Lecture 16: Clustering

Machine Learning, Summer Term 2019

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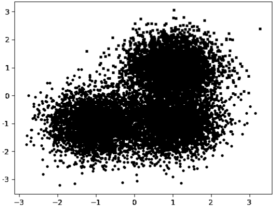
Lecture Overview

What is Cluster Analysis?

Also called: clustering, segmentation analysis, taxonomy analysis, automatic classification, numerical taxonomy, botryology, typological analysis, community detection, ...

(Plot modified from scikit-learn clustering tutorial)



Unsupervised task:

Group objects such that objects within a group are more similiar/related to each other *(in some sense)* than to objects of another group.

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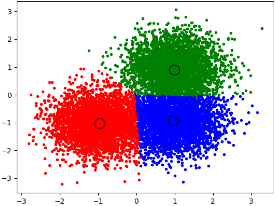

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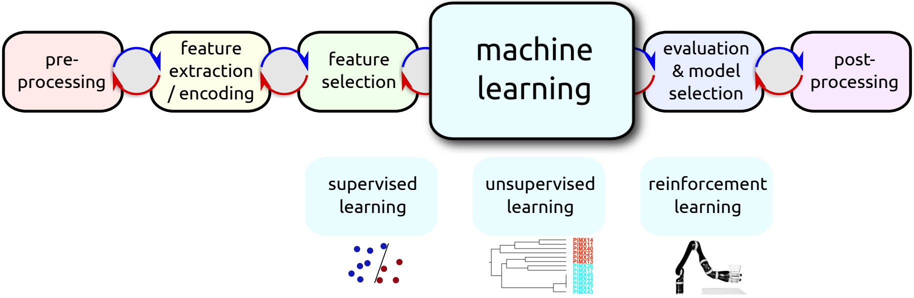
Group objects such that objects within a group are more similiar/related to each other *(in some sense)* than to objects of another group.

ML Design Cycle



Cluster analysis is an unsupervised learning task

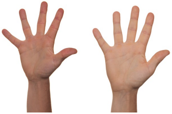
- Ground truth about clusters is not provided $\rightarrow$ evaluation is tricky!

Given:

- N high dimensional data points $\mathbf{x}_i \in \mathbb{R}^D$ with $i = 1 \ldots N$.
- Data is collected in matrix $\mathbf{X} \in \mathbb{R}^{N \times D}$

y missing

Applications



Example Applications (I)

- Medical imaging (fMRI, CT, PET): differentiate between different types of tissues, find tissue boundaries
- Biology: determine communities of organisms in space and time, compute data-driven phylogenetic trees
- Genetics: group DNA sequences into gene families
- Biochemistry / chemistry / pharmacology: group compounds according to their reaction mechanism
- Market research: detect clusters of customers with similar behavior, find market segments
- Social networks: recognize communities
- Search engines: Post-processing of search results into groups of hits that refer to vastly different topics

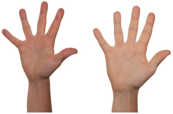
Example Applications (II)

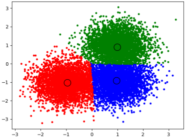
- Image segmentation: border detection, track objects
- Anomaly detection: identify outliers in data streams, network attacks, misbehaving software, sensor failures (robotics, production lines), predictive maintenance
- Finance: find stock clusters of similar behaviour
- Text analysis: clustering of documents into topics
- ...

Lecture Overview

How could Clusters be Determined?

Which metrics might be used to define clusters?





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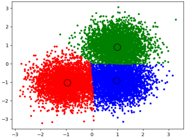


Zoo of clustering methods available, that exploit e.g.:

- distance/similarity function (between cluster members, between members of different clusters)
- connectivity structure using distances $\rightarrow$ single/avg/max linkage clustering, graph-based $\rightarrow$ clique
- centroid + neighborhood
- densities
- expected distributions

Lecture Overview

K-Means Clustering (Steinhaus, 1957)

Find set $C = C_1, ..., C_k$ of k clusters represented by cluster centroids μ_k such, that the clusters have equal variance.

$\rightarrow$ Minimize the *inertia* or *within-cluster sum-of-squares* criterion:

$$\underset{C}{\operatorname{argmin}} \sum_{i=1}^{k} \sum_{\mathbf{x} \in C_i} ||\mathbf{x} - \mu_j||^2$$

Observations:

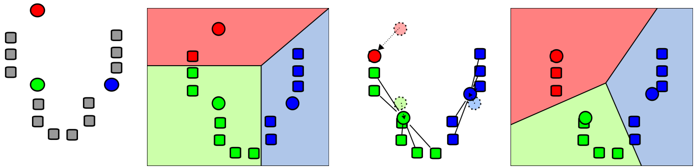
- Cluster centroids μ_j do not need to be points of the training data sets
- Unfortunately NP-hard problem!
- Clustering can be represented by Voronoi tesselation

K-Means Clustering

Practical solution by heuristic approximation
(e.g. Lloyd's algorithm (1957, 1982), similar to expectation-maximization):

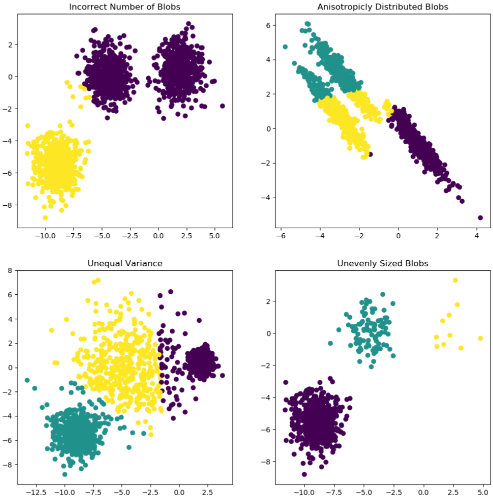
`Initialize` k `data points as cluster centroids.`
`Then iterate these two steps until convergence of the centroids:`

1. `Assign each data point to its nearest centroid`
   `(`$\rightarrow$ `approximations necessary for high dimensions!)`
2. `Create k new centroids by taking the mean value of all of the data points assigned to each novel centroid`
   `(`$\rightarrow$ `approximations necessary for many data points)`



K-Means Clustering

Problematic data sets for k-means:



K-Means Clustering

Pros:

- conceptually simple algorithm
- mini-batches and different kind of initialization strategies are available ($\rightarrow$ k-means++)
- scales to many data points (if approximations are utilized)

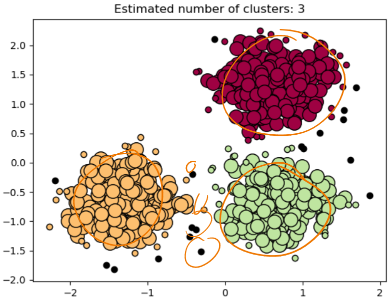
Cons:

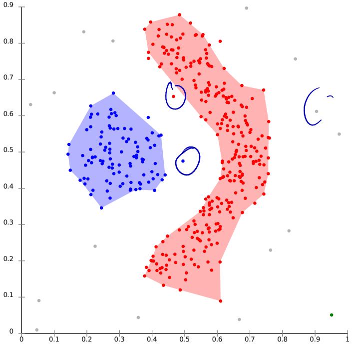
- sensitive to initialization of centroids
- can not model noise or outliers
- concave cluster shapes are problematic
- can not deal with uneven variance between clusters
- number k of clusters needs to be provided

Lecture Overview

DBSCAN

- DBSCAN (Ester et al., 1996) is a density-based, non-parameteric clustering method.
- It received the **test of time award** at KDD conference in 2014.





DBSCAN: A Cluster has High Density

DBSCAN: A Cluster has High Density

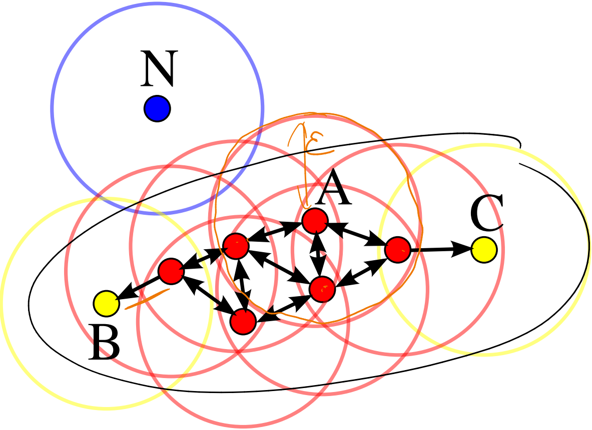
- A **core point** p is a data point in an area of high density. It is defined by having at least `minPts` points (including p) within an `eps`-neighborhood.

$p \longrightarrow q$

- A point q is **directly reachable** from $\cancel{q}$ p, if p is in the eps neighborhood of a core point q.
- A point q is **reachable** from p if there is a path along the points $p_1, ..., p_n$ with $p_1 = p$ and $p_n = q$, where each p_{i+1} is directly reachable from p_i. Note that this implies that all points on the path must be core points, with the possible exception of q (if q is on the fringe of a cluster).
- All points not reachable from any other point are considered **outliers** or **noise** points.

If p is a core point, then it forms a cluster together with all points (core or non-core) that are reachable from it.

DBSCAN



Example with `minPts`=4. The `eps`-neighborhoods are indicated by circles.

DBSCAN Algorithm

DBSCAN creates clusters by sequentially considering the training data points, starting with an arbitrary point:

1. Find the points in the `eps` neighborhood of every point, and identify the core points with more than `minPts` neighbors.
2. Find the connected components of core points on the neighbor graph, ignoring all non-core points.
3. Assign each non-core point to a nearby cluster if the cluster is an `eps` neighbor, otherwise assign it to noise.

Pseudocode for DBSCAN

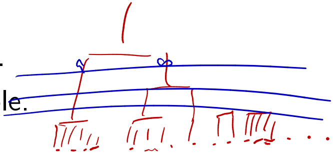
```
DBSCAN(DB, distFunc, eps, minPts) {
   C = 0                                                     /* Cluster counter */
   for each point P in database DB {
      if label(P) ≠ undefined then continue                  /* Previously processed in inner loop */
      Neighbors N = RangeQuery(DB, distFunc, P, eps)         /* Find neighbors */
      if |N| < minPts then {                                 /* Density check */
         label(P) = Noise                                    /* Label as Noise */
         continue
      }
      C = C + 1                                              /* next cluster label */
      label(P) = C                                           /* Label initial point */
      Seed set S = N \ {P}                                   /* Neighbors to expand */
      for each point Q in S {                                /* Process every seed point */
         if label(Q) = Noise then label(Q) = C               /* Change Noise to border point */
         if label(Q) ≠ undefined then continue               /* Previously processed */
         label(Q) = C                                        /* Label neighbor */
         Neighbors N = RangeQuery(DB, distFunc, Q, eps)      /* Find neighbors */
         if |N| ≥ minPts then {                              /* Density check */
            S = S ∪ N                                        /* Add new neighbors to seed set */
         }
      }
   }
}
```

```
RangeQuery(DB, distFunc, Q, eps) {
   Neighbors = empty list
   for each point P in database DB {                         /* Scan all points in the database */
      if distFunc(Q, P) ≤ eps then {                         /* Compute distance and check epsilon */
         Neighbors = Neighbors ∪ {P}                         /* Add to result */
      }
   }
   return Neighbors
}
```

Characteristics of DBSCAN

Pros:

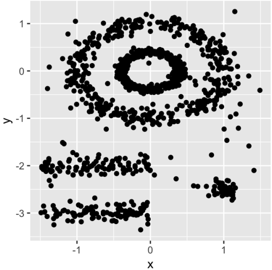
- DBSCAN is fast! With n data points: $O(n^2)$ as worst case (all points belong to single cluster), but $O(n \log(n))$ with good data structures and for typical data.
- DBSCAN is deterministic for a fixed processing sequence.
- Number of clusters is determined automatically.
- Hyperparameter ~~min samples~~ minPts can express prior knowledge about noise.
- Different distance metrics can be utilized.
- Hierarchical variant HDBSCAN is available.



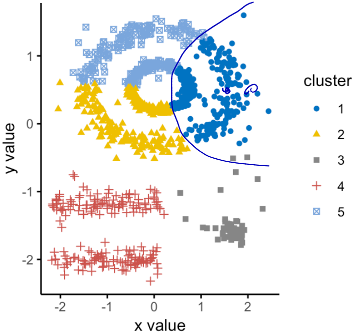
Cons:

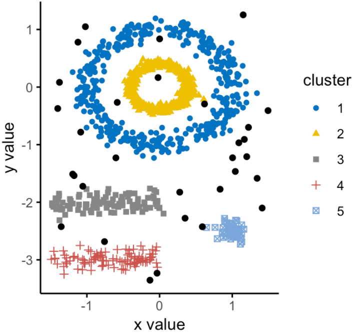
- Varying the sequence of data points processed can lead to different clusterings.
- Hyperparameter eps is critical, no good default!

Comparison of K-Means and DBSCAN

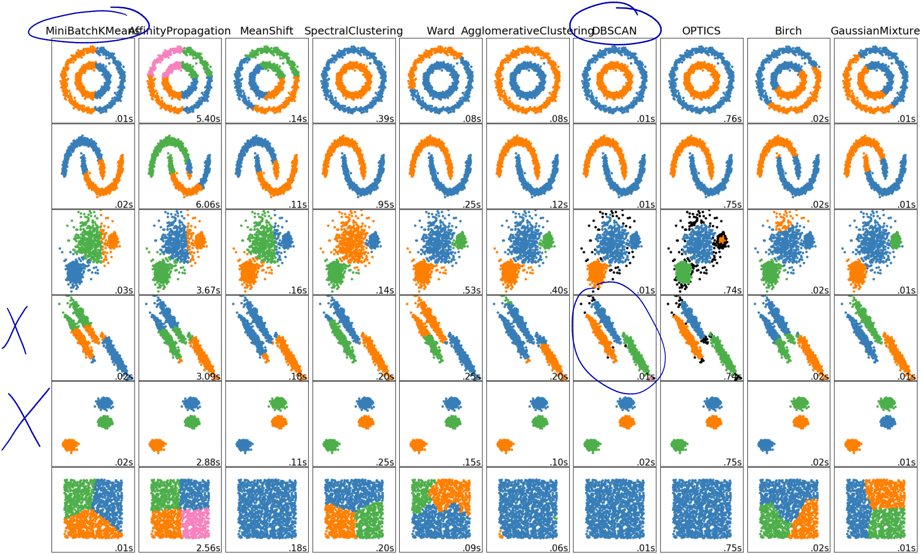


k-means





A few Clustering Algorithms on Toy Data



https://scikit-learn.org/stable/modules/clustering.html

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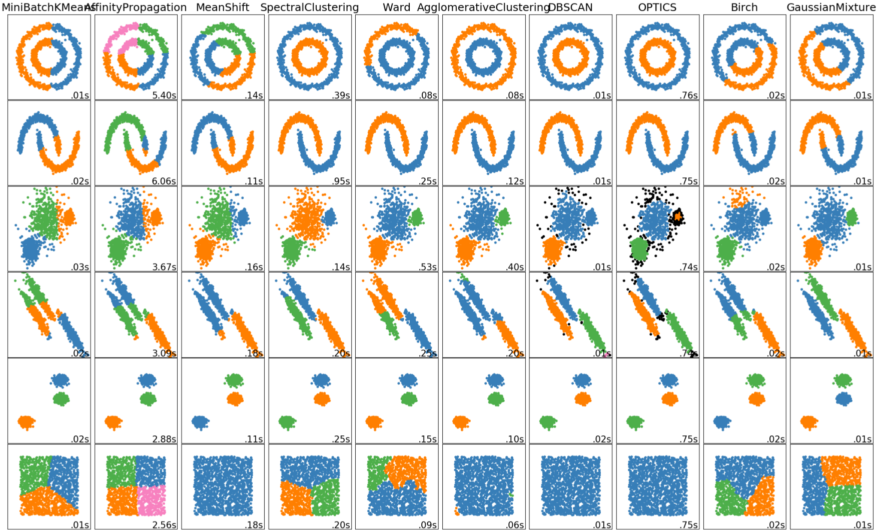

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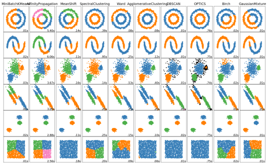
Criteria for the Choice of Clustering Algorithms



Does the algorithm...

- expects each cluster to follow a specific distribution? (e.g. Gaussian)?
- considers density of data points?
- deal well with noisy data / high-dimensional data / redundant dimensions / irrelevant dimensions?
- deliver hard / soft clustering?
- deliver a strict partitioning (i.e. each object belongs to exactly one cluster)?
- deliver a hierarchical clustering?

Wrap-Up: Summary by Learning Goals

Having heard this lecture and doing the assigment on clustering, you will be able to:

- Explain, which metrics can be used to create a clustering from unlabeled data
- formulate the optimization problem for k-means clustering and implement an iterative heuristic
- Describe pros and cons of k-means and DBSCAN
- Derive a metric for the quality of a given clustering (e.g. via the "**silhouette score**", see assignment)