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dbscan: Fast Density-Based Clustering with R

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Abstract

This article describes the implementation and use of the R package **dbscan**, which provides complete and fast implementations of the popular density-based clustering algorithm DBSCAN and the augmented ordering algorithm OPTICS. Package **dbscan** uses advanced open-source spatial indexing data structures implemented in C++ to speed up computation. An important advantage of this implementation is that it is up-to-date with several improvements that have been added since the original algorithms were publications (e.g., artifact corrections and dendrogram extraction methods for OPTICS). We provide a consistent presentation of the DBSCAN and OPTICS algorithms, and compare **dbscan**'s implementation with other popular libraries such as the R package **fpc**, **ELKI**, **WEKA**, **PyClustering**, **SciKit-Learn**, and **SPMF** in terms of available features and using an experimental comparison.

Keywords: DBSCAN, OPTICS, density-based clustering, hierarchical clustering.

1. Introduction

Clustering is typically described as the process of finding structure in data by grouping similar objects together, where the resulting groups are called clusters. The premise of many clustering algorithms is that objects assigned to the same cluster should be more similar to each other than to objects in other clusters. Similarity is often captured through some notion of distance, stemming from the fact that objects are assumed to be data points embedded in a data space in which a distance measure can be defined. Typical clustering methods either focus on solving the k-means problem (MacQueen *et al.* 1967) or rely on parametric mixture models, each of which cluster by finding the parameters of a probabilistic model from which the observed data were most likely to have arisen. For these methods well-established software packages are available (e.g., **mclust**, Scrucca, Fop, Murphy, and Raftery 2016; **mixtools**, Benaglia, Chauveau, Hunter, and Young 2009). Another approach is hierarchical clustering, which uses a similarity measure and a linkage criterion nested groupings of objects, often represented as a tree structure. Detailed reviews of popular clustering algorithms are provided by Kaufman and Rousseeuw (1990), Jain, Murty, and Flynn (1999), and more recently in Aggarwal and Reddy (2013).

Many of these approaches assume clusters with convex, hyper-spherical shapes (Jain *et al.* 1999). In contrast, density-based clustering approaches have become increasingly popular due to their ability to capture clusters of arbitrary shapes, including non-convex shapes. Density-based approaches posit merely that clusters are contiguous dense regions in the data space (i.e., regions of high point density), separated by areas of low density (Sander 2011). Density-based clustering also can handle noise, where points that reside in areas of very low density are not assigned a cluster label, but instead, are treated as outliers or noisy observations. These properties provide advantages for many applications. For example, geospatial data may be fraught with noisy data points due to estimation errors in GPS-enabled sensors (Chen, Ji, and Wang 2014) and may have non-convex cluster shapes caused by the topology of the physical space in which the data was captured. Density-based clustering has also shown advantages for characterizing high-dimensional data (Kailing, Kriegel, and Kröger 2004), where partitions are challenging to discover, and where the physical shape constraints assumed by model-based methods are more likely to be violated.

This paper focuses on an efficient implementation of the DBSCAN algorithm (Ester, Kriegel, Sander, Xu *et al.* 1996), one of the most popular density-based clustering algorithms, whose impact earned it the SIGKDD 2014's Test of Time Award (SIGKDD 2014), and OPTICS (Ankerst, Breunig, Kriegel, and Sander 1999), often thought of as an extension of DBSCAN. While surveying software tools that implemented various density-based clustering algorithms, it was discovered that existing implementations vary significantly in performance (Kriegel, Schubert, and Zimek 2016) and may also lack important components and corrections. Specifically, for the statistical computing environment R (R Core Team 2019), only naive DBSCAN implementations without the use of fast spatial data structures are available. An example is the implementation in the well-known Flexible Procedures for Clustering package **fpc** (Hennig 2019). OPTICS was not available for R before the introduction of **dbscan**. This motivated the development of a R package for density-based clustering with DBSCAN and related algorithms called **dbscan**.

This article presents an overview of the R package **dbscan**, focusing on the operation of DBSCAN and OPTICS. It also provides a comparison of **dbscan** with a number of other open-source implementations on various benchmark datasets. We start with a brief introduction of the concepts of density-based clustering and the DBSCAN and OPTICS algorithms in Section 2. The section also gives a short review of existing software packages implementing these algorithms. Section 3 contains detailed examples that show how to use DBSCAN and OPTICS in **dbscan**. A performance evaluation is presented in Section 4. Concluding remarks are offered in Section 5.

2. Density-based clustering

Density-based clustering is now well-studied. Conceptually, the idea behind density-based clustering is simple: given a set of data points, define a structure that accurately reflects the underlying density (Sander 2011). An important distinction between density-based clustering and alternative approaches to cluster analysis, such as (Gaussian) mixture models (see, e.g., Jain *et al.* 1999), is that the latter represents a parametric approach in which the observed data are assumed to have been produced by a mixture of parametric distributions (often assumed to be Gaussian). While useful in many applications, parametric approaches naturally assume clusters will exhibit some convex (hyper-spherical or hyper-elliptical) shape. Other approaches, such as k-means clustering (where the k parameter signifies the user-specified number of clusters to find), share this common theme by assuming that good clusters can be found by minimizing some measure of intra-cluster variance (often referred to as cluster cohesion) and maximizing the inter-cluster variance (cluster separation, Arbelaitz, Gurrutxaaga, Muguerza, Pérez, and Perona 2013) leading also to convex cluster shapes. Conversely, density-based clustering methods do not assume parametric distributions or use variance, and thus are capable of finding arbitrarily-shaped clusters, handle varying amounts of noise, and require no prior knowledge regarding how to set the number of clusters. Next, we discuss the most popular density-based clustering algorithm, called DBSCAN.

2.1. DBSCAN: Density-based spatial clustering of applications with noise

As one of the most cited density-based clustering algorithms (Microsoft Academic Search 2017), DBSCAN (Ester *et al.* 1996) is likely the most used density-based clustering algorithm in the scientific community today. The central idea behind DBSCAN and its extensions and revisions is the notion that points are assigned to the same cluster if they are *density-reachable* from each other. To understand this concept, we have to go through the most important definitions used in DBSCAN and related algorithms first. The definitions and the presented pseudo code follows the original by Ester *et al.* (1996), but are adapted to provide a more consistent presentation with the other algorithms discussed in this paper.

Clustering starts with a dataset D containing a set of points $p \in D$. Density-based algorithms need to obtain a density estimate over the data space. DBSCAN estimates the density around each point using the concept of ϵ-neighborhood.

Definition 1 ϵ-neighborhood. *The ϵ-neighborhood, $N_\epsilon(p)$, of a data point p is the set of points within a specified radius ϵ around p.*

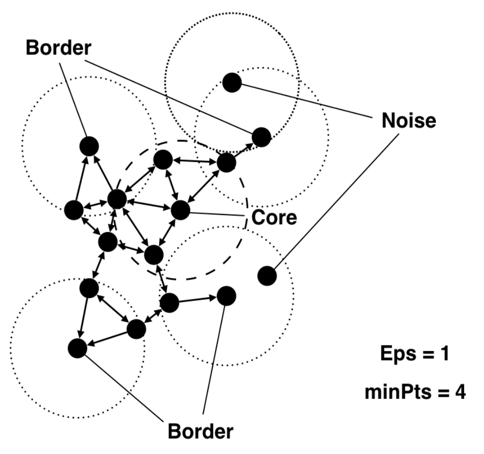
$$N_\epsilon(p) = \{q \in D \mid d(p, q) < \epsilon\}$$

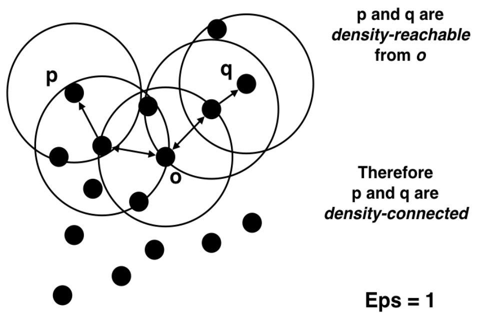
where d is some distance measure and $\epsilon \in \mathbb{R}^+$. Note that together with $p \in D$ this definition implies that point p is always part of its own ϵ-neighborhood, i.e., $p \in N_\epsilon(p)$ always holds.

Following this definition, the size of the neighborhood $|N_\epsilon(p)|$ can be seen as a simple unnormalized kernel density estimate around p using a uniform kernel with a bandwidth of ϵ. DBSCAN uses $N_\epsilon(p)$ and a threshold called *minPts* to detect dense regions and to classify the points in a dataset into *core*, *border*, or *noise* points.

Definition 2 Point classes. *A point $p \in D$ is classified as*

- *a* core point *if $N_\epsilon(p)$ has high density, i.e., $|N_\epsilon(p)| \geq minPts$ where $minPts \in \mathbb{Z}^+$ is a user-specified density threshold,*
- *a* border point *if p is not a core point, but it is in the neighborhood of a core point $q \in D$, i.e., $p \in N_\epsilon(q)$, or*
- *a* noise point*, otherwise.*





(a) (b)

Figure 1: Concepts used in the DBSCAN family of algorithms. (a) shows examples for the three point classes, core, border, and noise points, (b) illustrates the concept of density-reachability and density-connectivity.

An example of different point classes is shown in Figure 1(a). The size of the neighborhood for some points is shown as a circle, and their class is shown as an annotation.

To form contiguous dense regions from individual points, DBSCAN defines the notions of reachability and connectedness.

Definition 3 Directly density-reachable. *A point $q \in D$ is directly density-reachable from a point $p \in D$ with respect to ϵ and minPts if, and only if,*

1. $|N_\epsilon(p)| \geq minPts$, and

2. $q \in N_\epsilon(p)$.

That is, p is a core point and q is in its ϵ-neighborhood.

Definition 4 Density-reachable. *A point p is density-reachable from q if there exists in D an ordered sequence of points $(p_1, p_2, \ldots, p_n)$ with $q = p_1$ and $p = p_n$ such that p_{i+1} directly density-reachable from p_i $\forall$ $i \in \{1, 2, \ldots, n-1\}$.*

Definition 5 Density-connected. *A point $p \in D$ is density-connected to a point $q \in D$ if there is a point $o \in D$ such that both p and q are density-reachable from o.*

Figure 1(b) gives examples of density-reachable and density connected points.

The notion of density-connection can be used to form clusters as contiguous dense regions.

Definition 6 Density-based cluster. *A density-based cluster C is a non-empty subset of D satisfying the following conditions:*

1. Maximality*: If $p \in C$ and q is density-reachable from p, then $q \in C$.*

2. Connectivity*: $\forall$ $p, q \in C$, p is density-connected to q.*

The DBSCAN algorithm identifies all such clusters by systematically finding all core points and expanding each to all density-reachable points. The algorithm begin with an arbitrary point p and retrieves its ϵ-neighborhood. If it is a core point, then it will start a new cluster that is expanded by assigning all points in its neighborhood to the cluster. If an additional core point is found in the neighborhood, then the search is expanded to include also all points in its neighborhood. If no more core points are found in the expanded neighborhood, then the cluster is complete, and the remaining points are searched to see if another core point can be found to start a new cluster. After processing all points, points which were not assigned to a cluster have to be noise points.

Determining the appropriate values for the two parameters, ϵ and *minPts*, is not always easy. The parameters depend on the dataset and influence each other. For example, increasing *minPts* typically also requires increasing ϵ and vice versa. The clustering result is often also quite sensitive to small parameters changes. We present examples of how this issue can be addressed in Section 3.2.

In the DBSCAN algorithm, core points are always part of the same cluster, independent of the order in which the points in the dataset are processed. This is different for border points. Border points might be density-reachable from core points in several clusters and the original DBSCAN algorithm assigns them to the first of these clusters processed which depends on the order of the data points and the particular implementation of the algorithm. To alleviate this behavior, Campello, Moulavi, Zimek, and Sander (2015) suggest a modification called DBSCAN* which considers all border points as noise instead and leaves them unassigned.

2.2. OPTICS: Ordering points to identify clustering structure

The inability to find clusters of varying density is a notable drawback of DBSCAN resulting from the fact that a combination of a specific neighborhood size with a single density threshold *minPts* is used to determine if a point resides in a dense neighborhood. There are many instances where it would be useful to detect clusters of varying density. From identifying regions of similar seawater characteristics (Birant and Kut 2007), to network intrusion detection systems (Ertöz, Steinbach, and Kumar 2003), point of interest detection using geo-tagged photos (Kisilevich, Mansmann, and Keim 2010), classifying cancerous skin lesions (Celebi, Aslandogan, and Bergstresser 2005), the motivations for detecting clusters of varying densities are numerous.

In 1999, some of the authors of DBSCAN developed OPTICS (Ankerst *et al.* 1999) to address this concern. OPTICS borrows the core density-reachable concept from DBSCAN. But while DBSCAN may be thought of as a clustering algorithm, searching for natural groups in data, OPTICS is an *augmented ordering algorithm* from which either flat or hierarchical clustering results can be derived. OPTICS requires the same ϵ and *minPts* parameters as DBSCAN. However, the ϵ parameter is theoretically unnecessary and is only used for the practical purpose of reducing the runtime complexity of the algorithm. To describe OPTICS, we introduce two additional concepts called *core-distance* and *reachability-distance.*

Definition 7 Core-distance. *The core-distance of a point $p \in D$ with respect to minPts and ϵ is defined as*

$$\text{core-dist}(p; \epsilon, \mathit{minPts}) = \begin{cases} \mathit{UNDEFINED} & \mathit{if}\ |N_\epsilon(p)| < \mathit{minPts}, \mathit{and} \\ \mathit{minPts}\text{-}\mathit{dist}(p) & \mathit{otherwise.} \end{cases}$$

where $minPts$-$dist(p)$ is the distance from p to its $minPts - 1$ nearest neighbor, i.e., the minimal radius a neighborhood of size minPts centered at and including p would have.

Definition 8 Reachability-distance. *The reachability-distance of a point $p \in D$ to a point $q \in D$ parameterized by ϵ and minPts is defined as*

$$\text{reachability-dist}(p, q; \epsilon, \mathit{minPts}) = \begin{cases} \mathit{UNDEFINED} & \mathit{if}\ |N_\epsilon(p)| < \mathit{minPts}, \mathit{and} \\ \max(\text{core-dist}(p), d(p, q)) & \mathit{otherwise.} \end{cases}$$

The reachability-distance of a core point p with respect to object q is the smallest neighborhood radius such that p would be directly density-reachable from q. Note that the parameters, although they have the same name, work differently than in DBSCAN. In OPTICS, ϵ is typically set to a very large value compared to DBSCAN. Therefore, OPTICS will considered more nearest neighbors in the core-distance calculation and *minPts* affects the smoothness of the reachability distribution, where larger values will lead to a smoother reachability distribution. This needs to be kept in mind when choosing appropriate parameters. It is worth noting that the ϵ parameter is strictly there for computational reasons—it is used to restrict the number of points considered in the neighborhood search. It can safely be set to the maximum k-nearest neighbor distance, where $k = minPts$, and achieve the same result as if ϵ were set to ∞.

OPTICS provides an augmented ordering. The algorithm starts with a point and expands its neighborhood like DBSCAN, but it explores new points in the order of lowest to highest core-distance. The order in which the points are explored along with each point's core- and reachability-distance is the final result of the algorithm. An example result of OPTICS is shown in the form of a reachability plot in Figure 2. The data points are shown in the resulting order on the x-axis, while the reachability-distance of each point is shown on the y-axis. Low reachability-distances are shown as valleys represent clusters separated by peaks representing points with larger distances. This density representation essentially conveys similar information as a dendrogram, a tree structure often used to represent the result of hierarchical clustering. This is why OPTICS is often also presented as a visualization tool. Sander, Qin, Lu, Niu, and Kovarsky (2003) showed how the output of OPTICS could be converted into an equivalent dendrogram, and that under certain conditions, the dendrogram produced by hierarchical clustering with single linkage is equivalent to running OPTICS with $minPts = 2$. Ankerst *et al.* (1999) discuss two ways to group points into clusters based on the order discovered by OPTICS. We will refer to these as the ExtractDBSCAN method and the Extract-ξ method summarized below:

1. *ExtractDBSCAN* uses a single global reachability-distance threshold ϵ' to extract a clustering. This can be seen as a horizontal line in the reachability plot in Figure 2. Peaks above the cut-off represent noise points and separate the clusters.

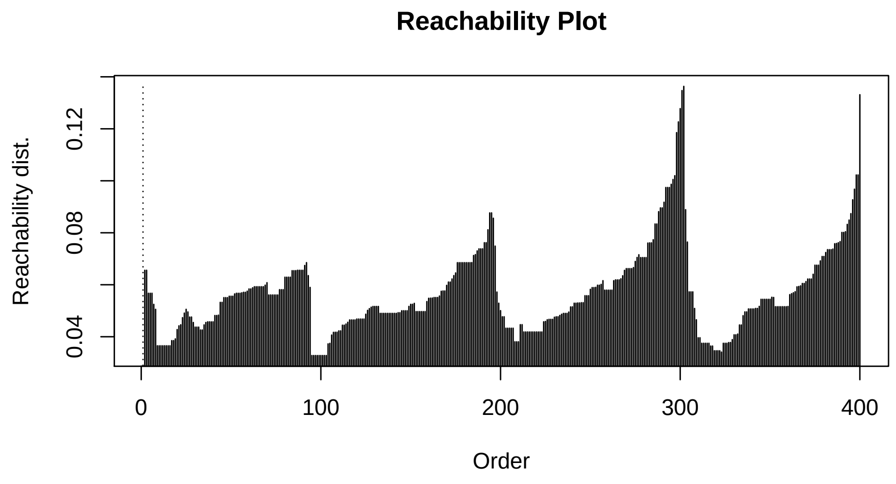


Figure 2: OPTICS reachability plot example for a dataset with four clusters of 100 data points each.

2. *Extract-ξ* identifies clusters *hierarchically* by scanning through the ordering that OPTICS produces to identify significant, relative changes in reachability-distance. The authors of OPTICS noted that clusters could be thought of as identifying 'dents' in the reachability plot.

The ExtractDBSCAN method extracts a clustering similar to DBSCAN* (i.e., DBSCAN where border points stay unassigned). Because this method extracts clusters like DBSCAN, it is hard to identify partitions that exhibit very significant differences in density. Clusters of significantly different density can only be identified if the data is well separated and very little noise is present. The second method, Extract-ξ[1], identifies a cluster hierarchy and replaces the data dependent global ϵ' used in ExtractDBSCAN parameter with ξ, a data-independent density-threshold parameter ranging between 0 and 1. One interpretation of ξ is that it describes the relative magnitude of the change of cluster density (i.e., reachability). Significant changes in relative reachability allow for clusters to manifest themselves hierarchically as dents in the ordering structure. Extract-ξ finds a hierarchical clustering which allows us to find clusters of varying densities.

With its two ways of extracting clusters from the ordering, whether through either the global ϵ' or relative ξ threshold, OPTICS can be seen as a generalization of DBSCAN. For applications where one needs to find clusters of similar density, OPTICS's ExtractDBSCAN yields a DBSCAN-like solution, while for other applications, Extract-ξ can generate a hierarchy representing clusters of varying density. It is thus interesting to note that while DBSCAN has reached critical acclaim, even motivating numerous extensions (Rehman, Asghar, Fong, and Sarasvady 2014), OPTICS has received decidedly less attention. Perhaps one of the reasons for this is because the powerful Extract-ξ method for grouping points into clusters has gone largely unnoticed, as it is not implemented in most open-source software packages that advertise an implementation of OPTICS. This includes implementations in **WEKA** (Hall, Frank, Holmes, Pfahringer, Reutemann, and Witten 2009), **SPMF** (Fournier-Viger *et al.* 2014), and

[1]In the original OPTICS publication (Ankerst *et al.* 1999), the algorithm was outlined in Figure 19 and called the *ExtractClusters* algorithm, where the clusters extracted were referred to as ξ-clusters. To distinguish the method uniquely, we refer to it in **dbscan** as the Extract-ξ method.

Library/Package	*DBSCAN*	*OPTICS*	*ExtractDBSCAN*	*Extract-ξ*
dbscan	✓	✓	✓	✓
ELKI	✓	✓	✓	✓
SPMF	✓	✓	✓	
PyClustering	✓	✓	✓	
WEKA	✓	✓	✓	
SciKit-Learn	✓			
fpc	✓			

Library/Package	*Index Acceleration*	*Dendrogram for OPTICS*	*Language*
dbscan	✓	✓	R
ELKI	✓	✓	Java
SPMF	✓		Java
PyClustering	✓		Python
WEKA			Java
SciKit-Learn	✓		Python
fpc			R

Table 1: A comparison of DBSCAN and OPTICS implementations in various open-source statistical software libraries and packages. A ✓ symbol denotes availability.

the **PyClustering** (Novikov 2019) and **SciKit-Learn** (Pedregosa *et al.* 2011) libraries for Python (Van Rossum *et al.* 2011). To the best of our knowledge, the only other open-source library currently providing a complete implementation of OPTICS is **ELKI** (Schubert, Koos, Emrich, Züfle, Schmid, and Zimek 2015), written in Java (Gosling, Joy, Steele, and Bracha 2000).

In fact, perhaps due to the (incomplete) implementations of OPTICS cluster extraction across various software libraries, there has been some confusion regarding the usage of OPTICS, and the benefits it offers compared to DBSCAN. Several papers motivate DBSCAN extensions or devise new algorithms by citing OPTICS as incapable of finding density-heterogeneous clusters (Ghanbarpour and Minaei 2014; Chowdhury, Mollah, and Rahman 2010; Gupta, Liu, and Ghosh 2010; Duan, Xu, Guo, Lee, and Yan 2007). Along the same line of thought, others cite OPTICS as capable of finding clusters of varying density, but either use the DBSCAN-like global density threshold extraction method or refer to OPTICS as a clustering algorithm, without mention of which cluster extraction method was used in their experimentation (Verma, Srivastava, Chack, Diswar, and Gupta 2012; Roy and Bhattacharyya 2005; Liu, Zhou, and Wu 2007; Pei, Jasra, Hand, Zhu, and Zhou 2009). However, OPTICS returns an ordering of the data points which can be post-processed to extract either (1) a flat clustering with clusters of relatively similar density or (2) a cluster hierarchy, which is adaptive to representing local densities within the data. To clear up this confusion, it seems to be important to add complete implementations to existing software packages and introduce new complete implementations of OPTICS like the R package **dbscan** described in this paper.

2.3. Current implementations of DBSCAN and OPTICS

Implementations of DBSCAN and OPTICS are available in many statistical software packages. We focus here on open-source solutions. These include the Waikato Environment for Knowledge Analysis (**WEKA**, Hall *et al.* 2009), the Sequential Pattern Mining Framework

(**SPMF**, Fournier-Viger *et al.* 2014), the Environment for Developing KDD-Application supported by Index Structures (**ELKI**, Schubert *et al.* 2015), the Python library **SciKit-Learn** (Pedregosa *et al.* 2011), the **PyClustering** Data Mining library (Novikov 2019), the Flexible Procedures for Clustering R package (Hennig 2019), and the **dbscan** package (Hahsler and Piekenbrock 2019) introduced in this paper. Table 1 presents a comparison of the features offered by these packages. All packages support DBSCAN and most use some form of index acceleration to speed up the ϵ-neighborhood queries involved in both DBSCAN and OPTICS algorithms, the known bottleneck that typically dominates the runtime and is essential for processing larger datasets. **dbscan** supports index acceleration for Euclidean distance using k-d trees with 5 different splitting methods (see Mount and Arya 2010 for more details). Other software libraries mentioned also may support a variety of other distance measures and other methods of index acceleration. OPTICS with ExtractDBSCAN is also widely implemented, but the Extract-ξ method, as well as the use of dendrograms with OPTICS, are features currently only available in **dbscan** and **ELKI**.

3. The dbscan package

The package **dbscan** provides high performance code for DBSCAN and OPTICS through a C++ implementation (interfaced via the **Rcpp** package by Eddelbuettel and François 2011) using the k-d tree data structure implemented in the C++ library **ANN** (Mount and Arya 2010) to improve k nearest neighbor (kNN) and fixed-radius nearest neighbor search speed. DBSCAN and OPTICS share a similar interface.

```
dbscan(x, eps, minPts = 5, weights = NULL, borderPoints = TRUE, ...)
optics(x, eps, minPts = 5, ...)
```

The first argument `x` is the dataset in form of a `data.frame` or a `matrix`. The implementations use by default Euclidean distance for neighborhood computation. Alternatively, a precomputed set of pair-wise distances between data points stored in a `dist` object can be supplied. Using precomputed distances, arbitrary distance metrics can be used, however, note that k-d trees are not used for distance data, but lists of nearest neighbors are precomputed. For `dbscan()` and `optics()`, the parameter `eps` represents the radius of the ϵ-neighborhood considered for density estimation and `minPts` represents the density threshold to identify core points. Note that `eps` is not strictly necessary for OPTICS but is only used as an upper limit for the considered neighborhood size used to reduce computational complexity. `dbscan()` also can use weights for the data points in `x`. The density in a neighborhood is calculated as the sum of the weights of the points inside the neighborhood. By default, each data point has a weight of one, so the density estimate for the neighborhood is the number of data points inside the neighborhood. Using weights, the importance of points can be changed.

The original DBSCAN implementation assigns border points to the first cluster it is density-reachable from. Since this may result in different clustering results if the data points are processed in a different order, Campello *et al.* (2015) suggest for DBSCAN* to consider all border points as noise. This can be achieved by using `borderPoints = FALSE`. All functions accept additional arguments. These arguments are passed on to the fixed-radius nearest neighbor search. More details about the implementation of the nearest neighbor search will be presented in Section 3.1 below.

To extract clusters from the linear order produced by OPTICS, **dbscan** implements the cluster extraction methods for ExtractDBSCAN and Extract-ξ:

```
extractDBSCAN(object, eps_cl)
extractXi(object, xi, minimum = FALSE, correctPredecessor = TRUE)
```

`extractDBSCAN()` extracts a clustering from an OPTICS ordering that is similar to what DBSCAN would produce with a single global ϵ' set to `eps_cl`. `extractXi()` extracts clusters hierarchically based on the steepness of the reachability plot. `minimum` controls whether only the minimal (non-overlapping) cluster are extracted. `correctPredecessor` corrects a common artifact known of the original ξ method presented in Ankerst *et al.* (1999) by pruning the steep up area for points that have predecessors not in the cluster (see technical note in Appendix A for details).

3.1. Nearest neighbor search

The density-based algorithms in **dbscan** rely heavily on forming neighborhoods, i.e., finding all points belonging to an ϵ-neighborhood. A simple approach is to perform a linear search, i.e., always calculating the distances to all other points to find the closest points. This requires $O(n)$ operations, with n being the number of data points, for each time a neighborhood is needed. Since DBSCAN and OPTICS process each data point once, this results in a runtime complexity of $O(n^2)$. A naive solution is to compute a distance matrix with all pairwise distances between points and sort the distances for each point (row in the distance matrix) to precompute the nearest neighbors for each point. However, this method has the drawback that the size of the full distance matrix is on the order of $O(n^2)$, and becomes very large for medium to large datasets.

To avoid computing the complete distance matrix, **dbscan** relies on a space-partitioning data structure called a k-d tree (Bentley 1975). This data structure allows **dbscan** to identify the kNN or all neighbors within a fixed radius *eps* more efficiently in sub-linear time using on average only $O(log(n))$ operations per query. This results in a reduced runtime complexity of $O(n\, log(n))$ for DBSCAN and OPTICS. However, note that k-d trees are known to degenerate for high-dimensional data requiring $O(n)$ operations and leading to a performance no better than linear search. Fast kNN search and fixed-radius nearest neighbor search are used in DBSCAN and OPTICS, but we also provide a direct interface in **dbscan**, since they are useful in their own right.

```
kNN(x, k, sort = TRUE, search = "kdtree", bucketSize = 10,
  splitRule = "suggest", approx = 0)
frNN(x, eps, sort = TRUE, search = "kdtree", bucketSize = 10,
  splitRule = "suggest", approx = 0)
```

The interfaces only differ in the way that `kNN()` requires to specify `k` while `frNN()` needs the radius `eps`. All other arguments are the same. `x` is the data, and the result will be a list with the neighbors for each point in `x`. `sort` controls if the returned points are sorted by the distance. `search` controls what searching method should be used. Available search methods are `"kdtree"`, `"linear"` and `"dist"`. The linear search method does not build a search data structure but performs a complete linear search to find the nearest neighbors. The dist method precomputes a dissimilarity matrix which is very fast for small datasets, but problematic for large sets. The default method is to build a k-d tree. k-d trees are implemented in C++ using a modified version of the **ANN** library (Mount and Arya 2010) compiled for Euclidean distances. Parameters `bucketSize`, `splitRule` and `approx` are algorithmic parameters which control the way the k-d tree is built. `bucketSize` controls the maximal size of the k-d tree leaf nodes. `splitRule` specifies the method how the k-d tree partitions the data space. We use `"suggest"`, which uses the best guess of the **ANN** library given the data. `approx` greater than zero uses approximate *NN* search to significantly speed up search, however, some actual neighbors may be omitted. Note that using this feature for DBSCAN or OPTICS is discouraged since it will lead to incorrect results by introducing spurious clusters and noise points. For more details, we refer the reader to the documentation of the **ANN** library (Mount and Arya 2010). `dbscan()` and `optics()` use internally `frNN()` and the additional arguments in `...` are passed on to the nearest neighbor search method.

3.2. Clustering with DBSCAN

In this section, we present how to use DBSCAN, find appropriate values for the two parameters, and evaluate parameter sensitivity. As an example, we use a very simple artificial dataset of four slightly overlapping Gaussians in two-dimensional space with 100 points each. We load **dbscan**, set the seed of the random number generator to make the results reproducible and create the dataset.

```
R> library("dbscan")
R> set.seed(2)
R> n <- 400
R> x <- cbind(x = runif(4, 0, 1) + rnorm(n, sd = 0.1),
+    y = runif(4, 0, 1) + rnorm(n, sd = 0.1))
R> true_clusters <- rep(1:4, time = 100)
R> plot(x, col = true_clusters, pch = true_clusters)
```

The resulting dataset is shown in Figure 3.

To apply DBSCAN, we need to decide on the neighborhood radius `eps` and the density threshold `minPts`. The rule of thumb for setting `minPts` is to use at least the number of dimensions of the dataset plus one. In our case, this is 3. To find a suitable value for `eps`, we can plot the points' kNN distances (i.e., the distance of each point to its k-th nearest neighbor) in decreasing order and look for a knee in the plot. The idea behind this heuristic is that points located inside of clusters will have a small k-nearest neighbor distance, because they are close to other points in the same cluster, while noise points are more isolated and will have a rather large kNN distance. **dbscan** provides a function called `kNNdistplot()` to make this easier. For k we use the `minPts` value of 3.

```
R> kNNdistplot(x, k = 3)
R> abline(h = 0.05, col = "red", lty = 2)
```

The kNN distance plot is shown in Figure 4. A knee is visible at around a 3-NN distance of 0.05. We have added a horizontal line manually for reference.

Now we can perform the clustering with the chosen parameters.

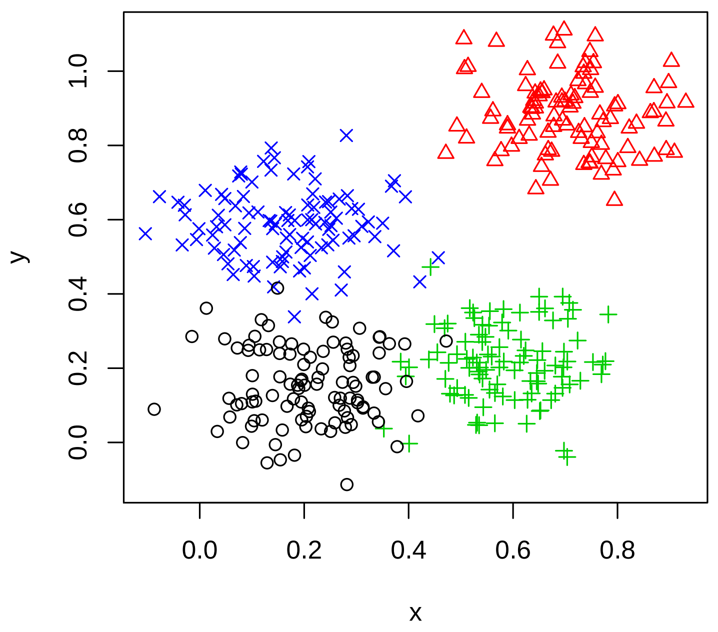


Figure 3: The sample dataset, consisting of 4 noisy Gaussian distributions with slight overlap.

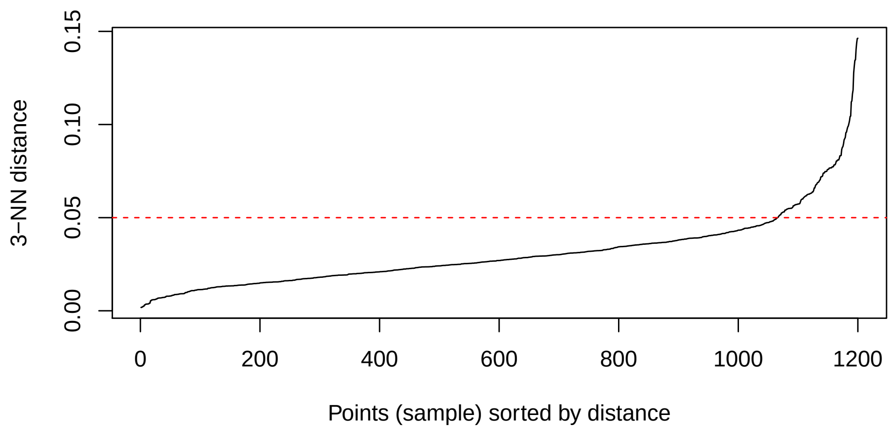


Figure 4: k-nearest neighbor distance plot.

```
R> res <- dbscan(x, eps = 0.05, minPts = 3)
R> res


DBSCAN clustering for 400 objects.
Parameters: eps = 0.05, minPts = 3
The clustering contains 6 cluster(s) and 30 noise points.

  0   1   2   3   4   5   6
 30 185  87  89   3   3   3

Available fields: cluster, eps, minPts
```

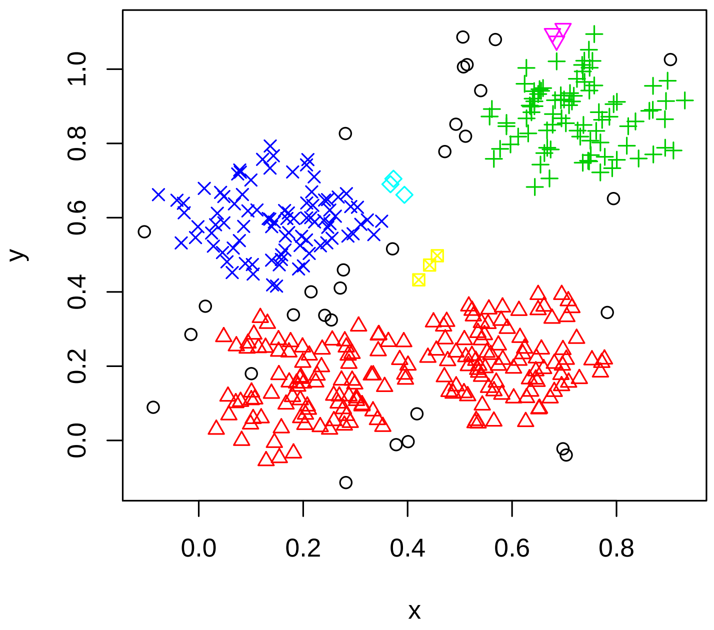


Figure 5: Result of clustering with DBSCAN. Noise is represented as black circles.

The resulting clustering identifies one large cluster with 185 member points and two medium size clusters of between 87 and 89 points, three very small clusters and 30 noise points (represented by cluster id 0). The available fields can be directly accessed using the list extraction operator `$`. For example, the cluster assignment information can be used to plot the data with the clusters identified by different labels and colors.

```
R> plot(x, col = res$cluster + 1L, pch = res$cluster + 1L)
```

Note that we add one to the cluster labels since noise points have a cluster label of zero and thus would not be visible in the plot. The resulting scatter plot in Figure 5 shows that the clustering algorithm correctly identified the upper two clusters, but merged the lower two clusters because the region between them has a high enough density. The small clusters are isolated groups of 3 points (passing *minPts*) and the noise points (black circles) are isolated points. **dbscan** also provides a plot that adds convex cluster hulls to the scatter plot shown in Figure 6.

```
R> hullplot(x, res)
```

A clustering can also be used to find out to which clusters new data points would be assigned using `predict(object, newdata = NULL, data, ...)`. The predict method uses nearest neighbor assignment to core points and needs the original dataset. Additional parameters are passed on to the nearest neighbor search method. Here we obtain the cluster assignment for the first 25 data points. Note that an assignment to cluster 0 means that the data point is considered noise because it is not in the ϵ-neighborhood of any core point.

```
R> predict(res, x[1:25, ], data = x)
```

```
[1] 1 2 1 0 1 2 1 3 1 2 1 3 1 0 1 3 1 2 0 3 1 2 1 3 1
```

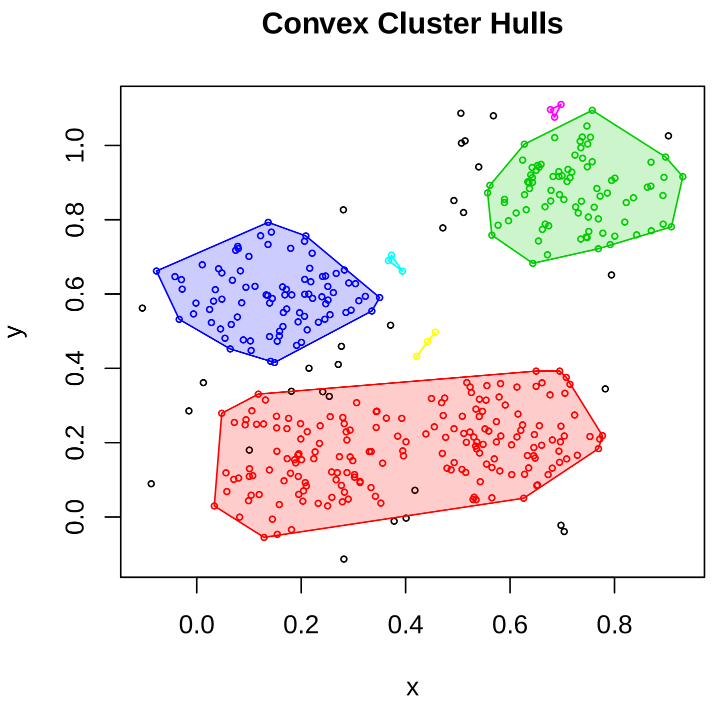


Figure 6: Convex hull plot of the DBSCAN clustering. Noise points are black. Note that density-based clusters do not need to be convex and thus noise points and points of another cluster may lie within the convex hull of a different cluster.

Even using the method based on the k-nearest neighbor distance plot described above, it is sometimes hard to find appropriate parameter values. This is in part because the parameters are interrelated and the algorithm can be very sensitive to small parameter changes. We show here how a simple sensitivity analysis can be performed. The idea is to create a grid of parameter combinations, cluster with each combination, and then calculate the clustering quality using a cluster validity measure. Here we have ground truth information (the correct cluster label) available, and therefore we can use the adjusted Rand index (ARI) (Hubert and Arabie 1985), a well-known external cluster validity measure. ARI compares the fraction of pairs of objects in agreement across the ground truth partition and the partition given by the clustering to be evaluated. The index is adjusted for agreement by chance. In the absence of a ground truth, internal cluster validity measures can be used.

We start with a reasonable grid.

```
R> minPts_grid <- 1:20
R> eps_grid <- seq(0.01, 0.2, by = 0.01)
```

Next, we define a function that clusters the data given a set of parameters and returns the adjusted Rand index (defined in package **mclust**, Scrucca *et al.* 2016). Note that the function uses the existing data, `x`, and the ground truth, `true_cluster`, from the parent environment. Finally, we apply the (vectorized) function to the grid of parameters.

```
R> library("mclust")
```

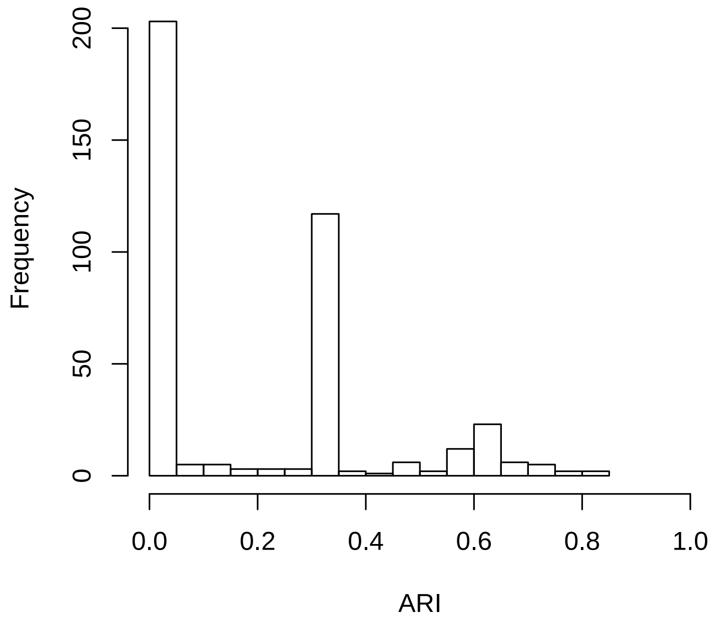


Figure 7: Histogram of the ARI values for ranges of settings of (`minPts`, `eps`).

```
R> clust <- function(minPts, eps) {
+    res <- dbscan(x, eps = eps, minPts = minPts)
+    adjustedRandIndex(res$cluster, true_clusters)
+ }
R> res_mat <- outer(minPts_grid, eps_grid, FUN = Vectorize(clust))
R> dimnames(res_mat) <- list(minPts_grid, eps_grid)
```

The sensitivity of the performance of DBSCAN to parameter variations can be assessed using a histogram of the ARI values.

```
R> hist(res_mat, breaks = 20, xlab = "ARI", xlim = c(0, 1), main = NULL)
```

The histogram in Figure 7 shows that many combinations of `minPts` and `eps` lead to an undesirable clustering result with low ARI. Only a very small number of combinations result in a reasonably high ARI of around 0.8 which indicates that the clustering captures much of the ground truth. The results of the sensitivity analysis can also be visualized as a color image to understanding how sensitive the DBSCAN algorithm is to parameter changes for the particular dataset. We use here the image plot provided in package **seriation** (Hahsler, Hornik, and Buchta 2008).

```
R> library("seriation")
R> pimage(res_mat, xlab = "eps", ylab = "minPts", key.lab = "ARI")
```

Figure 8 shows a band of higher ARI values where with increasing `minPts`, `eps` should be decreased. We can see that a good ARI value can be achieved by using `minPts` = 15 and `eps` = 0.09.

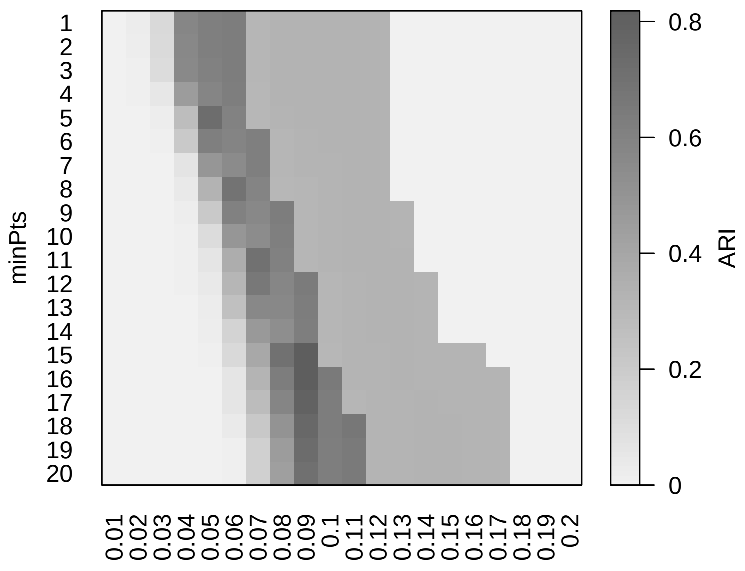


Figure 8: Image plot of the ARI values for a grid of settings of `minPts` and `eps`.

```
R> res <- dbscan(x, eps = 0.09, minPts = 15)
R> res

DBSCAN clustering for 400 objects.
Parameters: eps = 0.09, minPts = 15
The clustering contains 4 cluster(s) and 36 noise points.

 0  1  2  3  4
36 99 87 89 89

Available fields: cluster, eps, minPts

R> hullplot(x, res)
```

Figure 9 shows that the four clusters can be successfully identified with the parameters obtained using grid search with known ground truth.

3.3. Clustering with OPTICS

Unless OPTICS is purely used to extract a DBSCAN clustering, its parameters have a different effect than for DBSCAN: `eps` is typically chosen rather large (we use ten here) and `minPts` mostly affects core and reachability-distance calculation, where larger values have a smoothing effect. We also use 10, i.e., the core-distance is defined as the distance to the 9th nearest neighbor (spanning a neighborhood of 10 points including the point itself).

```
R> res <- optics(x, eps = 10, minPts = 10)
R> res
```

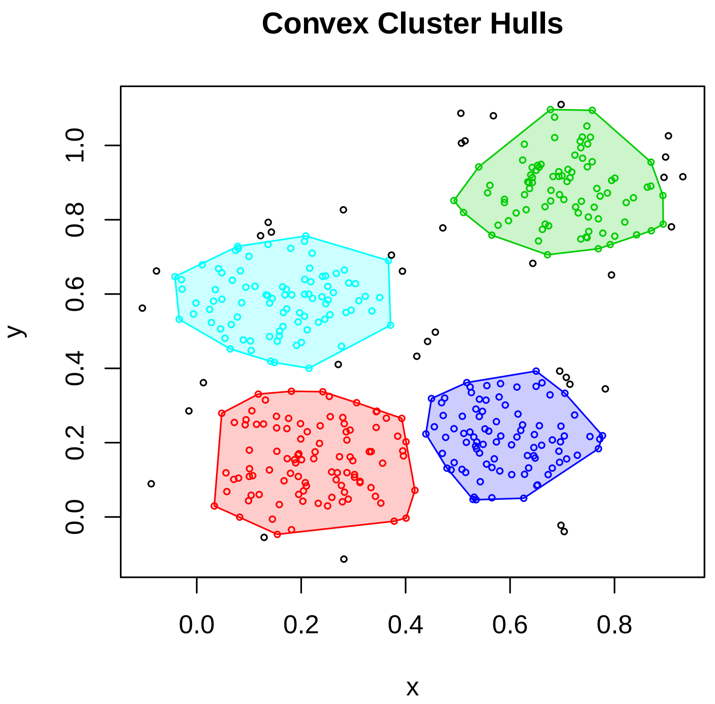


Figure 9: Convex hull plot of a DBSCAN clustering using `minPts` = 15 and `eps` = 0.09.

```
OPTICS ordering/clustering for 400 objects.
Parameters: minPts = 10, eps = 10, eps_cl = NA, xi = NA
Available fields: order, reachdist, coredist, predecessor,
                  minPts, eps, eps_cl, xi
```

OPTICS is an augmented ordering algorithm, which stores the computed order of the points it found in the `order` element of the returned object.

```
R> head(res$order, n = 15)
```

```
 [1]   1 363 209 349 337 301 357 333 321 285 281 253 241 177 153
```

This means that data point 1 in the dataset is the first in the order, data point 363 is the second and so forth. The density-based order produced by OPTICS can be directly plotted as a reachability plot.

```
R> plot(res)
```

The reachability plot in Figure 10 shows the reachability distance for points ordered by OPTICS. Valleys represent potential clusters separated by peaks. Very high peaks may indicate noise points. To visualize the order on the original datasets, we can plot a line connecting the points in order.

```
R> plot(x, col = "grey")
R> polygon(x[res$order, ])
```

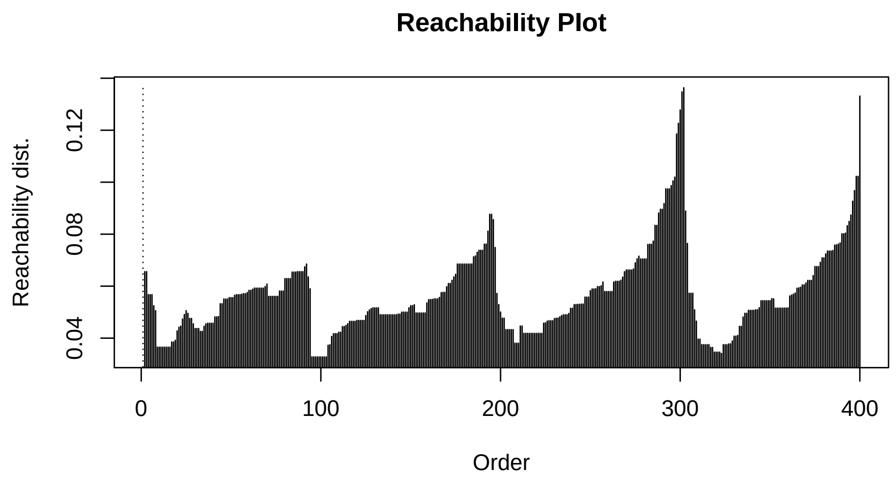


Figure 10: OPTICS reachability plot. Note that the first reachability value is always UNDEFINED.

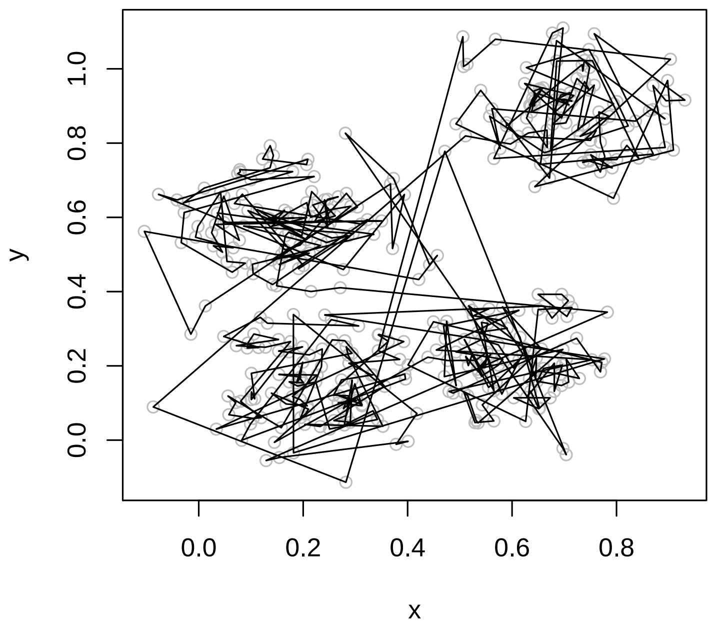


Figure 11: OPTICS order of data points represented as a line.

Figure 11 shows that points in each cluster are visited in consecutive order starting with the points in the center (the densest region) and then the points in the surrounding area.

As noted in Section 2.2, OPTICS has two primary cluster extraction methods using the ordered reachability structure it produces. A DBSCAN-type clustering can be extracted using `extractDBSCAN()` by specifying the global neighborhood size ϵ'. The reachability plot in Figure 10 shows four peaks, i.e., points with a high reachability-distance. These points indicate boundaries between clusters four clusters. A threshold that separates the four clusters can be visually determined. In this case we use `eps_cl` of 0.065.

```
R> res <- extractDBSCAN(res, eps_cl = 0.065)
```

```
R> res

OPTICS ordering/clustering for 400 objects.
Parameters: minPts = 10, eps = 10, eps_cl = 0.065, xi = NA
The clustering contains 4 cluster(s) and 92 noise points.

 0  1  2  3  4
92 81 84 72 71

Available fields: order, reachdist, coredist, predecessor,
                  minPts, eps, eps_cl, xi, cluster

R> plot(res)
R> hullplot(x, res)
```

The resulting reachability and corresponding clusters are shown in Figures 12 and 13. The clustering resembles the original structure of the four clusters with which the data were generated closely, with the only difference that points on the boundary of the clusters are marked as noise points.

dbscan also provides `extractXi()` to extract a hierarchical cluster structure. We use here a `xi` value of 0.05.

```
R> res <- extractXi(res, xi = 0.05)
R> res

OPTICS ordering/clustering for 400 objects.
Parameters: minPts = 10, eps = 10, eps_cl = NA, xi = 0.05
The clustering contains 7 cluster(s) and 1 noise points.

Available fields: order, reachdist, coredist, predecessor,
                  minPts, eps, eps_cl, xi, cluster,
                  clusters_xi
```

The ξ method results in a hierarchical clustering structure, and thus points can be members of several nested clusters. Clusters are represented as contiguous ranges in the reachability plot and are available the field `clusters_xi`.

```
R> res$clusters_xi

  start end cluster_id
1     1 194          1
2     1 301          2
3     8  23          3
4    94 106          4
5   196 288          5
6   302 399          6
7   308 335          7
```

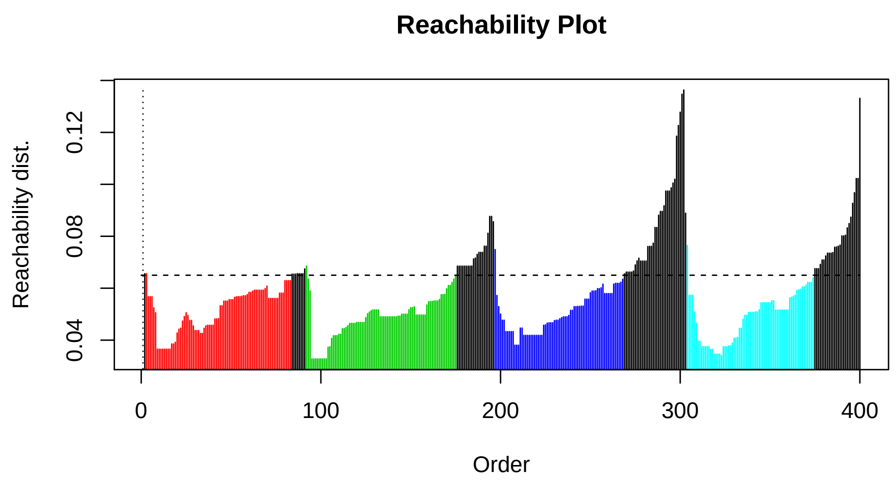


Figure 12: Reachability plot for a DBSCAN-type clustering extracted at global $\epsilon = 0.065$ results in four clusters.

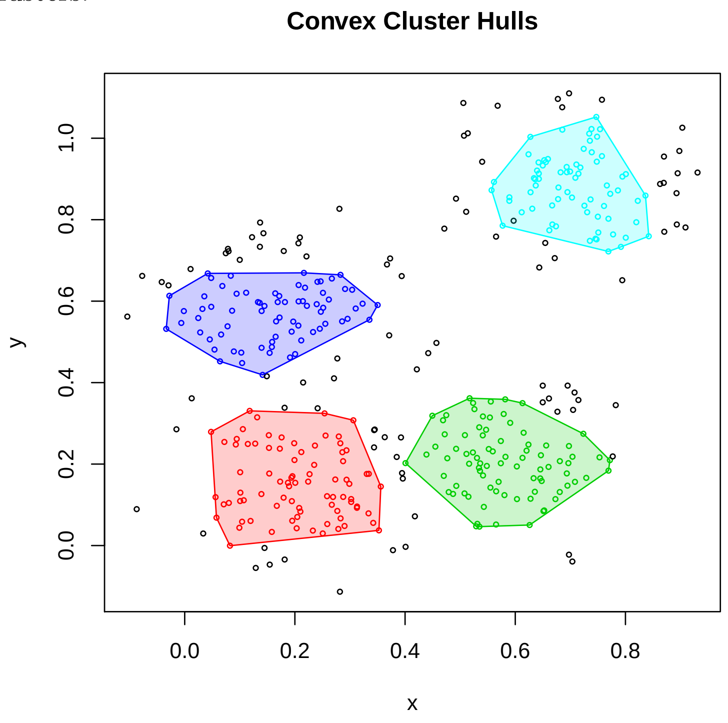


Figure 13: Convex hull plot for a DBSCAN-type clustering extracted at global $\epsilon = 0.065$ results in four clusters.

Here we have seven clusters. The clusters are also visible in the reachability plot.

```
R> plot(res)
R> hullplot(x, res)
```

Figure 14 shows the reachability plot with clusters represented using colors and vertical bars below the plot. The clusters themselves can also be plotted with the convex hull plot function

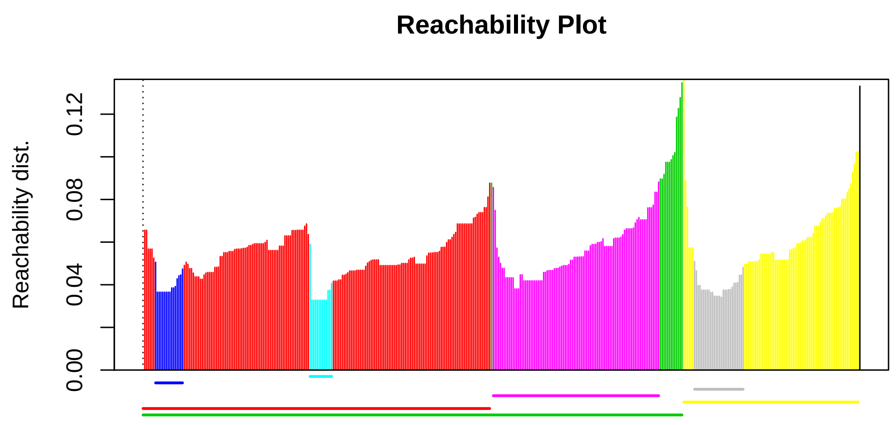


Figure 14: Reachability plot of a hierarchical clustering extracted with Extract-ξ.

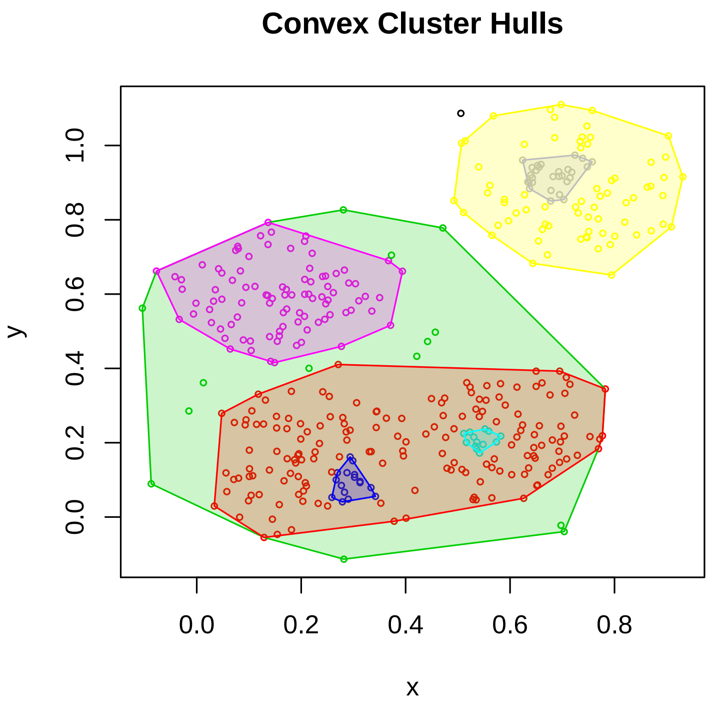


Figure 15: Convex hull plot of a hierarchical clustering extracted with Extract-ξ.

shown in Figure 15. Note how the nested structure is shown by clusters inside of clusters. Also note that it is possible for the convex hull, while useful for visualizations, to contain a point that is not considered as part of a cluster grouping.

3.4. Reachability and dendrograms

Reachability plots can be converted into equivalent dendrograms (Sander *et al.* 2003). **dbscan** contains a fast implementation of the reachability-to-dendrogram conversion algorithm

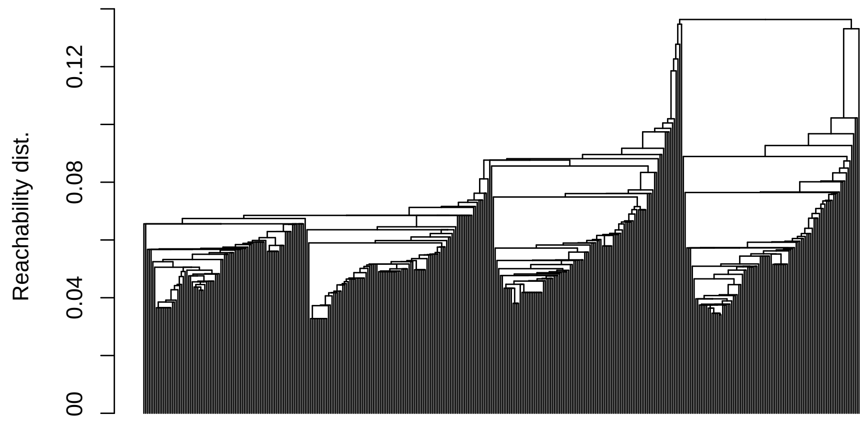


Figure 16: Dendrogram structure of OPTICS reordering.

through an implementation of the disjoint-set data structure (Cormen, Leiserson, Rivest, and Stein 2001; Patwary, Blair, and Manne 2010), allowing the user to choose which hierarchical representation they prefer. The conversion algorithm can be directly called for OPTICS objects using the coercion method `as.dendrogram()`.

```
R> dend <- as.dendrogram(res)
R> dend
```

```
'dendrogram' with 2 branches and 400 members total, at height 0.1363267
```

The dendrogram can be plotted using the standard plot method.

```
R> plot(dend, ylab = "Reachability dist.", leaflab = "none")
```

Note how the dendrogram in Figure 16 closely resembles the reachability plots with added binary splits. Since the object is a standard dendrogram (from package **stats**), it can be used like any other dendrogram created with hierarchical clustering.

4. Performance comparison

Finally, we compare the performance of **dbscan**'s implementation of DBSCAN and OPTICS with other open-source implementations. This is not a comprehensive performance evaluation study but is used rather to give the reader an idea about the performance of different DBSCAN and OPTICS implementations on datasets of varying sizes and number of dimensions. A comparative test was performed using both DBSCAN and OPTICS algorithms, where supported, for the libraries listed in Table 1 on page 8. The used datasets and their sizes are listed in Table 2. It is worth noting that we only consider Euclidean distance here. The datasets tested include s1 and s2, the randomly generated but moderately-separated Gaussian clusters often used for agglomerative cluster analysis (Fränti and Virmajoki 2006), the R15 validation dataset used for the maximum variance based clustering approach by Veenman, Reinders, and Backer (2002), the well-known spatial dataset DS3 used for validation of the CHAMELEON

Data set	*Size*	*Dimensionality*	*Type*
Aggregation	788	2	Benchmark
Compound	399	2	Benchmark
D31	3,100	2	Benchmark
flame	240	2	Benchmark
jain	373	2	Benchmark
pathbased	300	2	Benchmark
R15	600	2	Benchmark
s1	5,000	2	Benchmark
s4	5,000	2	Benchmark
spiral	312	2	Benchmark
t4.8k	8,000	2	Benchmark
CG6d_5k	5,000	6	Synthetic (Correlated)
CG6d_10k	10,000	6	Synthetic (Correlated)
CG6d_15k	15,000	6	Synthetic (Correlated)
UG6d_5k	5,000	6	Synthetic (Uncorrelated)
UG6d_10k	10,000	6	Synthetic (Uncorrelated)
UG6d_15k	15,000	6	Synthetic (Uncorrelated)
CG12d_5k	5,000	12	Synthetic (Correlated)
CG12d_10k	10,000	12	Synthetic (Correlated)
CG12d_15k	15,000	12	Synthetic (Correlated)
UG12d_5k	5,000	12	Synthetic (Uncorrelated)
UG12d_10k	10,000	12	Synthetic (Uncorrelated)
UG12d_15k	15,000	12	Synthetic (Uncorrelated)
CG18d_5k	5,000	18	Synthetic (Correlated)
CG18d_10k	10,000	18	Synthetic (Correlated)
CG18d_15k	15,000	18	Synthetic (Correlated)
UG18d_5k	5,000	18	Synthetic (Uncorrelated)
UG18d_10k	10,000	18	Synthetic (Uncorrelated)
UG18d_15k	15,000	18	Synthetic (Uncorrelated)

Table 2: Datasets used for comparison.

algorithm (Karypis, Han, and Kumar 1999), along with a variety of shape datasets commonly found in clustering validation papers (Gionis, Mannila, and Tsaparas 2007; Zahn 1971; Chang and Yeung 2008; Jain and Martin 2005; Fu and Medico 2007). To test higher-dimensional data, synthetic data was generated from both uncorrelated and correlated Gaussian sources (correlation has been shown to affect the performance of k-d trees in higher dimensions (Arya and Mount 1993)). The names of these datasets are abbreviated with whether they were generated from a correlated Gaussian (CG) or uncorrelated Gaussian (UG) source, followed by the dimensionality of the dataset, and the size of the dataset. For example, the dataset UG6d_10k refers to a 6-dimensional 10,000 point dataset generated from an uncorrelated multivariate Gaussian source distribution. The correlation between each dimension within the correlated datasets was randomly (uniformly) chosen between -1 and 1.

We perform a comparison with **ELKI** version 0.7, **PyClustering** 0.6.6, **fpc** 2.1-10, **dbscan** 0.9-8, **SPMF** v2.10, **WEKA** 3.8.0, **SciKit-Learn** 0.17.1 on a MacBook Pro equipped with a 2.5 GHz

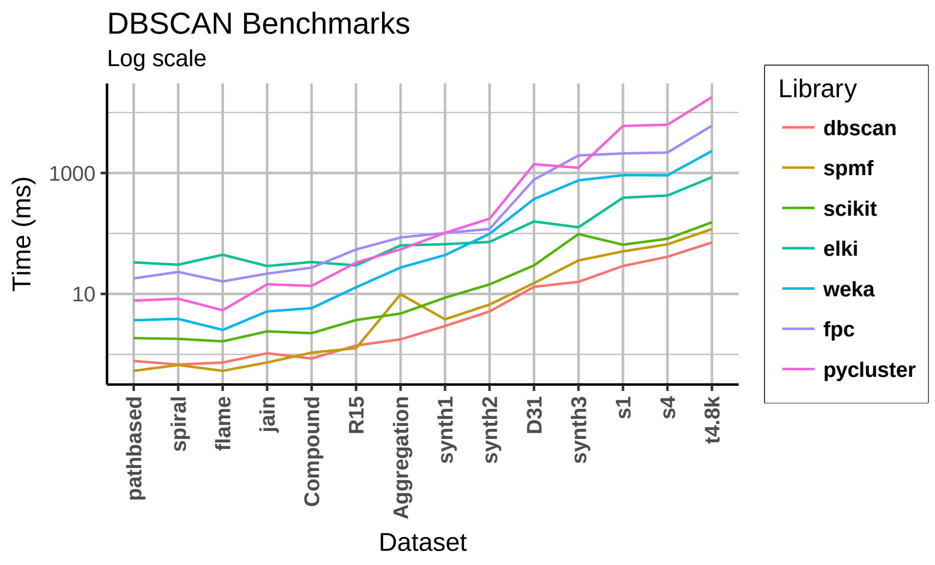


Figure 17: Runtime of DBSCAN in milliseconds (y-axis, logarithmic scale) vs. the name of the dataset tested (x-axis).

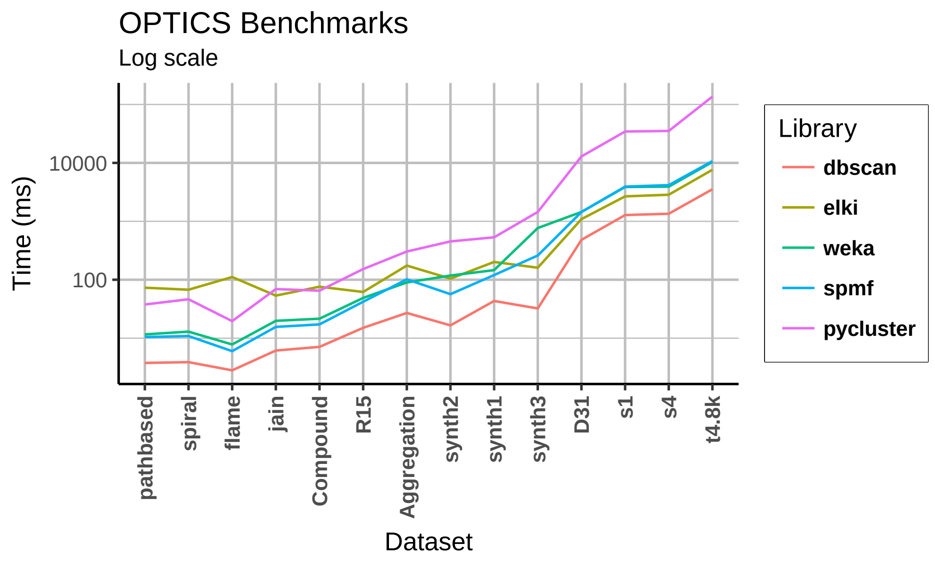


Figure 18: Runtime of OPTICS in milliseconds (y-axis, logarithmic scale) vs. the name of the dataset tested (x-axis).

Intel Core i7 processor, running OS X El Capitan 10.11.6. All datasets are normalized to the unit interval, $[0, 1]$, per dimension to standardize neighbor queries. For all datasets we use $minPts = 2$ and $\epsilon = 0.10$ for DBSCAN. For OPTICS, $minPts = 2$ with a large $\epsilon = 1$ is used. These parameters are explicitly chosen to be fairly large to test the scalability of the algorithms runtime performance. We replicate each run for each dataset 15 times and report the average runtime here. When possible, then we use the same parameters settings for libraries that support spatial-indexing acceleration (e.g., if it is possible to use a k-d tree, we use the same leaf size of 10). In total, $\approx 3,045$ tests were run for DBSCAN and $\approx\ 2,175$

tests were run for OPTICS. Figures 17 and 18 show the runtime results. The datasets are sorted from fastest to slowest, averaged across all libraries tested. The results show that the average runtime varies by many orders of magnitude between implementations, and that **dbscan** compares very favorably with other implementations.

5. Concluding remarks

The **dbscan** package offers a set of scalable, robust, and complete implementation s of popular density-based clustering algorithms from the DBSCAN family. The main features of **dbscan** are a simple interface to fast clustering and cluster extraction algorithms, extensible data structures and methods for both density-based clustering visualization and representation including efficient conversion algorithms between OPTICS ordering and dendrograms.

The density-based clustering field is still developing, and as new algorithms are introduced, we will try to incorporate them into **dbscan**. Initial versions of several algorithms related to density-based clustering have been added to **dbscan** recently. These algorithms include Hierarchical DBSCAN (HDBSCAN, Campello, Moulavi, and Sander 2013a), Local Outlier Factor (LOF, Breunig, Kriegel, Ng, and Sander 2000), Global-Local Outlier Scores from Hierarchies (GLOSH, Campello *et al.* 2015), the Framework for the Optimal Selection of Clusters (FOSC, Campello, Moulavi, Zimek, and Sander 2013b), and Jarvis-Patrick and Shared Nearest Neighbors clustering (Jarvis and Patrick 1973). **dbscan** will continue to incorporate state-of-the-art algorithms and methods used for density-based clustering and related problems.

Acknowledgments

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A. Technical note on OPTICS cluster extraction

Of the two cluster extraction methods outlined in this paper, the flat DBSCAN-type extraction method seems to remain the de facto clustering method implemented in most statistical software for OPTICS. However, this method produces clusters which are quite similar to the DBSCAN. To the best of the authors' knowledge, the only (other) library that has implemented the Extract-ξ method for finding ξ-clusters is the Environment for Developing KDD-Applications Supported by Index Structures (**ELKI**, Schubert *et al.* 2015). Perhaps much of the complication as to why nearly every statistical computing framework has neglected the Extract-ξ cluster method stems from the fact that the original specification (Figure 19 in Ankerst *et al.* 1999), while mostly complete, lacks important corrections that otherwise produce artifacts when clustering data. In the original specification of the algorithm, the dents in the ordering structure OPTICS produces are scanned for significant changes in reachability (specified by the ξ threshold). Clusters are identified as ranges of consecutive points separated by $1 - \xi$ density-reachability changes in the reachability plot. It is possible, however, after the recursive completion of the `update` algorithm (Figure 7 in Ankerst *et al.* 1999) that the next point processed in the ordering is not actually within the reachability distance of other members of the cluster being currently processed. To account for the missing details described above, a number of supplemental processing steps were added in the **ELKI** framework, which are mentioned in **ELKI**'s release notes (see `https://elki-project.github.io/releases/release_notes_0.7`). These steps correct artifacts through the addition of a small filtering step, thus improving the ξ-cluster method from the original implementation mentioned in the original OPTICS paper. This correction was not introduced until 2015, 16 years after the original publication of OPTICS and the Extract-ξ method. **dbscan** has incorporated these important changes in `extractXi()` via the option `correctPredecessors` which is by default enabled.

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