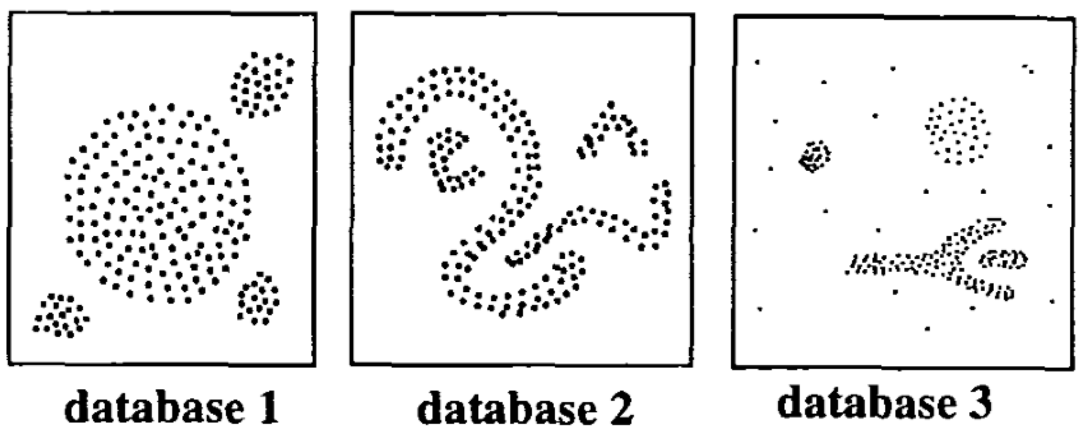
Chapter 19

DBSCAN: Density-Based Clustering

DBSCAN (**Density-Based Spatial Clustering and Application with Noise**), is a **density-based clusering** algorithm, introduced in Ester et al. 1996, which can be used to identify clusters of any shape in a data set containing noise and outliers.

The basic idea behind the density-based clustering approach is derived from a human intuitive clustering method. For instance, by looking at the figure below, one can easily identify four clusters along with several points of noise, because of the differences in the density of points.

Clusters are dense regions in the data space, separated by regions of lower density of points. The DBSCAN algorithm is based on this intuitive notion of "clusters" and "noise". The key idea is that for each point of a cluster, the neighborhood of a given radius has to contain at least a minimum number of points.



(From Ester et al. 1996)

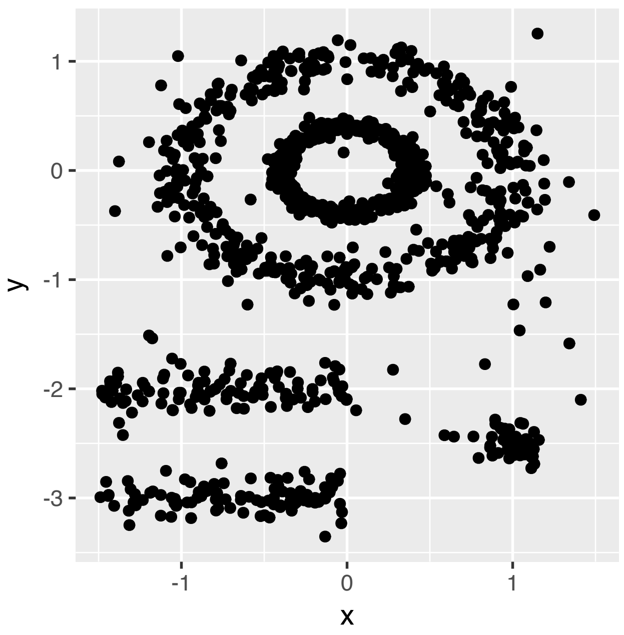
In this chapter, we'll describe the DBSCAN algorithm and demonstrate how to compute DBSCAN using the *fpc* R package.

19.1 Why DBSCAN?

Partitioning methods (K-means, PAM clustering) and hierarchical clustering are suitable for finding spherical-shaped clusters or convex clusters. In other words, they work well only for compact and well separated clusters. Moreover, they are also severely affected by the presence of noise and outliers in the data.

Unfortunately, real life data can contain: i) clusters of arbitrary shape such as those shown in the figure below (oval, linear and "S" shape clusters); ii) many outliers and noise.

The figure below shows a data set containing nonconvex clusters and outliers/noises. The simulated data set *multishapes* [in *factoextra* package] is used.



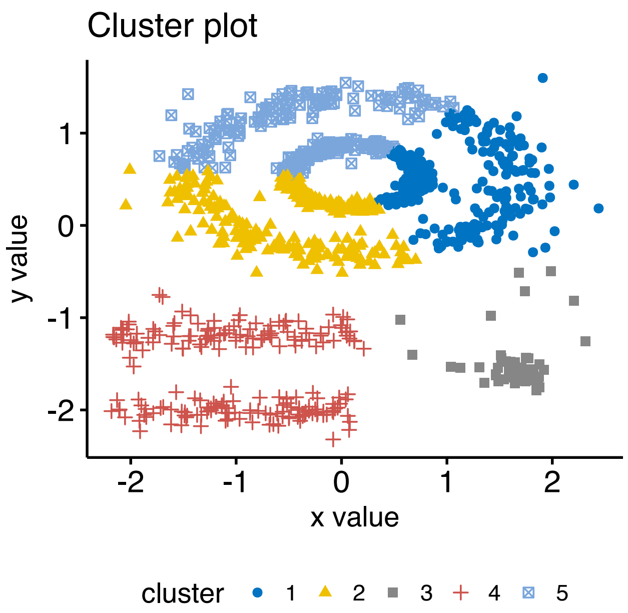
The plot above contains 5 clusters and outliers, including:

- 2 ovales clusters
- 2 linear clusters
- 1 compact cluster

Given such data, k-means algorithm has difficulties for identifying theses clusters with arbitrary shapes. To illustrate this situation, the following R code computes k-means algorithm on the multishapes data set. The function *fviz_cluster*()[*factoextra* package] is used to visualize the clusters.

First, install factoextra: install.packages("factoextra"); then compute and visualize k-means clustering using the data set multishapes:

```r
library(factoextra)
data("multishapes")
df <- multishapes[, 1:2]
set.seed(123)
km.res <- kmeans(df, 5, nstart = 25)
fviz_cluster(km.res, df,  geom = "point",
             ellipse= FALSE, show.clust.cent = FALSE,
             palette = "jco", ggtheme = theme_classic())
```



We know there are 5 five clusters in the data, but it can be seen that k-means method inaccurately identify the 5 clusters.

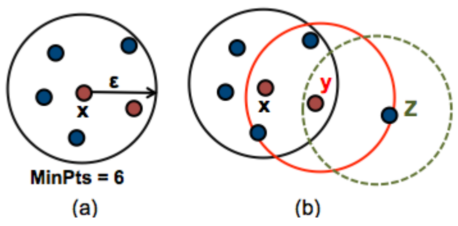
19.2 Algorithm

The goal is to identify dense regions, which can be measured by the number of objects close to a given point.

Two important parameters are required for DBSCAN: *epsilon* ("eps") and *minimum points* ("MinPts"). The parameter *eps* defines the radius of neighborhood around a point x. It's called called the ϵ-neighborhood of x. The parameter *MinPts* is the minimum number of neighbors within "eps" radius.

Any point x in the data set, with a neighbor count greater than or equal to *MinPts*, is marked as a *core point*. We say that x is *border point*, if the number of its neighbors is less than MinPts, but it belongs to the ϵ-neighborhood of some core point z. Finally, if a point is neither a core nor a border point, then it is called a noise point or an outlier.

The figure below shows the different types of points (core, border and outlier points) using MinPts = 6. Here x is a core point because $neighbours_\epsilon(x) = 6$, y is a border point because $neighbours_\epsilon(y) < MinPts$, but it belongs to the ϵ-neighborhood of the core point x. Finally, z is a noise point.



We start by defining 3 terms, required for understanding the DBSCAN algorithm:

- *Direct density reachable*: A point "A" is directly density reachable from another point "B" if: i) "A" is in the ϵ-neighborhood of "B" and ii) "B" is a core point.
- *Density reachable*: A point "A" is density reachable from "B" if there are a set of core points leading from "B" to "A.
- *Density connected*: Two points "A" and "B" are density connected if there are a core point "C", such that both "A" and "B" are density reachable from "C".

A density-based cluster is defined as a group of density connected points. The algorithm of density-based clustering (DBSCAN) works as follow:

1. For each point x_i, compute the distance between x_i and the other points. Finds all neighbor points within distance *eps* of the starting point (x_i). Each point, with a neighbor count greater than or equal to *MinPts*, is marked as *core point* or *visited*.

2. For each *core point*, if it's not already assigned to a cluster, create a new cluster. Find recursively all its density connected points and assign them to the same cluster as the core point.

3. Iterate through the remaining unvisited points in the data set.

Those points that do not belong to any cluster are treated as outliers or noise.

19.3 Advantages

1. Unlike K-means, DBSCAN does not require the user to specify the number of clusters to be generated

2. DBSCAN can find any shape of clusters. The cluster doesn't have to be circular.
3. DBSCAN can identify outliers

19.4 Parameter estimation

- MinPts: The larger the data set, the larger the value of minPts should be chosen. minPts must be chosen at least 3.
- ϵ: The value for ϵ can then be chosen by using a k-distance graph, plotting the distance to the k = minPts nearest neighbor. Good values of ϵ are where this plot shows a strong bend.

19.5 Computing DBSCAN

Here, we'll use the R package *fpc* to compute DBSCAN. It's also possible to use the package *dbscan*, which provides a faster re-implementation of DBSCAN algorithm compared to the fpc package.

We'll also use the *factoextra* package for visualizing clusters.

First, install the packages as follow:

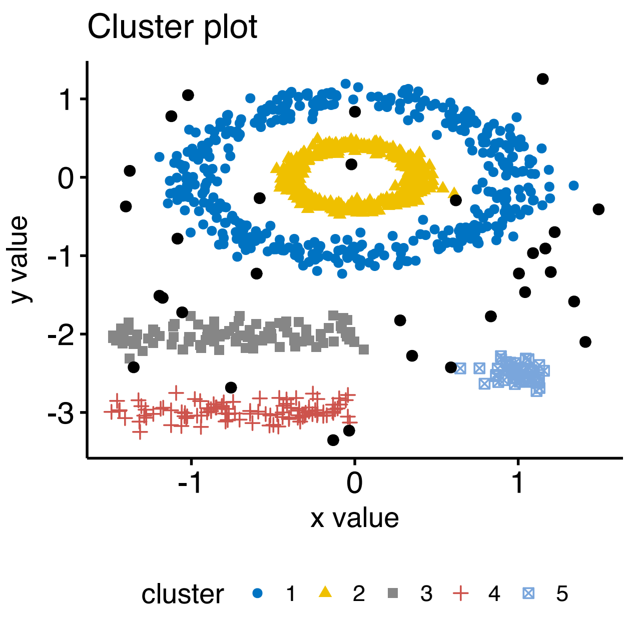
```r
install.packages("fpc")
install.packages("dbscan")
install.packages("factoextra")
```

The R code below computes and visualizes DBSCAN using multishapes data set [factoextra R package]:

```r
# Load the data
data("multishapes", package = "factoextra")
df <- multishapes[, 1:2]

# Compute DBSCAN using fpc package
library("fpc")
set.seed(123)
db <- fpc::dbscan(df, eps = 0.15, MinPts = 5)
```

```r
# Plot DBSCAN results
library("factoextra")
fviz_cluster(db, data = df, stand = FALSE,
             ellipse = FALSE, show.clust.cent = FALSE,
             geom = "point",palette = "jco", ggtheme = theme_classic())
```



Note that, the function *fviz_cluster*() uses different point symbols for core points (i.e, seed points) and border points. Black points correspond to outliers. You can play with *eps* and *MinPts* for changing cluster configurations.

It can be seen that DBSCAN performs better for these data sets and can identify the correct set of clusters compared to k-means algorithms.

The result of the *fpc::dbscan*() function can be displayed as follow:

```r
print(db)
```

```
## dbscan Pts=1100 MinPts=5 eps=0.15
##         0   1   2   3  4  5
## border 31  24   1   5  7  1
## seed    0 386 404  99 92 50
## total  31 410 405 104 99 51
```

In the table above, column names are cluster number. Cluster 0 corresponds to outliers (black points in the DBSCAN plot). The function *print.dbscan*() shows a statistic of the number of points belonging to the clusters that are seeds and border points.

```
# Cluster membership. Noise/outlier observations are coded as 0
# A random subset is shown
db$cluster[sample(1:1089, 20)]
```

```
##  [1] 1 3 2 4 3 1 2 4 2 2 2 2 2 2 1 4 1 1 1 0
```

DBSCAN algorithm requires users to specify the optimal *eps* values and the parameter *MinPts*. In the R code above, we used *eps = 0.15* and *MinPts = 5*. One limitation of DBSCAN is that it is sensitive to the choice of ϵ, in particular if clusters have different densities. If ϵ is too small, sparser clusters will be defined as noise. If ϵ is too large, denser clusters may be merged together. This implies that, if there are clusters with different local densities, then a single ϵ value may not suffice.

A natural question is:

How to define the optimal value of *eps*?

19.6 Method for determining the optimal eps value

The method proposed here consists of computing the k-nearest neighbor distances in a matrix of points.

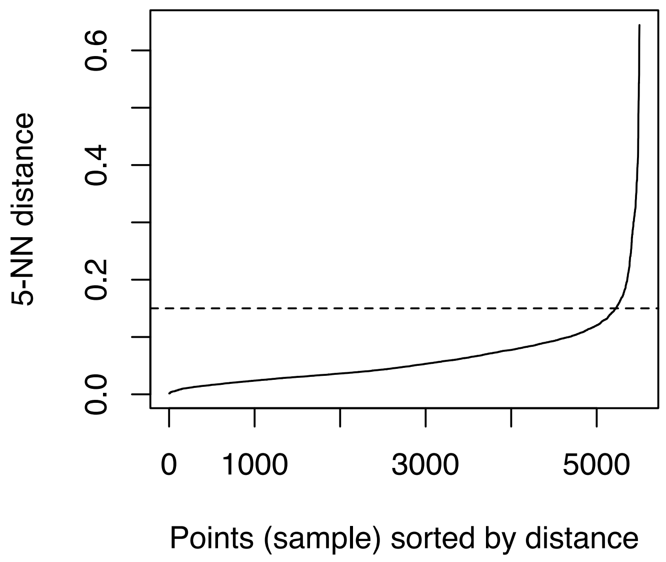
The idea is to calculate, the average of the distances of every point to its k nearest neighbors. The value of k will be specified by the user and corresponds to *MinPts*.

Next, these k-distances are plotted in an ascending order. The aim is to determine the "knee", which corresponds to the optimal *eps* parameter.

A knee corresponds to a threshold where a sharp change occurs along the k-distance curve.

The function *kNNdistplot*() [in *dbscan* package] can be used to draw the k-distance plot:

```
dbscan::kNNdistplot(df, k =  5)
abline(h = 0.15, lty = 2)
```



It can be seen that the optimal *eps* value is around a distance of 0.15.

19.7 Cluster predictions with DBSCAN algorithm

The function *predict.dbscan(object, data, newdata)* [in *fpc* package] can be used to predict the clusters for the points in *newdata*. For more details, read the documentation (*?predict.dbscan*).