line 12, we can skip the point with maximum density, since we know that it does not have a dependent point. On Lines 13–14, for each point, we find k^{dep} neighbors of x_i on each round, and if any of the neighbors have a higher density than x_i , we can return the closest such neighbor as the dependent point. We then double k_i^{dep} for the next round (Line 15). A similar doubling optimization is used in Chen et al. [16], but with a cover tree. Furthermore, their algorithm is sequential. On Line 16, we compute the set of points $P_{\text{unfinished}}$ that have not found their dependent point.

Example. On the example dataset from Figure 1, points a , c , e , and f would find their dependent point within their k -nearest neighbor ($k = 1$) on Lines 7–8 because their nearest neighbor has higher density than themselves. b is the point with maximum density and is skipped. For the remaining point d , on the first round we have $k^{\text{dep}} = 2$, and so $\mathcal{N}_{\text{candidates}} = \{e, f\}$. This does not contain any point with a higher density than d , and so we double $k^{\text{dep}} = 2$ and try again. On the second round, $k^{\text{dep}} = 4$, and so $\mathcal{N}_{\text{candidates}} = \{b, c, e, f\}$, which contains d 's dependent point c .

3.2 Performance Optimizations

Dependent Point Finding. Now we explain the two integer parameters L_d and `threshold`. The while-loop on Line 11 checks if $|P_{\text{unfinished}}| > \text{threshold}$, and when that is no longer true, we do a brute force k -nearest neighbor computation for the remaining points in $P_{\text{unfinished}}$ on Lines 17–18. This optimization is useful because for the points with relatively high density, it can be challenging for the index to find a dependent point (as most neighbors have lower density than them), and for these last few points it is faster to just brute force search than continue to double k^{dep} . Furthermore, when few points are remaining, there is less parallelism available when calling FINDKNN, each of which is sequential, compared to the brute force search, which is highly parallel. In our experiments, we set `threshold` to 300, which we found to work well in practice.

L_d is a tunable parameter that is $> k$ (Line 10) and indicates the initial number of nearest neighbors to search for to find a dependent point (Line 13). A larger value of L_d leads to fewer iterations. However, points that require fewer than L_d nearest neighbors to find a dependent point will do some extra work (as they search for more nearest neighbors than necessary). On the other hand, points that require at least L_d nearest neighbors to find a dependent point will

do less work overall (they do not need to waste work on the initial rounds where they would not find a dependent point anyway).

Vamana Graph Construction. Vamana [26, 55] is one of the graph-based indices that we use for ANNS. Its parallel construction algorithm [26] builds the graph by running greedy search (from Algorithm 1) on each point x_i (in batches), and then adds edges from x_i to points visited during the search (\mathcal{V}). It requires a degree bound parameter R , such that in the constructed graph each vertex has at most R out-neighbors. If adding edges between x_i and \mathcal{V} causes a vertex's degree to exceed R , a pruning procedure is called to iteratively select at most R out-neighbors. The pruning algorithm also has a parameter $\alpha \geq 1$ that controls how aggressive the pruning is; a higher α corresponds to more aggressive pruning, which can lead to less than R neighbors being selected. Intuitively, this heuristic prunes the long edge of a triangle, with a slack of α . The details of the pruning algorithm can be found in [55].

The original Vamana graph construction algorithm [26, 55] starts the greedy search from a single point, which is the medoid of P . Starting from a single point can make the algorithm require a high degree bound and beam width to achieve good results on clustered data because a search can be trapped within the cluster that the medoid is in. To improve performance without needing a large degree bound and beam width (which degrades performance), we use an optimization where we randomly sample a set of starting points for the Vamana graph construction algorithm instead of starting from the medoid alone. This random sampling heuristic is also explored in [62].

4 Applications of PECANN

PECANN allows users to plug in functions that can be combined to obtain new clustering algorithms. In this section, we describe several functions and provide their work and span bounds. Section 5 gives the overall bounds of PECANN using the combination of functions that gives the best performance in practice.

4.1 Indices

Here we describe several approaches for building indices for k -nearest neighbor search. Let the work and span of constructing G be \mathcal{W}_G and \mathcal{S}_G , respectively.

Brute Force. The brute force approach corresponds to not having an index at all. When searching for the exact k -nearest neighbors of x_i , it uses a PAR-SELECT to find the k^{th} smallest distance to x_i , and a PAR-FILTER to filter for the points with smaller distances to x_i . In this case, \mathcal{W}_G and \mathcal{S}_G are $O(1)$, while \mathcal{W}_{nn} and \mathcal{S}_{nn} are $O(n)$ and $O(\log n \log \log n)$, respectively.

Tree Indices. Another option is to use a tree index, such as a kd -tree or a cover tree [16]. For a parallel kd -tree, $\mathcal{W}_G = O(n \log n)$ and $\mathcal{S}_G = O(\log n \log \log n)$ [94]. A parallel cover tree can be constructed in $O(n \log n)$ expected work and $O(\log^3 n \log \log n)$ span with high probability [43]. A k -nearest neighbor search in a kd -tree takes $O(n)$ work and $O(\log n)$ span. A k -nearest neighbor search in a cover tree takes $O(c^7(k + c^3) \log k \log \Delta)$ expected work and span [32, 43], where c is the expansion constant of P and Δ is the aspect ratio of P . However, note that these tree indices usually suffer from the curse of dimensionality and do not perform well on high-dimensional datasets.

Graph Indices. Graph-based ANNS algorithms have been shown to be efficient and accurate in finding approximate nearest neighbors in high dimensions [26, 92, 95]. Our framework includes three parallel graph indices from the ParlayANN library [26]: Vamana [55], HCNNG [72], and PyNNDescent [69]. Similar to Vamana, HCNNG also uses the parameter α to prune edges. HCNNG and PYNNDESCENT also accept a *num_repeats* argument, which represents how many times they will independently repeat the construction process before merging the results together.

When the number of returned neighbors is less than k , we use the brute force method to find the exact k -nearest neighbors. Although these graph indices have been shown to work well in practice, there are only a few works that theoretically analyze their query complexity [50, 59, 73, 75, 82]. Indyk and Xu [50] show that Vamana construction takes $\mathcal{W}_c = O(n^2(R + \log n))$ work. In practice, we find that the work is usually much lower. Using the batch insertion method [26], which inserts points in batches of doubling size, Vamana construction takes $\mathcal{S}_c = O(n \log n(R + \log n))$ span.

4.2 Density Functions

In this section, we describe the density functions F_{density} that we implement in PECANN. Other density functions used in the literature are discussed in Section 7.

kth. The density of x_i is $\rho_i = \frac{1}{D(x_i, x_j)}$ where x_j is the furthest neighbor from x_i in \mathcal{N}_i , i.e., the distance to the exact or approximate k^{th} nearest neighbor of x_i [16, 35]. Each density computation is $O(k)$ work and $O(\log k)$ span to find the furthest neighbor in \mathcal{N}_i .

The density can also be normalized [47]. The normalized density (**normalized**) is $\rho'_i = \frac{\rho_i k}{\sum_{j \in \mathcal{N}_i} \rho_j}$. Intuitively, this function normalizes a point's density with an average of the densities of its neighbors. Each normalization takes an extra $O(k)$ work and $O(\log k)$ span.

exp-sum. The density of x_i is $\rho_i = \exp(-\frac{\sum_{j \in \mathcal{N}_i} D(x_i, x_j)^2}{k})$, which is exponential in the negative of the average squared distance between x_i and its k -nearest neighbors [28]. Each density computation takes $O(k)$ work and $O(\log k)$ span by using a parallel sum.

sum-exp. The density of x_i is $\rho_i = \frac{\sum_{j \in \mathcal{N}_i} \exp(-D(x_i, x_j)^2)}{k}$ [102]. Each density computation is $O(k)$ work and $O(\log k)$ span to compute the summation using a parallel sum. It can also be viewed as a variant of the kernel density of the original DPC algorithm [77].

sum. The density of x_i is $\rho_i = -\sum_{j \in \mathcal{N}_i} D(x_i, x_j)$, which is the negative sum of distances to the k -nearest neighbors. Each density computation takes $O(k)$ work and $O(\log k)$ span to compute the summation using a parallel sum. We include this as a simple baseline.

4.3 Center Functions

In this section, we describe the center functions F_{center} that we implement in PECANN. Recall from Section 2 that $\delta_i = D(x_i, \lambda_i)$ is the dependent distance of x_i .

Threshold Center. F_{center} obtains the center points by selecting the points whose distance to their dependent point is greater than δ_{\min} , a user-defined parameter. This can be implemented with a *par-filter*, whose work and span are $O(n)$ and $O(\log n)$, respectively. This method is used in [5, 6, 102].

Product Center. This method takes as input n_c , a user-defined parameter that specifies how many clusters to output. We compute the product $\delta_i \times \rho_i$ for all points x_i . The n_c points with the largest products are the center points. This function can be implemented with a *PAR-SELECT* to find the n_c^{th} largest product t , and then a *PAR-FILTER* to filter out the points with product less than t . The work and span are $O(n)$ and $O(\log n \log \log n)$, respectively. This method is used in [47, 56, 64, 77].

Local Center. For this method, a point is a center point if it has the highest density among its k -nearest neighbors. This can be implemented using a parallel filter with $O(nk)$ work and $O(\log n)$ span. This density finder is usually accompanied by further steps to merge and refine the initial DPC clusters [35, 87].

There are also methods that plot a decision graph for visualization and pick the cluster centers manually [29, 30]. Finally, some iterative methods have been proposed (e.g., [1, 64, 98]), but they have been infrequently used.

4.4 Noise Function

We implement a noise function F_{noise} , which returns the points x_i with density $\rho_i < \rho_{\min}$. These points are then ignored in the remainder of the algorithm. This can be implemented using a parallel filter with $O(n)$ work and $O(\log n)$ span. A noise function of this form is used by [5, 6, 77].

This noise function is the only one that PECANN currently implements because it is the most commonly used, but alternative noise function definitions can be supported. For example, Abbas et al. [1] define noise points based on the number of neighborhoods a point belongs in, and Xie et al. [98] compute noise points by using a threshold on the dependent distance.

5 Analysis of PECANN

The work and span of PECANN (Algorithm 2) depend on the specific index construction algorithm and the specific implementations of the functions F_{density} , F_{noise} , and F_{center} . Here, we will choose the functions that give the best performance in our experiments (*kth* density, product center, and default noise functions).

We first analyze the work and span of computing dependent points as shown in Algorithm 3 (this is called on Line 6 of Algorithm 2). Let $n_{\text{can}} = |\mathcal{N}_{\text{candidates}}|$. Lines 1–5 take $O(n_{\text{can}})$ work and $O(\log n_{\text{can}})$ span. Thus, Lines 7–8 take $O(nk)$ work and $O(\log k)$ span, because $|\mathcal{N}_i| = k$ and $|P| = n$. Line 9 takes $O(n)$ work and $O(\log n)$ span.

On Lines 11–16, for each point, we call *G.FINDKNN* $O(\log n)$ times since we double k^{dep} after each round. Let the work and span of finding the k nearest neighbors using *G* be $\mathcal{W}_{nn}(k)$ and $\mathcal{S}_{nn}(k)$, respectively. Let $\mathcal{W}_{nn} = \sum_{j=0}^{O(\log n)} \mathcal{W}_{nn}(2^j)$ and $\mathcal{S}_{nn} = \sum_{j=0}^{O(\log n)} \mathcal{S}_{nn}(2^j)$. The filter on Line 16 takes $O(n \log n)$ work and $O(\log^2 n)$ span across $O(\log n)$ rounds. The total work and span across all rounds is $O(n\mathcal{W}_{nn})$ and $O(\mathcal{S}_{nn} + \log^2 n)$. The brute force computation on Lines 17–18 takes $O(n)$ work and $O(\log n)$ span, as only $O(1)$ points remain after the loop on Lines 11–16.

Thus, the work and span of Algorithm 3 are $O(n\mathcal{W}_{nn})$ and $O(\mathcal{S}_{nn} + \log^2 n)$, respectively.

We now analyze the remaining steps of Algorithm 2. Lines 2–3 compute the k -nearest neighbors of all points, which takes $O(n\mathcal{W}_{nn}(k))$ work and $O(n\mathcal{S}_{nn}(k))$ span. Lines 4–5 compute the densities of all

Name	n	d	Description	# Clusters
S2	5,936	2	Standard benchmark	15
Unbalanced	6,500	2	Standard benchmark	8
gaussian	10^5 to 10^8	128	Standard benchmark	10 to 10000
MNIST	70,000	784	Raw images	10
ImageNet	1,281,167	1024	Image embeddings	1000
birds	84,635	1024	Image embeddings	525
reddit	420,464	1024	Text embeddings	50
arxiv	732,723	1024	Text embeddings	180

Table 2: The datasets used in our experiments, along with their sizes (n), their dimensionality (d), and the number of ground truth clusters.

points. Using the k th density function, this takes $O(nk)$ work and $O(\log k)$ span. Lines 7–8 using the product center and default noise functions take $O(n)$ work and $O(\log n \log \log n)$ span. The union-find operations on Lines 9–13 take $O(n\alpha(n, n))$ work and $O(\log n)$ span.

The following theorem gives the overall work and span of PECANN.

THEOREM 1. *The work and span of PECANN using the k th density, product center, and the default noise functions are $O(W_c + nW_{nn})$ and $O(S_c + S_{nn} + \log^2 n)$, respectively.*

6 Experiments

Computational Environment. We use *c2-standard-60* instances on the Google Cloud Platform. These are 30-core machines with two-way hyper-threading with Intel 3.1 GHz Cascade Lake processors that can reach a max turbo clock-speed of 3.8 GHz. The instances have two non-uniform memory access (NUMA) nodes, each with 15 cores. Except for the experiments specifically investigating how performance scales with the number of threads, we use all 60 hyper-threads for our experiments.

Datasets. We use a variety of real-world and artificial datasets, summarized in Table 2 and described below.

- S2 and Unbalanced [36] are small baseline datasets used in prior clustering papers.
- gaussian is a synthetic mixture of datasets generated from a Gaussian distribution. To generate a gaussian dataset of dimension $d = 128$ with size n and c clusters, we first sample c centers x_i uniformly from $[0, 1]^d$, and then we sample n/c points from a Gaussian centered at each x_i with variance 0.05.
- MNIST [24] is a standard machine learning dataset that consists of 28 \times 28 dimensional images of grayscale digits between 0 and 9. The i th cluster corresponds to all occurrences of digit i .
- ImageNet [23] is a standard image classification benchmark with more than one million images, each of size $224 \times 224 \times 3$. The images are from 1000 classes of everyday objects. Unlike for MNIST, we do not cluster the raw ImageNet images, but instead first pass each image through ConvNet [65] to get an embedding. Each ground truth cluster contains the embeddings corresponding to a single image class from the original ImageNet dataset.
- birds [39] is a dataset that contains images of 525 species of birds. The images have the same number of dimensions as ImageNet, and we pass it through the same ConvNet model to obtain an embedding dataset. The ground truth clusters are the 525 species of birds. This dataset is interesting because it is out of distribution for the original ConvNet model.

Dataset	L	L_d	R	k
S2, Unbalanced	12	4	16	6
MNIST	32	32	32	16
ImageNet	128	128	128	16
reddit, arxiv	64	64	64	16
gaussian, birds	32	32	32	16

Table 3: Default parameters used for datasets.

- reddit and arxiv are text embedding datasets studied in the recent Massive Text Embedding Benchmark (MTEB) work [71]. We restrict our attention to embeddings from the best model on the current MTEB leaderboard, GTE-large [61]. We also restrict our attention to the two largest datasets from MTEB, reddit, where the goal is to cluster embeddings corresponding to post titles into subreddits, and arxiv, where the goal is to cluster embeddings corresponding to paper titles into topic categories.

Algorithms. We implement our algorithms using the ParlayLib [10] and ParlayANN [26] libraries. We use C++ for all implementations, and the gcc compiler with the `-O3` flag to compile the code. We also provide Python bindings for PECANN. We evaluate the following algorithms.

- PECANN: Our framework described in Section 3 with the different density functions described in Section 4. Unless specified otherwise, we use the k th density function without normalization with $k = 16$, the VAMANA graph index with $\alpha = 1.1$, and the product center function with n_c set to the number of ground truth clusters, and the default noise function. In Table 3, we give the rest of the default parameters that we used for each dataset.
- FASTDP [83]: A single-threaded approximate DPC algorithm that also uses graph-based ANNS to estimate densities. As a conservative estimate, we assume that FASTDP can be modified to have ideal parallel speedup, and denote this with FASTDP (SCALED). In other words, we divide all FASTDP runtimes by 60 in plots to get FASTDP (SCALED).
- k -MEANS: We use the FAISS [57] implementation of k -means, an extremely efficient k -means implementation. The k -means algorithm takes in k , the number of clusters, *niter*, the number of iterations, and *nredo*, the number of times to retry and choose the best clustering. Unless specified otherwise, the number of clusters used in k -means is the number of clusters in the ground truth clustering.
- BRUTEFORCE: An instantiation of PECANN, where we use a naive parallel brute force approach for every step. This method takes $O(n^2)$ work. It also first searches within the k -nearest neighbors to find the dependent point. We refer to the result of BRUTEFORCE as the "exact DPC" result.

We also tried a parallel exact DPC algorithm that uses a priority search kd -tree-based dependent point finding algorithm that was designed for low dimensions [48]. We changed the first step of Huang et al. [48] from a range search to a k -nearest neighbor search to match our framework. On MNIST, their algorithm takes 280s on our 30-core machine, which is 320 times slower than PECANN. This method is prohibitively slow because kd -trees suffer from the curse of dimensionality, where performance in high dimensions degrades to no better than a linear search [96]. We thus do not further compare against this method.

Evaluation. We evaluate clustering quality using the Adjusted Rand Index (ARI) [49], homogeneity, and completeness [78].

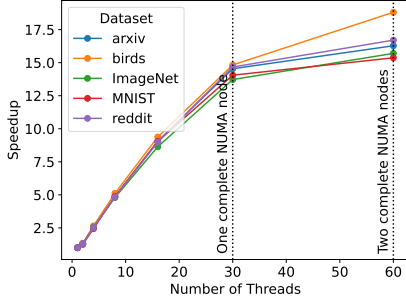


Figure 4: Self-relative parallel speedup across different numbers of hyper-threads.

Consider our clustering C and the ground-truth or exact clustering \mathcal{T} . Intuitively, ARI evaluates how similar C and \mathcal{T} are. Homogeneity measures if each cluster in C contains members from the same class in \mathcal{T} . Completeness measures whether all members in \mathcal{T} of a given class are in the same cluster in C .

Let n_{ij} be the number of objects in the ground truth cluster i and the cluster j generated by the algorithm, n_{i*} be $\sum_j n_{ij}$, n_{*j} be $\sum_i n_{ij}$, and n be $\sum_i n_{i*}$. The ARI is computed as

$$\frac{\sum_{i,j} \binom{n_{ij}}{2} - [\sum_i \binom{n_{i*}}{2} \sum_j \binom{n_{*j}}{2}] / \binom{n}{2}}{\frac{1}{2} [\sum_i \binom{n_{i*}}{2} + \sum_j \binom{n_{*j}}{2}] - [\sum_i \binom{n_{i*}}{2} \sum_j \binom{n_{*j}}{2}] / \binom{n}{2}}.$$

The ARI score is 1 for a perfect match, and its expected value is 0 for random assignments.

The formulas for homogeneity and completeness of clusters are defined as follows: homogeneity = $1 - \frac{H(C|\mathcal{T})}{H(C)}$; completeness = $1 - \frac{H(\mathcal{T}|C)}{H(\mathcal{T})}$. $H(C|\mathcal{T})$ is the conditional entropy of the class distribution given the cluster assignment, $H(C)$ is the entropy of the class distribution, $H(\mathcal{T}|C)$ is the conditional entropy of the cluster distribution given the class, and $H(\mathcal{T})$ is the entropy of the cluster distribution. For example, consider a ground-truth clustering \mathcal{T} where all classes have the same number of points. If C assigns every point to its own cluster of size 1, it has homogeneity score 1 and a low completeness score when $n_c \ll n$. On the other hand, if C assigns all points to a single cluster, it has completeness score 1 and homogeneity score 0.

Parallel Scalability. Figure 4 shows the parallel scalability of PECANN on our larger datasets. PECANN achieves an average of 14.36x self-relative speedup on one NUMA node with 30 hyper-threads and an average of 16.57x self-relative speedup on two NUMA nodes with 60 hyper-threads.

Scalability over Dataset Size. Figure 5 shows the runtime of PECANN as we increase the size of the synthetic gaussian dataset and vary the number of clusters. We use a linear fit on the logarithm of runtime and $\log n$ to get the slopes of the lines in Figure 5. The slope s reflects the exponent in the growth of runtime with respect to data size. We see that the slope ranges from 1.12–1.2 depending on the number of output clusters, and thus experimentally the clustering grows approximately as $O(n^{1.2})$ for this dataset. This shows that PECANN has good scalability with respect to n .

Runtime Decomposition. We present the runtime decomposition of PECANN on each dataset with all density methods and all values of

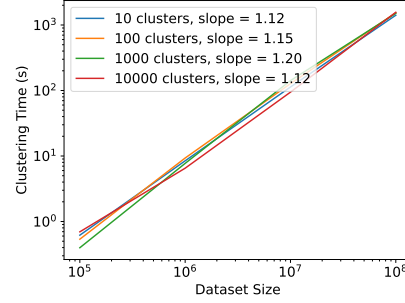


Figure 5: Running time (seconds) across gaussian datasets of different sizes and different numbers of clusters in log-log scale. The "slope" s is the slope of the line in the log-log plot, and means that the running time scales as $O(n^s)$.

Dataset	k	Index	Density	Dependent Point	Union-Find
arxiv	8	60.9	35.0	4.1	0.0
arxiv	32	52.5	45.6	1.9	0.0
MNIST	8	53.4	43.7	2.6	0.3
MNIST	32	34.8	63.7	1.4	0.1
reddit	8	54.6	36.9	8.4	0.1
reddit	32	58.6	40.1	1.2	0.1
birds	8	72.0	20.8	6.0	1.2
birds	32	55.2	38.8	5.1	0.9
ImageNet	8	70.0	27.3	2.6	0.1
ImageNet	32	59.0	39.0	2.0	0.0

Table 4: Runtime percentage breakdown with the k th density method with $k = 8, 32$ on large datasets.

k in Figure 6. As a summary, Table 4 presents the runtime breakdown for the k th density method for $k = 8, 32$. The bottleneck of the running time is the index construction time and the k -nearest neighbor time when computing densities. When k is larger, the k -nearest neighbor search time for density computation is longer, as expected. Computing clusters with union-find is fast because this step has low work, as discussed in Section 4. The dependent point computation time is significantly shorter than the density computation because the dependent point for some points can be obtained from the k -nearest neighbors (Lines 7–8 in Algorithm 3), so we do not need to run nearest neighbor searches for these points. Additionally, even when the dependent point is not in the k -nearest neighbors, our doubling technique finds a dependent point in the first few rounds for most points, thereby usually avoiding an expensive exhaustive search.

Comparison of Different Density Functions and Values of k . In Figure 7, we show the runtime vs. ARI of different density functions and values of k . We see that the k th density function is the most robust and achieves the highest ARI score on most datasets. We also observe that using $k = 16$ provides a good trade-off between quality and time.

Comparison of Different Graph Indices. We can easily swap in different graph indices into our framework and compare the results. In Figure 8, we show a Pareto frontier of the clustering quality vs. runtime on ImageNet for each of the following different graph indices: VAMANA [55], PYNNDESCENT [69], and HCNNG [72]. The Pareto frontier comprises points that are non-dominated, meaning no

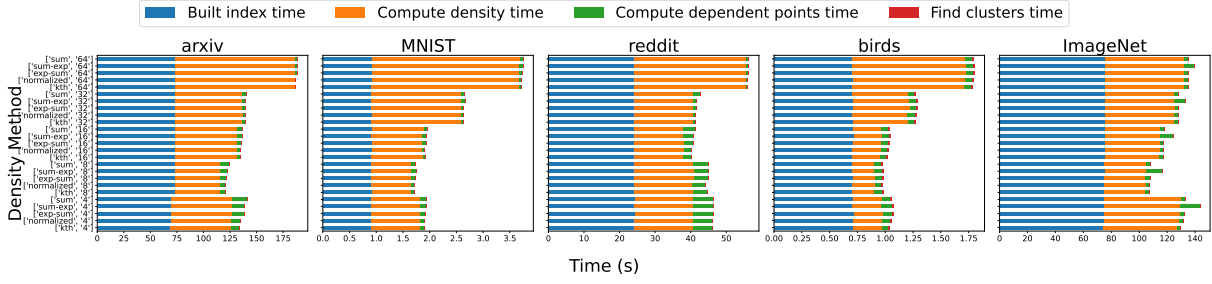


Figure 6: Runtime decomposition of PECANN with different density functions and values of k .

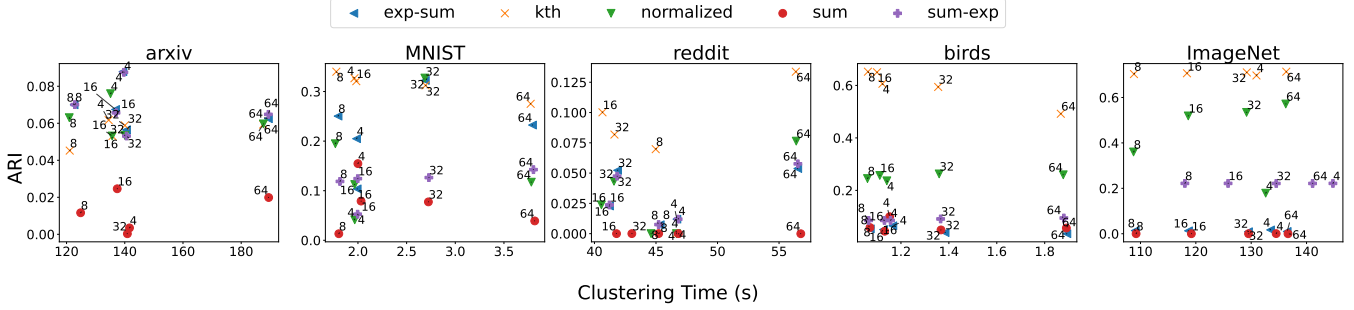


Figure 7: Clustering quality (ARI) vs. runtime of PECANN when using different density functions and values of k . The y -axis shows the ARI scores computed with respect to the ground truth. The x -axis shows the runtime in seconds. Each color represents a density function, and the number next to each data point is the value of k used.

point on the frontier can be improved in quality without worsening time and vice versa. In other words, the curve we plot represents the optimal trade-off in the parameter space between clustering time and quality.

To create the Pareto frontier, we do a grid search for each method over different choices of maximum degree R and the beam sizes for construction, k -nearest neighbor search, and dependent point finding. We choose all combinations of these four parameters from $[8, 16, 32, 64, 128, 256]^4$. We set the density method to be `kth` without normalization and $k = 16$. We set $\alpha = 1.1$ for VAMANA and PYNNDESCENT. HCNNG and PYNNDESCENT additionally accept a `num_repeats` argument, which represents how many times we should independently repeat the construction process before merging the results together; we set this parameter equal to 3. We see that all graph indices are able to achieve similar maximum ARI with respect to the ground truth: VAMANA, HCNNG, and PYNNDESCENT achieve maximum ARIs of 0.709, 0.715, and 0.713, respectively. HCNNG attains this maximum slightly faster than the other two indices, but when compared to the exact DPC result, HCNNG has a smaller maximum ARI, which means its clustering deviates more from the exact solution. Indeed, HCNNG has a maximum ARI compared to exact DPC of 0.918, while PYNNDESCENT and VAMANA attain a maximum ARI of 0.995 compared to exact DPC.

Clustering Quality-Time Trade-off vs. Exact DPC. In Figure 9, we plot the Pareto frontier of clustering quality (ARI with respect to the exact DPC clustering) vs. runtime of PECANN. To obtain the Pareto frontiers, we use the same parameter values as in the last experiment, except that for the smaller datasets with $n < 250,000$ we use a smaller range $[8, 16, 32, 64]^4$ for the parameter search space. We see

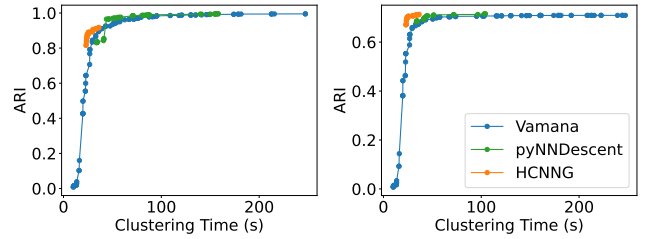


Figure 8: (Left) Pareto frontier of clustering quality with respect to exact DPC vs. runtime on ImageNet. (Right) Pareto frontier of clustering quality with respect to the ground truth clustering vs. runtime on ImageNet.

that PECANN is able to achieve results very close to the exact DPC clustering. On all datasets except `arxiv`, PECANN achieves at least 0.995 ARI with respect to exact DPC, and on `arxiv`, PECANN achieves 0.989 ARI with respect to exact DPC.

Comparison of Different Methods. We first show in Table 5 the runtime and ARI score with respect to the ground truth of all methods run using a single thread on the small datasets `S2` and `Unbalanced`. Compared to the density-based methods, k -MEANS has a slightly higher ARI on `S2`, but significantly worse ARI on `Unbalanced`. This shows that the relative performance of k -MEANS and density-based methods depends on the dataset, which we also observe below on large high-dimensional real-world datasets.

In Figure 10, we plot the Pareto frontier of clustering quality (ARI with respect to the ground truth clustering) vs. runtime for

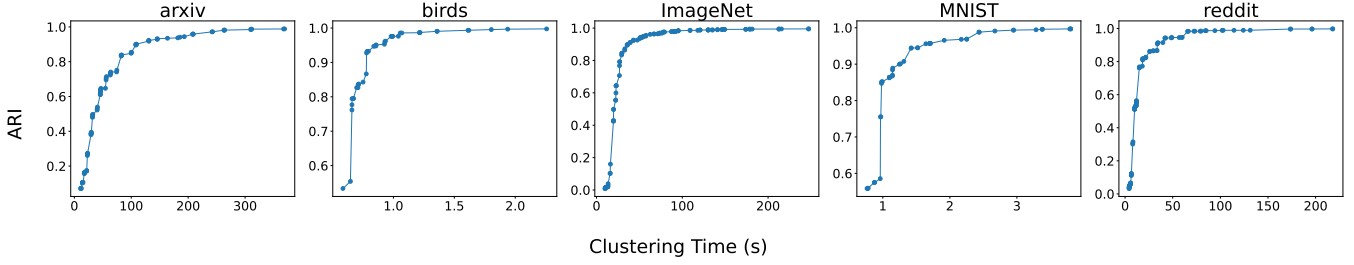


Figure 9: Pareto frontier of clustering quality of PECANN with respect to exact DPC.

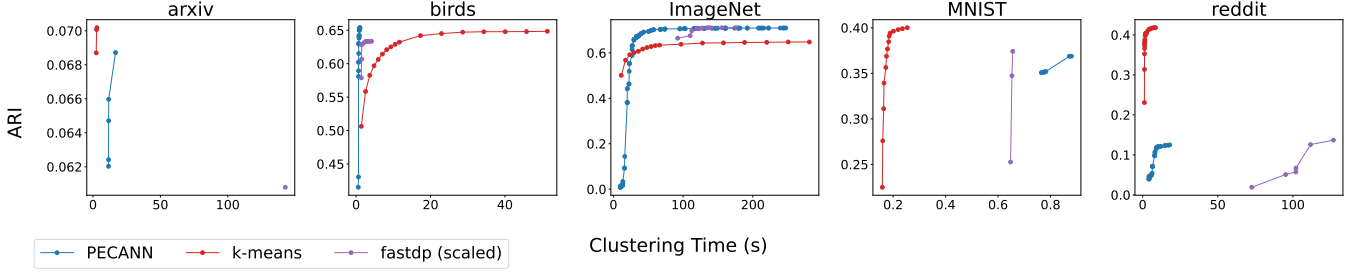


Figure 10: Pareto frontier of clustering quality of all methods with respect to ground truth vs. runtime. Up and to the left is better. PECANN is the best method on ImageNet and birds, has similar performance to the best method (k -MEANS) on arxiv, and is slower or has worse quality than the best method (k -means) on mnist and reddit. FASTDP is sequential, and in this plot we assume it achieves a perfect speedup of 60 to obtain FASTDP (SCALED).

Dataset	Algorithm	Details	Time	ARI
S2	FASTDP	N/A	0.172	0.933
S2	k -MEANS	$nredo = 1$	0.005	0.860
S2	k -MEANS	$nredo = 50$	0.237	0.940
S2	PECANN	product center finder	0.486	0.925
S2	PECANN	threshold center finder	0.473	0.925
S2	BRUTEFORCE	threshold center finder	0.499	0.925
Unbalanced	FASTDP	N/A	0.246	1.000
Unbalanced	k -MEANS	$nredo = 1$	0.003	0.691
Unbalanced	k -MEANS	$nredo = 50$	0.098	0.832
Unbalanced	PECANN	product center finder	0.737	0.843
Unbalanced	PECANN	threshold center finder	0.651	1.000
Unbalanced	BRUTEFORCE	threshold center finder	0.623	1.000

Table 5: Runtime and ARI score with respect to ground truth for all methods using a single thread on the small low-dimensional synthetic datasets S2 and Unbalanced. When using the threshold center finder, we set $\delta_{\min} = 102873$ for S2 and $\delta_{\min} = 30000$ for Unbalanced. We set $\rho_{\min} = 0$ for the noise function. For k -means, we used $niter = 20$.

different methods on the larger datasets. To obtain the Pareto frontiers, we use the same parameters for VAMANA as in the previous experiment. For k -MEANS, we use $nredo \in [1, 2, 3, 4]$ and $niter \in [1, 2, 3, \dots, 9, 10, 15, 20, 25, \dots, 40, 45]$, for all combinations where $niter * nredo < 100$. For FASTDP, we use $window_size \in [20, 40, 80, 160, 320]$ for all datasets (controlling query quality) and $max_iterations \in [1, 2, 4, 8, 16, 32, 64]$ (controlling graph construction quality).

We observe that FASTDP, even when given ideal parallel speedup, is slower than PECANN on all datasets except MNIST, where the two methods have similar performance. In terms of accuracy, PECANN has better maximum ARI on birds and arxiv, while FASTDP has better maximum ARI on reddit (although as we discuss below, reddit is not well suited to DPC).

Compared with k -MEANS, PECANN obtains better quality and is faster on ImageNet and birds, where the number of ground truth clusters is large, and performs about equal with k -MEANS on arxiv. However, PECANN has worse quality for a given time limit on reddit and mnist. We summarize the best ground truth ARI and the corresponding parallel running time that all three of these methods achieve, as well as BRUTEFORCE, in Table 6. Compared to density-based methods, PECANN achieves 37.7–854.3x speedup over BRUTEFORCE, 45–734x speedup over FASTDP, and 0.76–12.24x speedup over FASTDP (SCALED), while achieving comparable ARI.

For some more intuition on the runtime differences between PECANN and k -MEANS, we note that the work of each iteration of k -MEANS is linear in the number of clusters multiplied by n , and so k -MEANS is very fast on datasets like MNIST with a small number of ground truth clusters, while it is comparatively slower on datasets like birds and imagenet that have many clusters.

In terms of an explanation for the quality difference between PECANN and k -MEANS, PECANN gets better maximum accuracy on imagenet and birds, which may be because the ground truth clusters in these datasets form shapes that our density-based method PECANN can find, but that the geometrically constrained k -means cannot. On the other hand, for reddit, PECANN has lower quality than k -MEANS. Since we still obtain cluster quality very close to the exact DPC on reddit (see Figure 9), this dataset is a case where the density based DPC method is worse than the simpler k -means heuristic.

Varying Number of Clusters. In Figure 11, we show the ARI (with respect to ground truth) of PECANN using VAMANA and k -MEANS when we pass a number of clusters to the algorithm different than the ground truth (we plot the ratio between the number of clusters used and the number of ground truth clusters). Not knowing the

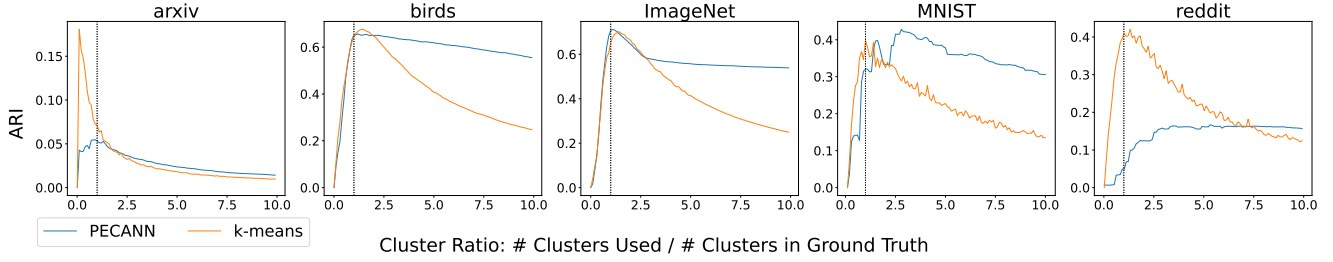


Figure 11: The ARI of PECANN using the VAMANA graph index vs. that of k -MEANS, when clustering with a different numbers of clusters than the ground truth. y -axis is the ARI with respect to the ground truth. x -axis is the ratio between the number of clusters used and the number of clusters in the ground truth. The vertical dotted line is $x = 1$, where the correct number of clusters is used.

Algorithm	Dataset	Time (s)	Maximum ARI
PECANN	arxiv	11.65	0.07
FASTDP (SCALED)	arxiv	142.63	0.06
BRUTEFORCE	arxiv	9953.15	0.07
KMEANS	arxiv	2.41	0.07
PECANN	birds	0.86	0.65
FASTDP (SCALED)	birds	2.15	0.63
BRUTEFORCE	birds	66.04	0.66
KMEANS	birds	28.66	0.65
PECANN	ImageNet	101.58	0.71
FASTDP (SCALED)	ImageNet	127.60	0.71
BRUTEFORCE	ImageNet	31979.98	0.71
KMEANS	ImageNet	188.17	0.65
PECANN	MNIST	0.87	0.37
FASTDP (SCALED)	MNIST	0.66	0.37
BRUTEFORCE	MNIST	32.80	0.34
KMEANS	MNIST	0.22	0.40
PECANN	reddit	14.90	0.12
FASTDP (SCALED)	reddit	127.03	0.14
BRUTEFORCE	reddit	2888.20	0.10
KMEANS	reddit	5.36	0.42

Table 6: The maximum ARI score with respect to the ground truth achieved by different clustering algorithms across different datasets, and their corresponding parallel running time. The sequential FASTDP runtime can be computed by multiplying FASTDP (SCALED) by 60.

number of ground truth clusters is common in real-world settings, so algorithm performance in this regime is important. We see that PECANN is better than k -MEANS when the number of clusters used is larger than the true number of clusters (except on *reddit*, where we have argued above that DPC is not suitable). When the number of clusters used is larger, the quality of k -MEANS decays quickly while the quality of PECANN is more robust. When the true number of clusters used is smaller than the ground truth, the quality of the two methods is similar on *birds*, *ImageNet*, and *MNIST*, while k -MEANS is better on *arxiv* and *reddit*.

As mentioned in Section 1, DPC variants can produce a hierarchy of clusters, which contains more information than k -means. Each run of k -means produces only a single cluster. Thus, to perform the experiment in Figure 11, in PECANN we can just redo the postprocessing step (Lines 7–14 of Algorithm 2), whereas for k -means we must rerun the algorithm from scratch for each choice of the number of clusters.

In Figure 12, we show a Pareto frontier of the completeness and homogeneity scores (with respect to the ground truth) of PECANN and k -MEANS on different datasets. We generate this Pareto frontier

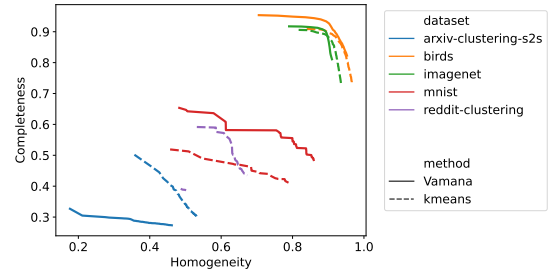


Figure 12: Pareto frontiers of completeness vs homogeneity of PECANN and k -MEANS on different datasets. Up and to the right is better.

using the same experiment setup as just described, except that now we record homogeneity and completeness instead of ARI as we vary the number of clusters given to each method. Thus, points along the Pareto frontier in Figure 12 are optimal tradeoffs between homogeneity and completeness as we vary the cluster granularity. We see that PECANN strictly dominates k -MEANS on *birds* and *MNIST*, and k -MEANS is better on *arxiv* and *reddit*. On *ImageNet*, PECANN achieves higher completeness and k -MEANS achieves higher homogeneity.

7 Related Work

Density peaks clustering (DPC) has gained considerable attention recently due to its effectiveness. Since the original DPC algorithm [77] was proposed, various adaptations and improvements have been developed. In this section, we give an overview of different DPC variations, particularly the ones that are based on k -nearest neighbors. We also briefly introduce other density-based clustering algorithms. Finally, we discuss recent advances on graph-based approximate nearest neighbor search.

Variants of DPC. The original DPC algorithm [77] uses a range search to compute the density of a point x . The density is the number of points in a ball centered at x with a user-defined radius. In contrast, our paper focuses on evaluating k -nearest neighbor-based DPC variants, which do not require a range search. We can let $k = n$ and let F_{density} be a range search. Using k -nearest neighbor-based density computation also reduces sensitivity to noise and outliers by focusing on local densities, thereby mitigating the impact of sparse data points prevalent in high-dimensional spaces [35]. However, in theory PECANN supports radius-based DPC variants. Some of these

(e.g. [35, 87, 98, 102]) methods have a refinement step after obtaining the initial DPC clustering. For these methods, PECANN can be also used to efficiently obtain the first DPC clustering before the refinement step.

Floros et al. [35] and Chen et al. [16] use the inverse of the distance to the k^{th} nearest neighbor as the density measure. Sieranoja and Fränti [83] propose FASTDP, which uses the inverse of the average distance to all k -nearest neighbors as the density measure, and finds the k -nearest neighbors by constructing an approximate k -nearest neighbor graph. Their motivation for not using the original DPC density function is that they are considering non-metric distance measures. Specifically, they use string similarity measures such as the Levenshtein distance and the Dice coefficient. In our experiments, we used the Euclidean distance measure for FASTDP to be consistent. Du et al. [29] propose a density function that depends on the shortest path distance in the k -nearest neighbor graph. Some works propose to normalize the density of each point by the density of its neighbors [38, 47, 86], as the normalization helps to reduce the influence of large density differences across clusters and is better for detecting clusters with different densities [47]. Yin et al. [103] use k -nearest neighbor searches to partition the data, which they show works well when the average density between clusters is very different. There are also works that propose to use density measures based on the mutual neighborhood [14, 60, 87], natural neighborhood [25, 107], order similarity [101], and the exponential of the sum of distances to neighbors [28, 60, 98, 102]. d’Errico et al. [31] propose a variant of DPC for high-dimensional data. It combines DPC with a non-parametric density estimator called PAK, but their algorithm is sequential. There are also algorithms that perform dimensionality reduction on the dataset before running DPC [14, 28], such as using principal components analysis.

Parallel, Approximate, and Dynamic DPC. Zhang et al. [104] propose an approximate DPC algorithm in the distributed (MapReduce) setting using locality-sensitive hashing. Their algorithm can also work in multicore environments. It partitions the data set into buckets, and searches within the bucket to find approximate dependent points. It resorts to scanning the whole dataset when the approximate dependent point does not seem accurate.

Amagata and Hara [5] propose a partially parallel exact DPC algorithm and two parallel grid-based approximate DPC algorithms. They show that their algorithms are faster than previous solutions, including LSH-DDP [104], CFSFDP-A [8], FastDPeak [16], and DPCG [99]. They also propose parallel static and dynamic² DPC algorithms for data in Euclidean space [4, 6]. Amagata and Hara [6] show that their dynamic algorithm outperforms previous dynamic DPC algorithms [41, 89]. Huang et al. [48] propose a fully parallel exact DPC algorithm based on priority kd -trees and show that their algorithm is faster than previous tree-index approaches [5, 76]. Lu et al. [66] propose speeding up DPC using space-filling curves. All of these algorithms [5, 6, 8, 48] are optimized for low-dimensional datasets, and suffer from the curse of dimensionality in high dimensions. Compared to these algorithms, PECANN is suitable for high dimensional data and can be used for distance metrics other than Euclidean distance.

Amagata [4] proposes an approximate dynamic DPC algorithm for metric data, but their algorithm is sequential, and only tested on datasets in up to 115 dimensions. In comparison, our framework is parallel and we experimented on datasets in up to 1024 dimensions. There are also dynamic algorithms for k -nearest neighbor-based DPC variants [27, 80].

Density-based Clustering Algorithms. DPC falls under the broad category of density-based clustering algorithms, which have the advantage of being able to detect clusters of arbitrary shapes. Density-based clustering algorithms come in different varieties. Some density-based clustering algorithms define the density of a point based on the number of points in its vicinity [3, 7, 17, 34, 35, 53, 77]. Others use a grid-based definition, which first quantizes the space into cells and then does clustering on the cells [45, 46, 81, 93]. In addition, some algorithms define density based on a probabilistic density function [58, 85, 93]. One popular density-based clustering algorithm is DBSCAN [34], which has many derivatives as well [7, 12, 13, 18, 33, 42, 88]. However, the original authors of DBSCAN state that it is difficult to use for high-dimensional data [79].

Graph-based Approximate Nearest Neighbor Search (ANNS). Finally, we give an overview of graph-based approximate nearest neighbor search methods, which have been empirically shown to be effective [26, 92, 95]. There are many graph-based indices, including Hierarchical Navigable Small World Graph (HNSW) [67], DiskANN (also called Vamana) [55], HCNNG [72], PyNNDescent [69], τ -MNG [74], and many others (e.g., [15, 20, 106]). We refer the readers to Dobson et al. [26] and Wang et al. [92] for comprehensive overviews of these methods and their comparisons with non-graph-based methods, such as locality-sensitive hashing, inverted indices, and tree-based indices.

The dependent point search in DPC can also be viewed as a filtered search, where the points’ labels are their density, and we filter for points with densities larger than the query point’s density. Various graph-based similarity search algorithms have been adapted recently to support filtering [40, 44, 91, 105]. Gollapudi et al. [40] propose the Filtered DiskANN algorithm, which supports filtered ANNS queries, where nearest neighbors returned must match the query’s labels. Gupta et al. [44] developed the CAPS index for filtered ANNS via space partitions, which supports conjunctive constraints while DiskANN does not. Both DiskANN [84] and CAPS can be made dynamic. However, these solutions use categorical labels, and a point can have multiple labels. Using this approach for dependent point finding requires quadratic memory just to specify the labels (the i^{th} least dense point would need $i - 1$ labels, which are the $i - 1$ smaller density values than its density), which is prohibitive. Indeed, we tried running the Filtered DiskANN code on our datasets but it ran out of space on our machine.

There are also works that explore the theoretical aspects of graph-based ANNS [50, 59, 73, 75, 82]. It is known that if we want to be able to find the exact nearest neighbor for any possible query via a greedy search, then the graph has to contain the classical Delaunay graph as a subgraph. However, in high dimensions, Delaunay graphs have high degrees and cannot be constructed in a reasonable amount of time [73, 75]. Laarhoven [59] provides bounds for nearest neighbor search on datasets uniformly distributed on a d -dimensional sphere with $d \gg \log n$ and provides time-space trade-offs for the

²Dynamic algorithms support updates to the dataset.

ANNS. Prokhorenkova and Shekhovtsov [75] extend Laarhoven [59]’s work and analyze the performance of graph-based ANNS algorithms in the low-dimensional ($d \ll \log n$) regime. Peng et al. [74] propose a new graph index and prove that if the distance between a query and its nearest neighbor is less than a constant, the search on their graph is guaranteed to find the exact nearest neighbor and the time complexity of the search is small. Indyk and Xu [50] study the worst-case performance of graph-based approximate nearest neighbor search algorithms, including DiskANN, HNSW, and NSG. They show non-trivial bounds on accuracy and query time for a "slow preprocessing" version of DiskANN, and provide examples of poor worst-case behavior for the regular version of DiskANN, HNSW, and NSG.

There has also been work that uses approximate nearest neighbor oracles for clustering problems other than DPC [90].

8 Conclusion

We have presented the PECANN framework for density peaks clustering variants in high dimensions. We adapt graph-based approximate nearest neighbor search techniques to support (filtered) proximity searches in density peaks clustering variants. PECANN is highly parallel and scales to large datasets. We show several example clustering algorithms that can be implemented using PECANN, and evaluate them on large high-dimensional datasets. We show significant improvements in running time and clustering quality over other clustering algorithms.

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