FISHDBC: Flexible, Incremental, Scalable, Hierarchical Density-Based Clustering for Arbitrary Data and Distance

Matteo Dell’Amico
Symantec Research Labs
matteo_dellamico@symantec.com

ABSTRACT
FISHDBC is a flexible, incremental, scalable, and hierarchical density-based clustering algorithm. It is flexible because it empowers users to work on arbitrary data, skipping the feature extraction step that usually transforms raw data into numeric arrays letting users define an arbitrary distance function instead. It is incremental and scalable: it avoids the $O(n^2)$ performance of other approaches in non-metric spaces and requires only lightweight computation to update the clustering when few items are added. It is hierarchical: it produces a "flat" clustering which can be expanded to a tree structure, so that users can group and/or divide clusters in sub- or super-clusters when data exploration requires so. It is density-based and approximates HDBSCAN*, an evolution of DBSCAN.

We evaluate FISHDBC on 8 datasets, confirming its scalability. Our quality metrics show that FISHDBC often performs comparably to HDBSCAN*, and sometimes FISHDBC’s results are even preferable thanks to a regularization effect.

1 INTRODUCTION
In exploratory data analysis (EDA), data are often large, complex, and arrive in a streaming fashion; clustering is an important tool for EDA, because it summarizes datasets—making them more amenable to human analysis—by grouping similar items. Data can be complex because of heterogeneity: consider, e.g., a database of user data as diverse as timestamps, IP addresses, user-generated text, geolocation information, etc. Clustering structure can be complex as well, involving clusters within clusters. Complexity requires clustering algorithms that are flexible, in the sense that they can deal with arbitrarily complex data, and are able to discover hierarchical clusters. Large datasets call for scalable solutions, and streaming data benefits from incremental approaches where the clustering can be updated cheaply as new data items arrive. In addition, it is desirable to distinguish signal from noise with algorithms that do not fit isolated data items into clusters.

As discussed in Section 2, while these problems have been considered previously in the literature, our proposal tackles all of them at once. FISHDBC, which stands for Flexible, Incremental, Scalable, Hierarchical Density-Based Clustering, is flexible because it is applicable to arbitrary data and distance functions; rather than being forced to convert data to numeric values through a feature extraction process that may lose valuable information, domain experts can encode as much domain knowledge as needed by defining any symmetric and possibly non-metric distance function, no matter how complex—our implementation accepts arbitrary Python functions as distance measures. FISHDBC is incremental: it holds a set of data structures to which new data can be added cheaply and from which clustering can be computed quickly; in a streaming context, new data can be added as they arrive, and clustering can be computed inexpensively. FISHDBC is also scalable, in the sense that it avoids in most common cases the $O(n^2)$ complexity that most clustering algorithms have when dealing with non-metric spaces; our experiments show that it can scale to millions of data items. It is hierarchical, recognizing clusters within clusters. FISHDBC belongs to the family of density-based algorithms inspired by DBSCAN [9], inheriting the ability to recognize clusters of arbitrary shapes and filtering noise.

FISHDBC approximates HDBSCAN* [4], an evolution of DBSCAN supporting hierarchical clustering and recognizing clusters with different densities; HDBSCAN*, however, has $O(n^2)$ computational complexity when using distance functions for which no accelerated indexing exists. The key idea that allows FISHDBC to be flexible and incremental while maintaining scalability is maintaining a data structure—a spanning tree connecting data items—which is updated as new items are added to the dataset. The problems of neighbor discovery and incremental model maintenance are separated, making the algorithm simpler to understand, implement and modify. In Section 3 we present the algorithm, together with an analysis of its time and space complexity and its relationship with HDBSCAN*.

We evaluate FISHDBC on 8 datasets varying by size, dimensionality, data type, and distance function used. In Section 4, we validate the scalability and show that clustering quality metrics are often close to the ones of HDBSCAN*, and sometimes they outperform it thanks to a regularization effect. We conclude by discussing when FISHDBC is preferable to existing approaches in Section 5.

2 BACKGROUND AND RELATED WORK
Several algorithms have a subset of the desirable properties discussed in Section 1: for example, spectral clustering [12] is not limited to spherical clusters; agglomerative methods [30] produce hierarchical clusters and can have incremental implementations. To the best of our knowledge, though, no other algorithm embodies at once all the properties that FISHDBC satisfies, being flexible, incremental, scalable, and providing hierarchical density-based clustering. Due to space limitations, we cannot cover all approaches that have some of the above properties. In the following, we focus on density-based clustering and approaches applicable to arbitrary data and (potentially non-metric) dissimilarity/distance functions.

Relational Clustering. These algorithms take as input a distance matrix $D$ containing all $O(n^2)$ pairwise distances. Among them, some are specialized towards arbitrary (non-metric) distances [11, 19]. Unfortunately, these methods are intrinsically not scalable because computing $D$ requires $O(n^2)$ time. FISHDBC scales better because not all pairwise distances are computed: rather than taking a matrix as input, FISHDBC takes a dataset of arbitrary items and a
Distance function to apply to them: the distance function will be called on a small subset of the \( O(n^2) \) item pairs.

Spectral clustering, which is expensive because it involves factorizing an \( O(n^2) \)-sized affinity matrix, can be accelerated via the Nyström method [13]: computing approximate eigenvectors by randomly sampling matrix rows. This sampling approach would be ineffective for density-based clustering as it would not retrieve a good approximation of each node’s local neighborhood, which density-based algorithms need to discover dense areas. FISHDBC is instead guided by an approximate neighbor search converging towards each node’s neighbors, discovering most of them cheaply.

Density-Based Clustering on Arbitrary Data. Density-based clustering was introduced with DBSCAN [9] and generalized to arbitrary data in GDBSCAN [37], in which clusters are connected dense areas: given a definition of an item’s neighborhood (in most cases, given a distance function, the items at distance smaller than a threshold \( \epsilon \)), a node is considered to be in a dense area if its neighborhood contains at least \( \text{MinPts} \) points, and each node in its neighborhood is considered to be in the same cluster. In the general case, GDBSCAN has \( O(n^2) \) complexity, even though indexing structures can lower the computational complexity of the algorithm, depending on the complexity of range queries [38] which are \( O(n) \) in the general case of arbitrary distance functions. Some subsequent pieces of work still require indexing structures to lower computational complexity [23], while others [2] are based on filter functions, i.e., cheap functions that return a superset of an item’s neighborhood: in this latter case, complexity depends on the filter’s function selectivity, i.e., how big their output is. Unlike these approaches, FISHDBC does not require users to provide an indexing structure or a filter function tailored to the distance function used, and it avoids \( O(n^2) \) complexity by introducing approximation.

NG-DBSCAN [22] is a distributed approximate DBSCAN implementation that discovers neighbors in arbitrary spaces with an approach inspired by NN-Descent [6] approximate nearest-neighbor algorithm. Other approaches [17, 21] use a similar strategy. Unlike FISHDBC, these approaches are not incremental: their results must be wholly recomputed as the dataset changes. Moreover, FISHDBC benefits from the better scalability of HNSWs over NN-Descent [1]. Finally, compared to these works, FISHDBC inherits the improvements of HDBSCAN* over DBSCAN: better clustering, one less parameter, and hierarchical output.

Incremental Density-Based Clustering. Unlike our work, existing incremental density-based clustering algorithms [10, 14, 18] have quadratic complexity in non-metric spaces; moreover, they generally report speed-up factors lower than 100 for incremental recomputation after adding a few elements. What we obtain (see Tables 3 and 8, “cluster” columns) is generally similar or better.

HDBSCAN*. Campello et al. [4] improve on DBSCAN while removing the cluster density threshold \( \epsilon \), which is tuned automatically and separately for each cluster. In addition to simplifying tuning, result quality improves because the output can include clusters having different density in the same simplifying.

HDBSCAN* introduces the concepts of core and reachability distance. A node \( a \)’s core distance \( c(a) \) is the distance of its \( \text{MinPts} \)th closest neighbor, while the reachability distance between items \( a \) and \( b \) is \( \max(d(a, b), c(a), c(b)) \) with \( d \) being the distance function. Reachability distance essentially factors in the computation the density of each node’s neighborhood. HDBSCAN* computes the minimum spanning tree (MST) \( T \) of a complete reachability graph \( RG \) having data items as nodes and their reachability distance as weights; the hierarchical clustering is obtained from \( T \) by removing all edges in order of decreasing weight. Because \( T \) is a spanning tree, edge removals split connected components into reciprocally disconnected ones. A \( m_{cs} \) parameter controls the minimum cluster size, and each split is added to the hierarchical clustering if both resulting components have size at least \( m_{cs} \); Campello et al. suggest to set \( m_{cs} = \text{MinPts} \). The non-hierarchical flat output consists of disjoint clusters selected from the hierarchical ones, selecting an \( \epsilon \) threshold for each branch of \( T \) to maximize cluster stability across a wide range of densities. Explicitly computing \( RG \) has \( O(n^2) \) complexity. McInnes and Healy [26] introduced a faster implementation that directly computes \( T \) thanks to accelerated lookup structures if the distance function belongs to a set of supported ones.

3 THE FISHDBC ALGORITHM

HDBSCAN* improves on DBSCAN in terms of result quality and by yielding hierarchical results recognizing clusters within clusters. Unfortunately, though, HDBSCAN* is not incremental—if new data arrives, results have to be recomputed from scratch—and it has \( O(n^2) \) complexity in the generic case of arbitrary distance functions; it also underperforms when lookup structures are ineffective, e.g., when datasets have very high dimensionality. As our analytic (Section 3.2) and empirical (Section 4) results show, FISHDBC instead supports incremental computation, maintains or even improves result quality, is accelerated with arbitrary distance functions in most common cases and has a moderate memory footprint.

The core idea of FISHDBC is maintaining an approximate version of the \( T \) MST described in Section 2 and updating it incrementally, at a low cost, as new data arrive. We discover candidate edges for \( T \) by carefully adapting HNSWs (Hierarchical Navigable Small Worlds [24]). HNSWs are indexes conceived for near-neighbor querying in non-metric spaces; however, rather than first building an HNSW representing our dataset and then querying it to find each node’s neighbors, we piggyback on all calls to the distance function performed by building the index, and generate batches of \( (a, b, d(a, b)) \) triples that we consider for inclusion in \( T \). This strategy allows us to significantly improve FISHDBC’s efficiency because no query is ever performed on the HNSW; moreover, we tune the HNSW for speed: as we will see, settings that speed up index construction but would result in low accuracy for nearest-neighbor querying hit desireable trade-offs for our clustering task.

The crux of FISHDBC’s approximation lies in that not all \( (a, b) \) pairs are computed, and the clustering result only depends on known distances—as proven in Theorem 3.4. FISHDBC’s results are equivalent to assuming \( d(a, b) = \infty \) for non-computed distances. While this may seem to imply a loss in clustering quality, in machine learning [36] and clustering in particular [16] subsampling the distance matrix can improve the results by working as a regularization step that avoids overfitting. As discussed in Section 2, uniformly sampling the distance matrix would not be effective in our case;
Algorithm 1 FISHDBC.

1: procedure setup(d, MinPts, ef)  d is the distance function
2:     self.MinPts ← MinPts
3:     self.mst ← {}  approx. MST
4:     mst is a hashtable mapping (x, y) edges to weights
5:     self.neighbors ← {}  MinPts neighbors per node
6:     maps HNSW to max-heaps of (distance, neighbor) pairs
7:     self.HNSW ← HNSW(d, MinPts, ef)
8:     HNSW’s k parameter (neighbors per node) is MinPts
9:     self.candidates ← {}  Candidate edges
10:    mapping of (x, y) edges to weights
11: procedure add(x)
12:     self.HNSW.add(x)
13:     self.neighbors[x] ← MinPts closest neighbors found
14:     for each time d(x, y) is called by HNSW returning v do
15:         rd ← max(v, core distances of x and y)
16:         self.candidates[x, y] ← rd  Reachability distance
17:         if we found a new top-MinPts neighbor for y then
18:             update self.neighbors[y]
19:         for all neighbor z of y at distance w < v do
20:             if core distance of z is less than v then
21:                 rd ← max(w, core distances of y and z)
22:                 candidates[y, z] ← rd
23:                 reachability distance for (y, z) decreased
24:         if |candidates| > α |neighbors| then call update_MST
25:     We guarantee that candidates has O(n) size
26: procedure update_MST
27:     mst ← Kruskal(mst ∪ candidates)
28:     candidates ← {}  temporary set of candidate edges
29: function cluster(m_t)
30:     if candidates is not empty then call update_MST
31:     compute clustering from MST
32:     using McInnes and Healy [26]’s approach

hence, we resort to HNSWs which provide a good approximation of a node’s neighborhood to estimate local density.

A second regularization effect benefiting FISHDBC is that there are often multiple valid MSTs of a given reachability graph, because several edges connected to a same node can have the same weight (e.g., because they correspond to that node’s reachability distance). FISHDBC tends to privilege edges towards nodes that are higher up in the HNSW hierarchy, leading to MSTs with a lower diameter (because the top of the HNSW hierarchy is reached more quickly), which in turn corresponds to final outputs with smaller and larger clusters, and with shallower hierarchies. As a consequence of these two factors, some results of Section 4 indeed show that FISHDBC outperforms HDBSCAN\(^*\) in terms of quality metrics.

Our implementation is available at https://github.com/matteodellamicco/flexible-clustering.

3.1 The Algorithm in Detail

Algorithm 1 shows FISHDBC in pseudocode. The state consists of four objects: (1) the HNSW; (2) neighbors: each node’s MinPts closest discovered neighbors and their distance; (3) the current approximated MST and, for each edge (a, b) in it, the corresponding value of d(a, b); (4) candidates, a temporary collection of candidate MST edges. Setup initializes the state.

Add is called to incrementally add a new element x to the dataset. It adds x to the HNSW, updates the max-heap of x’s neighbors with those discovered in the HNSW, and then processes all the pairs (x, y) whose distance has been computed while adding x to the HNSW. Each of them is considered as a candidate edge for our MST; in addition, we add to the candidate MST edges candidates all those for which the reachability distance decreased due to the new edge. Since neighbor’s contains max-heaps, each item’s core distance—i.e., the distance of the m\(^{th}\) closest neighbor—is accessible at the top of the heap. If candidates became larger than an, we call update_MST to free memory. α has a moderate impact on runtime, and should be chosen as large as possible while guaranteeing that FISHDBC’s state will fit in memory.

Update_MST processes the temporary set of candidate edges candidates. Any minimum spanning forest algorithm can be called on the union of the current MST and the new candidates; in our implementation, we use Kruskal’s algorithm. Technically, the approximate MST might be a forest—an acyclic graph with multiple connected components—rather than a tree; as shown in Theorem 3.4, this has no effect on final results. In a streaming context when data arrives incrementally, this procedure can be called during idle time.

The output is finally computed using the bottom-up strategy by McInnes and Healy [26] after calling update_MST.

About HNSWs and the FISHDBC Design. HNSWs represent each dataset as a set of layered approximated k-nearest neighbor graphs, where the bottom layer contains the whole dataset, and each other one contains approximately 1/k-th of the elements in the layer below it. Neighbors are found through searching starting at the top layer and continuing in the lower ones when a local minimum is found in the above layer. Since we want to find the MinPts nearest neighbors, we set k = MinPts. The ef parameter controls the effort spent in the search; in Section 4 we show that ef ∈ [20, 50] yields a good trade-off between speed and quality of results.

One may think that FISHDBC could have a simpler design, computing the MST based on the nearest neighbor distances in the bottom graph of the HNSW which represents the whole dataset, similarly to other approaches [17, 21]. This, however, is not optimal as information about farther away items is important to avoid breaking up large clusters: often, small clusters having around close to MinPts nodes are disconnected from other (close) clusters in the nearest neighbor graph. By gradually converging towards closest nodes during neighbor search, we obtain enough information about other nodes to ensure that local clusters remain connected.

3.2 Properties of FISHDBC

We now give proofs relative to FISHDBC’s complexity in terms of space and time, as well as studying its relationship with HDBSCAN\(^*\).

Space Complexity. The asymptotic memory footprint of FISHDBC is rather small: this is confirmed in Section 4, where we show that FISHDBC can handle datasets that are too large for HDBSCAN\(^*\).
**Theorem 3.1. FISHDBC’s state has size \(O(n \log n)\).**

Proof. FISHDBC’s state consists of (1) the HNSW \(O(n \log n)\) size [24]); (2) neighbors: each node’s MinPts closest discovered neighbors and their distance \(O(n)\) size; (3) MST: the current approximated MST stored as a mapping between edges and their weight \((n\) nodes and at most \(n - 1\) edges, hence \(O(n)\) size); (4) the temporary set candidates of candidate edges \(O(n)\) size, because each call to \(\text{ADD}\) will add to \(\text{candidates}\) at most \(n - 1\) elements. The union of these four objects has therefore size \(O(n \log n)\). □

**Time Complexity.** This theorem justifies why computation time grows slowly as dataset size increases (e.g., Fig. 2).

**Theorem 3.2. Adding elements to FISHDBC and recomputing clustering has average time complexity \(O(t + n \log n)\), where \(t\) is the number of calls to \(d(\cdot)\) performed by the HNSW.**

The time complexity of FISHDBC depends on HNSWs: if they require few distance calls, computation cost remains low. We experimentally see that this is true in most real-world cases; moreover, Malkov and Yashunin [24] show that HNSWs have \(t = O(l \log n)\) for adding \(l\) elements under some assumptions. Malkov and Yashunin provide experimental results that support this, similarly to our own results which also show a coherent behavior. When this holds, incrementally processing \(l\) elements has time complexity \(O(l \log^2 n + n \log n)\), and processing a whole dataset has complexity \(O(n \log^2 n)\). Our experiments show that most computation is spent in incrementally building and updating the MST, while computing clustering is orders of magnitude cheaper (e.g., Table 3).

Proof. We will call \(\text{ADD}(x)\) for each new element \(x\) to update the model, and then \(\text{CLUSTER}\) to obtain the clustering.

Core distance lookups have \(O(1)\) cost as they are accessible at the top of each heap in \(\text{neighbors}\). The complexity of adding elements to the HNSW is \(O(t)\) where \(t\) is the number of calls to \(d(\cdot)\). In the rest of the \text{ADD} procedure (see Algorithm 1), the most computationally intensive part is the inner loop of lines 19–23. This loop is executed at most \(O(t \log \text{MinPts})\) times: the \(O(t)\) factor is due to the outer loop (line 14) and \(O(\log \text{MinPts})\) to the inner loop. The hashtable lookup at line 22 has complexity \(O(1)\), for an average complexity of \(O(\log \text{MinPts})\) for the whole time spent in the \text{ADD} procedure, excluding \text{UPDATE_MST} calls.

The cost of \text{UPDATE_MST} is determined by the MSF algorithm. Kruskal’s algorithm, which we use, has time complexity \(O(E \log E)\) where \(E\) is the number of input edges. Since \(E \in O(n)\) here, a call of \text{UPDATE_MST} has cost \(O(n \log n)\). This function will be called \(O(t/n + 1)\) times, resulting in a computational complexity of \(O(t/n + 1)n \log n = O(t(n + 1) \log n)\) for this procedure.

The call to \text{CLUSTER} has complexity \(O(n \log n)\) [26].

The dominant cost is the time spent in \text{UPDATE_MST}, yielding a total complexity of \(O(t(n + 1) \log n)\). □

**Approximation of HDBSCAN*.** We show that the only reason for the approximation is that we do not compute all pairwise distances: FISHDBC computes a valid result of HDBSCAN* when the latter is passed a distance matrix in which all the pairwise distances that are not computed are set to infinity. If \(d(\cdot)\) is called on all the \(O(n^2)\) pairwise distances, we will indeed be proving that FISHDBC is equivalent to HDBSCAN*.

We first prove that, in a reachability graph, edges with weight \(\infty\) can be safely removed without any effect on the resulting clustering.

**Lemma 3.3. Consider two reachability graphs \(RG\) and \(RG'\), where \(RG'\) is obtained by removing all edges weighted \(\infty\) from \(RG\). Clusterings resulting from \(RG\) and \(RG'\) are equivalent.**

Proof. The procedure we use to compute clustering [26] starts by considering each node as a cluster, iterates through MST edges grouped by increasing weight, and joins in the same cluster the nodes connected by those edges. When clusters of size at least \(m_{cs}\) are joined, they are added to the hierarchical clustering—excluding the root cluster which contains all nodes.

Let us consider the minimum spanning forests \(F\) and \(F'\) obtained respectively from \(RG\) and \(RG'\). Because \(RG\) is a full graph, \(F\) is a spanning tree, while \(F'\) may not be. If \(F = F'\), the thesis is proven. If \(F \neq F'\), it must be because all edges of \(F'\) are present in \(F\), and one or more edges having weight \(\infty\) are present in \(F\). Since edges of the MST are processed by increasing weight, these \(\infty\)-weighted edges are processed last, hence the output for \(F\) and \(F'\) will be the same until then; joining edges in this last step will necessarily result in the root cluster containing all nodes which is not returned in the final results. The two outputs will therefore be the same. □

We can now prove our theorem.

**Theorem 3.4. The output of FISHDBC is a valid output of HDBSCAN* run on a distance matrix \(D'\) such that \(D'_{i,j} = d(i,j)\) if \(d(i,j)\) has been called, and \(D'_{i,j} = \infty\) otherwise.**

Proof. HDBSCAN* can have several valid outputs because it is based on computing a spanning tree of the reachability graph, which may not be unique if several edges have the same weight. We prove the equivalence for at least one of the valid spanning trees.

We base ourselves on a result by Eppstein [8, Lemma 1], which proves that minimum spanning forests (MSFs) can be built incrementally: rather than taking as input a whole graph \(G\) at once we can take a subgraph \(G'\), compute its MSF \(F'\) and ignore the rest of \(G'\). We can later add to \(F'\) the parts of \(G\) that were not in \(G'\) and compute an MSF of the resulting graph: it will be a correct MSF \(F\) of \(G\). Hence, we can add edges incrementally in batches and keep memory consumption low (while \(G\) has size \(O(n^2)\), \(F\) has size \(O(n)\)). More formally, given a graph \(G = (V,E)\) and a subgraph of it \(G' = (V' \subseteq V,E' \subseteq E)\), for every MSF \(F'\) of \(G'\), there exists an MSF \(F\) of \(G\) such that \((E' \setminus F') \cap F = \emptyset\).

Given the reachability graph \(RG\) obtained from \(D'\) we consider \(RG'\), which is \(RG\) without all the edges having weight \(\infty\). Due to Lemma 3.3, our goal reduces to showing that FISHDBC will end up having in \(\text{MST}\) a minimum spanning forest of \(RG'\).

Recall the \text{UPDATE_MST} procedure of Algorithm 1: we iteratively add elements from \(\text{candidates}\) to \(\text{MST}\) and discard the edges that are not part of the MSF. Thanks to the aforementioned result by Eppstein, our thesis is proven if all edges of \(RG'\) eventually end up in \(\text{candidates}\): this is actually done in line 16; the reachability distance might not be correct if some neighbors are not yet known, but this will be eventually updated to the correct value (line 26) when neighbors are discovered. We may include a single edge multiple times in \(\text{candidates}\), but the weight always decreases:
since we compute a minimum spanning forest, only the last (and correct) value for the weight will end up in $mst$ at last.

Since all edges of $RG'$ are eventually added to candidates with their correct weights, $mst$ will be a minimum spanning forest of $RG'$, which thanks to Lemma 3.3 proves our thesis.

4 EXPERIMENTAL EVALUATION

The key novelties of FISHDBC with respect to HDBSCAN* are incremental implementation and handling arbitrary data and distance functions while maintaining scalability. HDBSCAN* is regarded as an improvement on DBSCAN and known for the result quality [4, 38], and the accelerated implementation by McInnes et al. [27] is competitive in terms of runtime with many other algorithms [26]. In the following, we therefore use McInnes et al. [27]'s HDBSCAN* implementation as a strong state-of-the-art baseline for both speed and clustering quality which also handles arbitrary data and distance functions and returns hierarchical results, and evaluate where FISHDBC does (and does not) outperform it. We refer to McInnes and Healy [26] for comparisons between our reference HDBSCAN* implementation and other algorithms. We consider comparisons against distributed DBSCAN implementations [22, 39] as out of scope, also because of the difficulties in performing fair comparisons between single-machine and distributed approaches [28].

4.1 Experimental Setup

The goal is to test FISHDBC’s flexibility by evaluating it on several very diverse datasets and distance functions. We evaluate FISHDBC’s quality/runtime tradeoff on a single machine with 128 GB of RAM and different values of the $ef$ HNSW parameter: 20 for faster computation and, in some cases, lower quality, and 50 for slower computation and possibly better results. We performed experiments—reported where space allows—with other values ($ef \in [10, 200]$), which hit less desirable tradeoffs: this is remarkable, because Malkov and Yashunin [24] report a good tradeoff between speed and approximation with a value of $ef = 100$ for their problem of nearest neighbor search; in our clustering use case, we can significantly cut computation without large impacts on result quality by choosing lower values of $ef$. Following the advice of Schubert et al. [38], we use a low value of $MinPts = 10$; in additional experiments—not included due to space limitations—we see that $MinPts$ has only a minor effect on final results. HNSW parameters are set to the defaults of Malkov and Yashunin [24], except for $ef$.

Datasets. We validate FISHDBC on 8 datasets and 8 different distance functions (Table 1). While many related works are evaluated on large datasets with only a handful of dimensions, we are especially interested in high-dimensional cases, where ad-hoc lookup structures (and algorithms based on them) often do not scale well.

Blobs. Synthetic labeled datasets of isotropic Gaussian blobs (10 centers, 10,000 samples) generated with scikit-learn [33]. Results are averaged over generated datasets; the standard deviation is small enough that it would not be discernible in plots.

Docword. The DW-* datasets [7] represent text documents as high-dimensional bags of words; here, we use cosine distance.

Finefoods consists of unlabeled textual food reviews [25], which we cluster with the Jaro-Winkler edit distance [40].

Fuzzy Hashes are digests of binary files from the study of Pagani et al. [32]—digests can be compared to output a similarity score between files. We use three algorithms: lzjd [34], sdhash [3] and tlsh [31]. sdhash and tlsh have been evaluated as sound approaches by Pagani et al., while lzjd is a recent improvement [34]. Files have 5 labels each: program, package, version, compiler used to build it, and options passed to the compiler.

Household is a large unlabeled 7-dimensional dataset of power consumption data [7]. We use Euclidean distance.

Synth datasets are created with Cesario et al. [5]'s generator, simulating transactions as event sets. In each, we generate 5 clusters of transactions with no outliers, no overlapping and dimensionality varying between 640 and 2,048. We use Jaccard distance.

USPS. A set of 16x16-pixel images of handwritten letters [19]. Like other works [11, 19], we consider the 0 and 7 digits and discretize them to a bitmap using a threshold of 0.5, and we consider only those with at least 20 pixels having a value of 1, for a total of 2,196 elements. As in these works, we use the Simpson score as our distance function. Where & is the bitwise-and function and $c()$ is the function that returns the number of ‘1’ bits, the Simpson distance between bitmaps $x$ and $y$ is $1 - (c(x\&y)/\min(c(x),c(y)))$.

Quality metrics. We evaluate clustering on labeled datasets with external metrics: adjusted mutual information (AMI) and adjusted Rand index (ARI). These metrics vary between 0 (random clustering) and 1 (perfect matching). Like most density-based clustering algorithms, FISHDBC does not cluster all the elements, returning instead a set of unclustered “noise” elements: for this reason, we compute AMI and ARI by taking into account only the clustered elements. A metric like this, however, may reward clusterings that only group extremely similar items and mark as noise the rest of the dataset: hence, we use two additional metrics—respectively, AMI* and ARI*—that consider all noise items as a single additional cluster. While AMI/ARI evaluate whether clustered elements are grouped similarly to the reference labeling, AMI*/ARI* penalize outputs that do not cluster many items. Other options can be envisioned, such as treating each noise item as a single cluster, but this could trigger known problems as metrics such as AMI are biased against solutions with many small clusters [15]. Romano et al. [35] advise using AMI rather than ARI for unbalanced datasets; as this can be the case when some clusters are disproportionately recognized as noise, we always use AMI and include ARI when space allows it.

For unlabeled datasets, we resort to internal metrics, such as silhouette, intra- and inter-cluster distance [20]. Silhouette is expensive to compute and generally requires more memory than FISHDBC, hence we obtained out-of-memory errors (OOM) on larger datasets; for intra-cluster (lower is better) and inter-cluster distance (higher is better) we resorted, for the larger clusters, to sampling, choosing two random elements from the same cluster (intra-cluster) or different clusters (inter-cluster), normalizing the probability of choosing each cluster to ensure that each pair has the same probability of being selected. We use a sample size of 10,000.

We do not use the density-based clustering validation metric by Moulavi et al. [29], as besides having $O(n^2)$ complexity—it is designed for low-dimensional datasets: results are unstable and
Table 1: Evaluated datasets.

| Dataset       | Size    | Data type                      | Distance function(s) | Metric | Labeled | Results Quality | Runtime |
|---------------|---------|--------------------------------|----------------------|--------|---------|-----------------|---------|
| Blobs         | 10 000  | 1,000 to 10,000-d vectors      | Euclidean            | yes    | yes     | Table 6         | Fig. 3  |
| DW-Enron      | 39 861  | Sparse 914-d vectors           | cosine               | no     | no      | Table 7         | Table 8 |
| DW-NYTimes    | 300 000 | Sparse 2,120-d vectors         | cosine               | no     | no      | Table 7         | Table 8 |
| Finefoods     | 568 474 | Text (average 430 chars)       | Jaro-Winkler         | no     | no      | Table 7         | Table 8 |
| Fuzzy hashes  | 15 402  | File digests                   | lzjd, tlsh, sdhash   | no     | yes     | Fig. 1          | Table 2 |
| Household     | 2 049 280 | 7-d vectors                | Euclidean            | yes    | no      | Table 7         | Table 8 |
| Synth         | 10 000  | 640–2,048-d sparse bool vectors | Jaccard             | yes    | yes     | Table 4         | Table 3 |
| USPS          | 2 197   | 16x16 bitmaps                  | Simpson score        | no     | yes     | Table 5         | Table 8 |

4.2 Ad-Hoc Distance Measures

We now consider distance measures for which our reference HDBSCAN* implementation [27] does not provide accelerated support; in such cases, it is still possible to run HDBSCAN* by computing a pairwise distances matrix. Here, FISHDBC can scale better than HDBSCAN* because of the lower asymptotical complexity.

Fuzzy Hashes. This dataset has the interesting property of having overlapping class labels. We start by analyzing Fig. 1: here, computational cost is dominated by the calls to the distance function, and we clearly see a quadratic increase in runtime for HDBSCAN*—differences between HDBSCAN* results are essentially due to the differences in cost between the distance functions. FISHDBC consistently scales much better than HDBSCAN*.

The quality metrics of Table 2, where we evaluate AMI and AMI* for each fuzzy hash algorithm/labeling pair, inspire some considerations.
First, HDBSCAN\(^*\) consistently clusters more files than FISHDBC, but the AMI score of FISHDBC is often higher. This means that FISHDBC identifies more elements as noise, while outputting the other elements in more coherent clusters.

Second (with the single exception of sHash applied to the “program” label where FISHDBC’s approximation appears to impact result quality negatively), the AMI\(^*\) scores of HDBSCAN\(^*\) are generally equivalent or worse than those of FISHDBC, suggesting that the additional elements clustered by HDBSCAN\(^*\) are often not well clustered. This can be explained by the argument of Section 3, which suggests that—by working as regularization—FISHDBC’s approximation can improve output quality. By manually examining results, we confirm that the hierarchical clustering of FISHDBC is generally simpler, with fewer larger clusters and a shallower hierarchy.

| dim | FISHDBC (\(ef = 20\)) build | FISHDBC (\(ef = 50\)) build | FISHDBC (\(ef = 20\)) cluster | FISHDBC (\(ef = 50\)) cluster | HDBSCAN\(^*\) | AMI | AMI\(^*\) | ARI | ARI\(^*\) |
|-----|----------------------------|----------------------------|----------------------------|----------------------------|----------------|-----|---------|-----|---------|
| 640 | 67.5                       | 0.21                       | 109                        | 0.24                       | 115            | 1   | 0.38    | 1   | 0.38    |
| 1024| 65.7                       | 0.19                       | 103                        | 0.20                       | 100            | 1   | 0.40    | 1   | 0.40    |
| 2048| 82.2                       | 0.22                       | 126                        | 0.23                       | 155            |     |         |     |         |

Table 3: Synth: runtime (s). “Build” is the time to incrementally build the FISHDBC data structures, “cluster” the time to compute clustering using them as input.

| \(ef\) | dim = 640 | AMI\(^*\) | ARI\(^*\) | dim = 1,024 | AMI\(^*\) | ARI\(^*\) | dim = 2,048 | AMI\(^*\) | ARI\(^*\) |
|-------|-----------|-----------|-----------|-------------|-----------|-----------|-------------|-----------|-----------|
| 20    | 0.89      | 0.94      | 0.96      | 0.99        | 1         | 1         |             |           |           |
| 50    | 0.96      | 0.98      | 0.96      | 0.99        | 1         | 1         |             |           |           |
| HDBSCAN\(^*\) | 0.49  | 0.75      | 0.79      | 0.95        | 1         | 1         |             |           |           |

Table 4: Synth: external quality metrics.

Synth. Table 3 reports on runtime while varying \(ef\). FISHDBC spends most of the time building incrementally its data structures, while the cost of extracting a clustering from them is more than two orders of magnitude cheaper. Therefore clustering can be recomputed, cheaply, as the data structure grows; as shown in Table 8, this is the case in all our datasets. FISHDBC outperforms HDBSCAN\(^*\) here, with a margin growing as the dimensionality (and hence the cost of the distance function) grows. Compared to the Fuzzy Hashes dataset, the smaller difference is largely due to a cheaper distance function. Quality results in Table 4 are perhaps more surprising: for 640 and 1,024 dimensions, FISHDBC substantially outperforms HDBSCAN\(^*\); once again, we attribute this to the regularization effect described in Section 3. As the dimensionality grows, clusters become more separated and quality metrics values grow.

Finefoods. This dataset is rather large, and the Jaro-Winkler distance applied to it is quite expensive. We could not apply HDBSCAN\(^*\) to this dataset, as the full distance matrix would be very expensive to compute and could not fit in memory; this dataset allows us investigate FISHDBC’s scalability. In Fig. 2 we observe the average number of calls to the distance function performed per item as new elements get introduced in the FISHDBC data structure (a clustering is computed every time 2% of the dataset is added). We can see that, in the beginning, the number of comparisons grows as the dataset does, but it tends to plateau afterwards. Results for quality metrics and runtime are available in Tables 7 and 8.

USPS. In this smaller dataset, the runtime results of Table 8—while in any case small—are preferable for HDBSCAN\(^*\), as the advantages brought by asymptotical complexity are irrelevant here. Results in Table 5 are, on the other hand, quite interesting: once again, the regularization effects discussed in Section 3 improve the quality metrics on the results. In particular, AMI and ARI are both equal to 1, showing that FISHDBC always returns two clusters: one for each of the two labels in the original dataset (AMI\(^*\)/ARI\(^*\) values are still lower than 1 because many digits are still considered as noise). On the other hand, HDBSCAN\(^*\) returns a larger number of clusters (11), and some of them contain mixed labels.

Summary. FISHDBC enables performant clustering in cases where computing the full distance matrix falls short. Moreover, FISHDBC rarely fares worse than HDBSCAN\(^*\) in terms of quality metrics—in various cases, indeed, regularization effects improve result quality.

4.3 FISHDBC Versus Accelerated HDBSCAN\(^*\)

We now consider Euclidean and cosine distance, for which HDBSCAN\(^*\) provides a high-performance accelerated implementation.

Blobs. These datasets have between 1,000 and 10,000 dimensions. HDBSCAN\(^*\) uses a KD-tree here, but as the number of dimensions grows the effectiveness of such data structures decreases. In Fig. 3, we see how the computation for HDBSCAN\(^*\) increases quite steeply as dimensionality grows; on the other hand, growth is definitely
larger memory footprint; hence, FISHDBC can compute results in faster execution but the results on runtime in Table 8, however, are quite different: the metrics in Table 7 are again similar between FISHDBC and HDBSCAN*.

Quality metrics in Table 6 show that, here, FISHDBC pays a small price in terms of clustering quality. The experiment was repeated on 30 randomly generated datasets for each number of dimensions, and the standard deviation in AMI* and ARI* is, in all cases, 0.01 for FISHDBC and 0 for HDBSCAN*.

Household. In this 7-dimensional Euclidean dataset, one may speculate that FISHDBC would be largely outperformed by the accelerated ad-hoc HDBSCAN* implementation (it uses an elaborate dual-tree version of Borůvka’s algorithm). Actually, as reported in Table 8, HDBSCAN* is only slightly faster than FISHDBC. It is possible that optimizations on constant factors, e.g., swapping our pure Python HNSW implementation with a faster one, could make FISHDBC faster in this case as well. Intra- and inter-cluster quality metrics (Table 7) are better for HDBSCAN*, but FISHDBC produces a smaller number of clusters, which is arguably more desirable for data exploration because the summarization due to clustering is more succinct. While a considerable number of elements are categorized as noise in the flat clustering, almost all elements end up in a cluster when we consider the hierarchical clustering, which can facilitate data exploration tasks. This benefit is shared by both FISHDBC and HDBSCAN*, for most datasets reported in Table 7.

Docword. We conclude our evaluation by examining sparse vector datasets where we use cosine distance, which has an accelerated ad-hoc implementation in HDBSCAN* [27]. Internal quality metrics in Table 7 are again similar between FISHDBC and HDBSCAN*. Results on runtime in Table 8, however, are quite different: the lookup structures of HDBSCAN* result in faster execution but larger memory footprint; hence, FISHDBC can compute results for DW-NYTimes while HDBSCAN* fails with an out-of-memory error.

Summary. Ad-hoc lookup structures are appealing, but they do not always outperform the generic acceleration of FISHDBC. FISHDBC outperforms HDBSCAN* in very high-dimensional dense datasets like Blobs, and because of its lower memory footprint it can handle dataset that HDBSCAN* cannot like DW-NYTimes.

5 CONCLUSION

FISHDBC can deal with arbitrary distance functions and can handle datasets that are too large for our HDBSCAN* reference. Its core features are providing cheap, incremental computation while supporting arbitrary data and distance functions, avoiding $O(n^2)$ complexity without needing filter functions or lookup indices: domain experts are free to write arbitrarily complex distance functions reflecting the quirks of the data at hand. In addition to being incremental, scalable and flexible, FISHDBC supports hierarchical clustering. It is also an option for very high-dimensional datasets where lookup structures suffer from the curse of dimensionality: our results show that for datasets that have very high dimensionality FISHDBC can outperform ad-hoc accelerated approaches.

We believe that separating neighbor discovery from incremental model maintenance is a powerful approach, which allows for algorithms that are easier to reason about, implement and improve.

REFERENCES

[1] Martin Aumüller, Erik Bernhardsson, and Alexander Faithfull. 2017. ANN-Benchmarks: A Benchmarking Tool for Approximate Nearest Neighbor Algorithms. In Similarity Search and Applications (Lecture Notes in Computer Science), Christian Beecks, Felix Borutta, Peer Krüger, and Thomas Seidl (Eds.). Springer International Publishing, Munich, Germany, 34–49.

[2] Stefan Brecheisen, H-P Kriegel, and Martin Pfeifle. 2004. Efficient density-based clustering of complex objects. In Data Mining, 2004. ICDM’04. Fourth IEEE International Conference on. IEEE, Brighton, UK, 41–50.

[3] Frank Breitinger, Harald Baier, and Jesse Beckhaming. 2012. Security and implementation analysis of the similarity digest sDHash. In First international baltic conference on network security & forensics (NiSFo). Tartu, Estonia, 16.

[4] Ricardo J. G. B. Campello, Davoud Moulavi, and Jorg Sander. 2013. Density-Based Clustering Based on Hierarchical Density Estimates. In Advances in Knowledge Discovery and Data Mining (Lecture Notes in Computer Science), Jian Pei, Vincent S. Tseng, Longhui Cao, Hiroshi Motoda, and Guandong Xu (Eds.). Springer Berlin Heidelberg, Gold Coast, Australia, 168–172.

[5] Eugenio Cesarino, Giuseppe Manco, and Riccardo Ortolani. 2007. Top-down parameter-free clustering of high-dimensional categorical data. IEEE Transactions on Knowledge and Data Engineering 19, 12 (2007), 1607–1624.

[6] Wei Dong, Charikar Moses, and Kai Li. 2011. Efficient k-nearest neighbor graph construction for generic similarity measures. In WWW. ACM, Hyderabad, India, 577–586.

[7] Dhruv Posa and Casey Graff. 2017. UCIMachine Learning Repository. http://archive.ics.uci.edu/ml

[8] D. Eppstein. 1994. Offline Algorithms for Dynamic Minimum Spanning Tree Problems Journal of Algorithms 17, 2 (Sept. 1994), 237–250. https://doi.org/10.1006/jagm.1994.1033

[9] Martin Ester, Hans-Peter Kriegel, Jörg Sander, and Xiaowei Xu. 1996. A density-based algorithm for discovering clusters in large spatial databases with noise. In KDD. ACM, Portland, Oregon, USA, 226–231.

[10] Martin Ester and Rüdiger Württmann. 1998. Incremental generalization for mining in a data warehousing environment. In International Conference on Extending Database Technology. Springer, Valencia, Spain, 135–149.

[11] Maurizio Filippone. 2009. Dealing with non-metric dissimilarities in fuzzy central clustering algorithms. International Journal of Approximate Reasoning 50, 2 (2009), 363–384.

[12] Maurizio Filippone, Francesco Camastra, Francesco Masulli, and Stefano Rovetta. 2008. A survey of kernel and spectral methods for clustering. Pattern Recognition 41, 1 (2008), 176–190.
Table 7: Internal clustering quality metrics. OOM stands for out-of-memory errors when computing the Silhouette metric.

| Dataset     | Algorithm (ef) | Clusters | Silhouette | Average distance |
|-------------|----------------|----------|------------|------------------|
|              |                | flat     | hierarchical | intra-cluster | inter-cluster |
| Finefoods   | FISHDBC (20)   | 77 152   | 566 484    | 2 924          | 6 262         | OOM         | 0.282 | 0.372 |
| Household   | HDBSCAN*       | 1 395 980 | 2 049 273 | 61 902         | 2 4 0.532     | 0.375       | 0.967 |
|              | FISHDBC (50)   | 79 904   | 568 104    | 3 531          | 7 486         | OOM         | 0.226 | 0.363 |
|              |                 |          |            |                 |               |             |       |
| Table 8: Runtime (in seconds). |

| Dataset     | ef = 20 | ef = 50 | HDBSCAN* |
|-------------|---------|---------|----------|
| Blobs       | see Table 3 on page 8 |         |          |
| DW-Kos      | 27.4    | 0.102   | 37.1     | 0.103       | 1.06 (yes)   |          |
| DW-Enron    | 616     | 2.39    | 851      | 2.06        | 112          |          |
| DW-Nytimes  | 8 733   | 41.1    | 12 604   | 36.8        | OOM         | (yes)     |
| Finefoods   | 50 422  | 48.9    | 84 765   | 42.9        | OOM (no)    |          |
| Household   | 27 375  | 123     | 38 759   | 109         | 24 258      | OOM       |          |
| USPS        | 9.1     | 0.0500  | 12.1     | 0.0502      | 1.57 (no)   |          |

[13] C. Fowlkes, S. Belongie, F. Chung, and J. Malik. 2004. Spectral grouping using the Nyström method. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 26, 2 (Feb 2004), 214–225. https://doi.org/10.1109/TPAMI.2004.1262185

[14] Jun-Song Fu, Yun Liu, and Han-Chieh Chao. 2017. The impact of random models on clustering similarity. *The Journal of Machine Learning Research*, 18, 1 (2017), 3049–3076.

[15] Yanchi Liu, Zhongmou Li, Hui Xiong, Xuedong Gao, and Junjie Wu. 2010. Unsupervised k-NN based text clustering. In *Proceedings of the 12th International Conference on Digital Investigation*. IEEE, Sydney, Australia, 3888–3895. https://doi.org/10.1109/ijdig.2010.5697497

[16] Laura Ricci. 2015. Scalable k-NN based text clustering. In *Proceedings of the 13th International Conference on Security and Privacy*. IEEE, Anchorage, Alaska, 911–916. https://doi.org/10.1109/SP.2015.7024037

[17] Alexander J Gates and Yong-Yeol Ahn. 2017. The impact of random models on clustering similarity. *The Journal of Machine Learning Research*, 18, 1 (2017), 3049–3076.

[18] [19] Julian Laub and Klaus-Robert Müller. 2004. Feature discovery in non-metric pairwise data. *Journal of Machine Learning Research*, 5, Jul (2004), 801–818.

[20] [21] Alessandro Lulli, Thibault Debatty, Matteo Dell’Amico, Pietro Michiardi, and Laura Ricci. 2015. Scalable k-NN based text clustering. In *Proceedings of the 18th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*. ACM, Sydney, Australia, 911–916.

[22] [23] Alessandro Lulli, Matteo Dell’Amico, Pietro Michiardi, and Laura Ricci. 2016. NG-DISSCAN: scalable density-based clustering for arbitrary data. *Proceedings of the VLDB Endowment*, 9, 10 (2016), 157–168.

[24] [25] Son T. Mai, Ira Assent, Jon Jacobsen, and Martin Storgaard Dieu. 2018. Anytime parallel density-based clustering. *Data Mining and Knowledge Discovery*, 32, 4 (July 2018), 1121–1176. https://doi.org/10.1007/s10618-018-0562-1

[26] Y. A. Malkov and D. A. Yashunin. 2018. Efficient and robust approximate nearest neighbor search using Hierarchical Navigable Small World graphs. *IEEE Transactions on Pattern Analysis and Machine Intelligence* (2018), 1–1. https://doi.org/10.1109/TPAMI.2018.2899475

[27] [28] Julian John McAuley and Jure Leskovec. 2013. From amateurs to connoisseurs: modeling the evolution of user expertise through online reviews. In *Proceedings of the 22nd international conference on World Wide Web*. ACM, Rio de Janeiro, Brazil, 897–908.

[29] Leland McInnes and John Healy. 2017. Accelerated Hierarchical Density Based Clustering. In *Data Mining Workshops (ICDMW), 2017 IEEE International Conference on*. IEEE, New Orleans, LA, USA, 33–42.

[30] Leland McInnes, John Healy, and Steve Astels. 2017. hdbSCAN: Hierarchical density based clustering. The *Journal of Open Source Software*, 2, 11 (23 3 2017), 265. https://doi.org/10.21105/joss.00205

[31] Frank McSherry, Michael Ianderson, and Derek G. Murray. 2015. Scalability! But at what COST?. In *15th Workshop on Hot Topics in Operating Systems (HotOS XV)*. USENIX Association, Karlsruhe, Germany, Article 14, 6 pages. https://www.usenix.org/conference/hotos15/workshop-program/presentation/mcsherry

[32] Davoud Moulavi, Pablo A Jaskowiak, Ricardo J Campello, Arthur Zimek, and Jörg Sander. 2014. Density-based clustering validation. In *Proceedings of the 24th ACM International Conference on Information and Knowledge Management*. ACM, Pisa, Italy, 735–744.

[33] Fionn Murtagh and Pedro Contreras. 2012. Algorithms for hierarchical clustering: an overview. *Wiley Interdisciplinary Reviews: Data Mining and Knowledge Discovery*, 2, 1 (2012), 86–97.

[34] J. Oliver, C. Cheng, and Y. Chen. 2013. TLSH – A Locality Sensitive Hash. In *2013 Fourth Cybercrime and Trustworthy Computing Workshop*. IEEE, Sydney, Australia, 7–13. https://doi.org/10.1109/CTC.2013.9

[35] Fabio Pagani, Matteo D’Amico, and Davide Balzarotti. 2018. Beyond Precision and Recall: Understanding Uses (and Misuses) of Similarity Hashes in Binary Analysis. In *Proceedings of the Eighth ACM Conference on Data and Application Security and Privacy*. ACM, Tempe, AZ, USA, 354–365.

[36] P. F. Pedregosa, G. Varoquaux, A. Gramfort, V. Michel, B. Thirion, O. Grisel, M. Blondel, P. Prettenhofer, R. Weiss, V. Dubourg, J. Vanderplas, A. Passos, D. Cournapeau, M. Brucher, M. Perrot, and E. Duchesnay. 2011. Scikit-learn: Machine Learning in Python. *Journal of Machine Learning Research*, 12 (2011), 2825–2830.

[37] Edward Raff and Charles Nicholas. 2018. Lempel-Ziv Jaccard Distance, an effective alternative to Levenshtein distance. *Digital Investigation*, 15, 202 (2018), 34–49.
[35] Simone Romano, Nguyen Xuan Vinh, James Bailey, and Karin Verspoor. 2016. Adjusting for chance clustering comparison measures. The Journal of Machine Learning Research 17, 1 (2016), 4635–4666.

[36] Alessandro Rudi, Raffaello Camoriano, and Lorenzo Rosasco. 2015. Less is More: Nyström Computational Regularization. In Advances in Neural Information Processing Systems 28, C. Cortes, N. D. Lawrence, D. D. Lee, M. Sugiyama, and R. Garnett (Eds.). Curran Associates, Inc., Montréal, Canada, 1657–1665. http://papers.nips.cc/paper/5936-less-is-more-nystrom-computational-regularization.pdf

[37] Jörg Sander, Martin Ester, Hans-Peter Kriegel, and Xiaowei Xu. 1998. Density-based clustering in spatial databases: The algorithm GDBSCAN and its applications. Data mining and knowledge discovery 2, 2 (1998), 169–194.

[38] Erich Schubert, Jörg Sander, Martin Ester, Hans Peter Kriegel, and Xiaowei Xu. 2017. DBSCAN Revisited, Revisited: Why and How You Should (Still) Use DBSCAN. ACM Trans. Database Syst. 42, 3, Article 19 (July 2017), 21 pages. https://doi.org/10.1145/3068335

[39] Hwanjun Song and Jae-Gil Lee. 2018. RP-DBSCAN: A Superfast Parallel DBSCAN Algorithm Based on Random Partitioning. In Proceedings of the 2018 International Conference on Management of Data (SIGMOD ’18). ACM, New York, NY, USA, 1173–1187. https://doi.org/10.1145/3183713.3196887

[40] William E Winkler. 1999. The state of record linkage and current research problems. Technical Report. Statistical Research Division, US Census Bureau.