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Machine Learning II

Unsupervised Learning: Clustering

Outline

- Clustering Algorithms
  - K-Means
  - DBSCAN

Introduction to ML

Basic Types of Machine Learning Algorithms

- Supervised Learning
- Unsupervised Learning
- Reinforcement Learning

- NO Labeled data
- NO Direct and quantitative evaluation

- Explore structure of data

Clustering Algorithms

Definition

Cluster analysis or **clustering** is the task of **grouping a set of objects** in such a way that objects in the same group (called a cluster) are **more similar** (in some sense) to each other than to those in other groups (clusters). [Wikipedia]

Introduction to ML

Unsupervised Learning

Data without “labels” $(x_1, x_2, \ldots, x_n)$

- **Clustering**
- **Outlier Detection (e.g. Defect or Intrusion detection)**

Clustering Algorithms

Introduction

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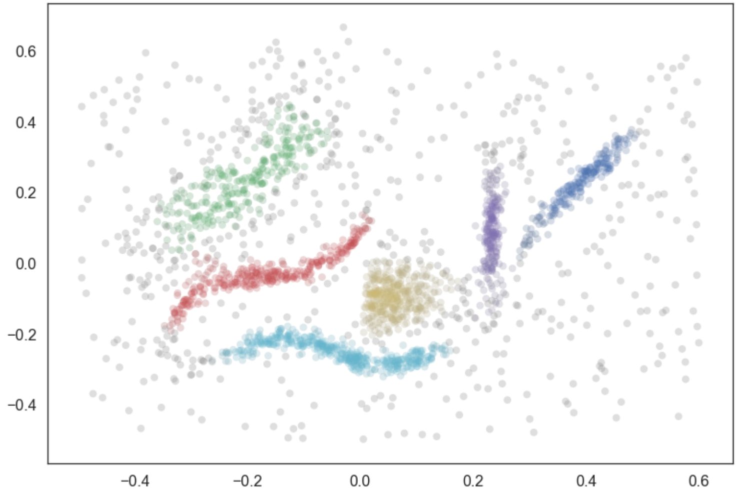


Example 2d data set

Clustering Algorithms

Motivation

- Standard technique for data exploration and anlysis
- Objective: find inherent structures in data
- Just like Multivariate Statistics
    - For high dimensional data
    - Geometric (manifold) and statistical motivations

Clustering Algorithms: K-Means

Definition:

Given a set of observations $(x_1, x_2, \ldots, x_n)$

where each observation is a *d*-dimensional real vector, **K-Means** clustering aims to partition the *n* observations into $k \leq n$

sets $S = \{S_1, S_2, \ldots, S_k\}$

so as to minimize the within-cluster sum of squares:

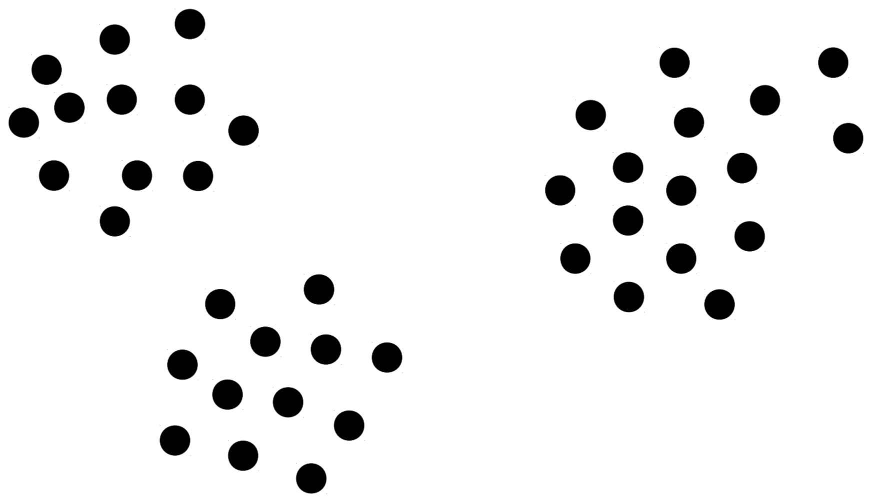
$$\arg\min[S] \sum_{i=1}^{k} \sum_{x \in S_i} \|x - \mu_i\|$$

Clustering Algorithms: K-Means

Intuition:

$$\arg\min[S] \sum_{i=1}^{k} \sum_{x \in S_i} ||x - \mu_i||$$

Data:

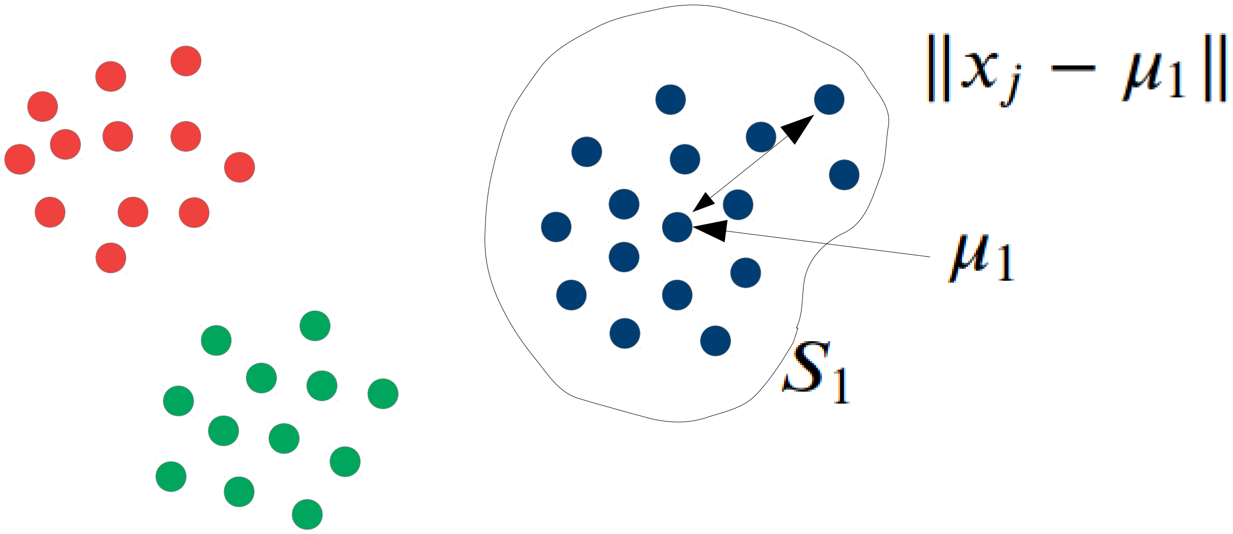


Clustering Algorithms: K-Means

Intuition:

$$\arg\min[S] \sum_{i=1}^{k} \sum_{x \in S_i} \|x - \mu_i\|$$

Clustering
for k=3



Clustering Algorithms: K-Means

Basic Algorithm:

Init (t=1): Select *k* random cluster centers

$$\mu_1^{(1)} := x_{r1}, \mu_2^{(1)} := x_{r2}, \ldots, \mu_k^{(1)} := x_{rk} \quad for \quad x_{rj} \in X$$

Repeat *n* times:

1. For step t: Assign all samples to “closest” center

$$S_i^{(t)} = \{x_p : \|x_p - \mu_i^{(t)}\|^2 \leq \|x_p - \mu_j^{(t)}\|^2 \quad \forall j, 1 \leq j \leq k\}$$

2. Re-Compute cluster centers

$$\mu_i^{(t+1)} = \frac{1}{|S_i^{(t)}|} \sum_{x_j \in S_i^{(t)}} x_j$$

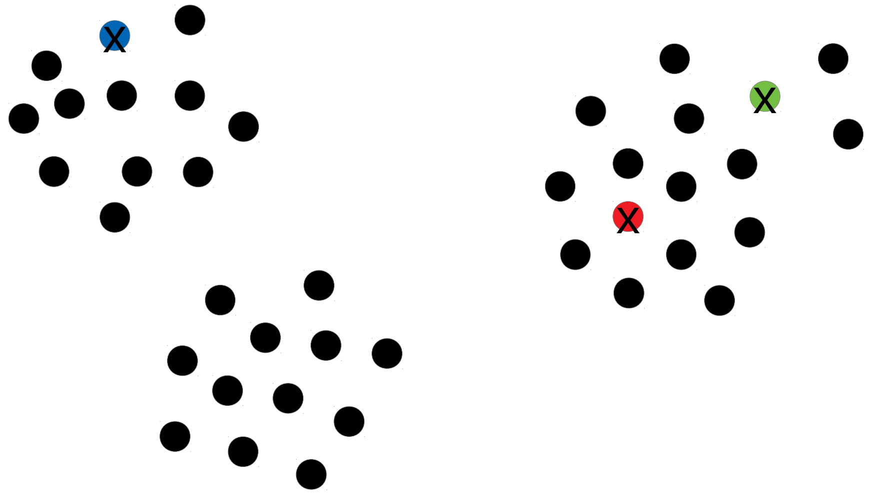
Clustering Algorithms: K-Means

Intuition:

$$\mu_1^{(1)} := x_{r1}, \mu_2^{(1)} := x_{r2}, \dots, \mu_k^{(1)} := x_{rk} \quad for \quad x_{rj} \in X$$

Random!

Init:



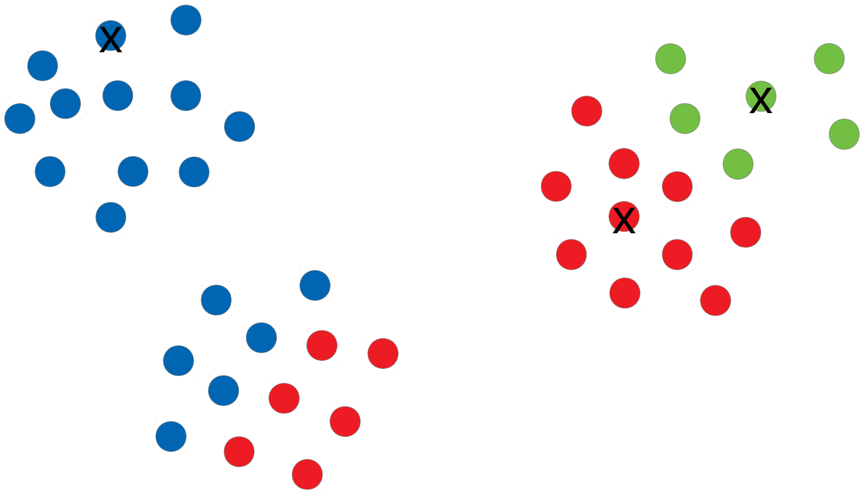
t=1

Clustering Algorithms: K-Means

Intuition:

$$S_i^{(t)} = \{x_p : \|x_p - \mu_i^{(t)}\|^2 \le \|x_p - \mu_j^{(t)}\|^2 \quad \forall j, 1 \le j \le k\}$$

Step 1:



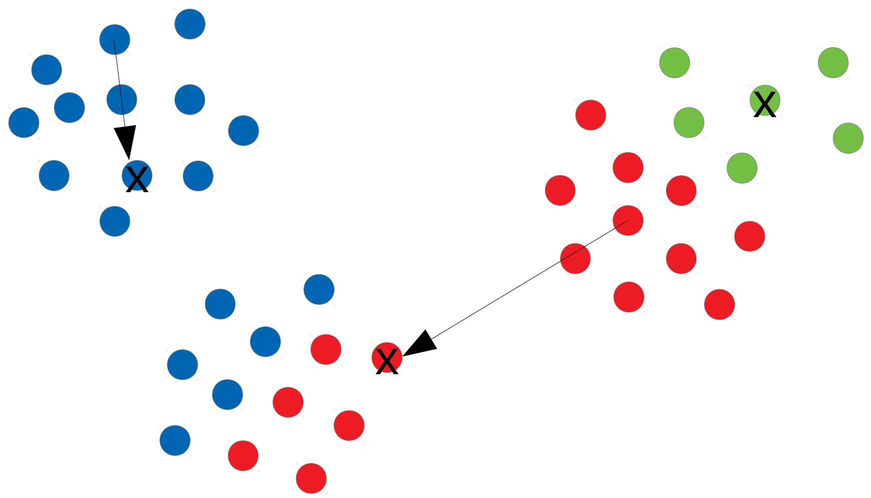
t=2

Clustering Algorithms: K-Means

Intuition:

$$\mu_i^{(t+1)} = \frac{1}{|S_i^{(t)}|} \sum_{x_j \in S_i^{(t)}} x_j$$

Step 2:



t=2

Clustering Algorithms: K-Means

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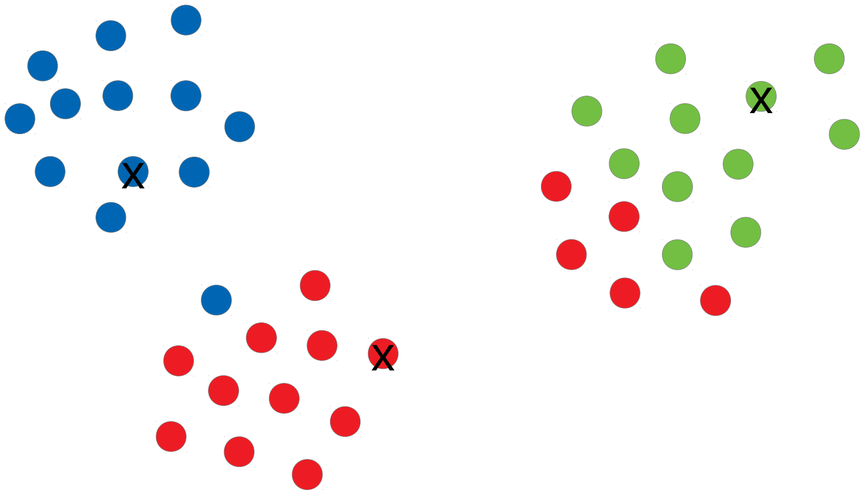

t=3

Clustering Algorithms: K-Means

Intuition:

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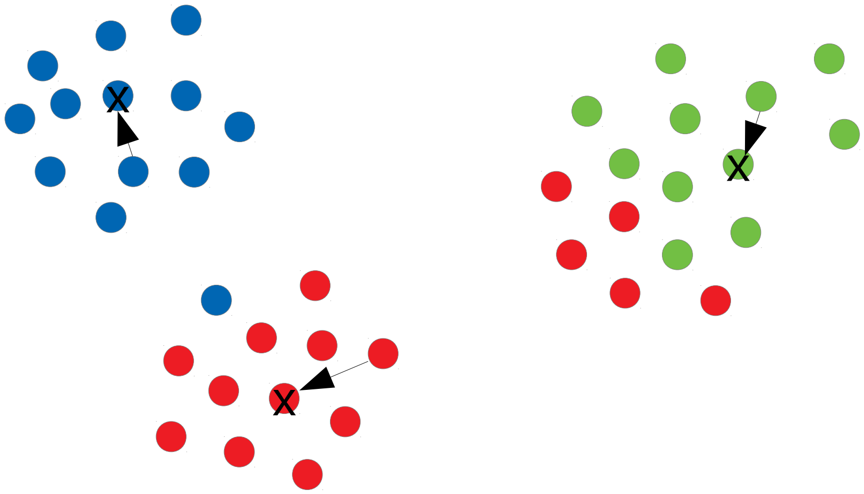

t=3

Clustering Algorithms: K-Means

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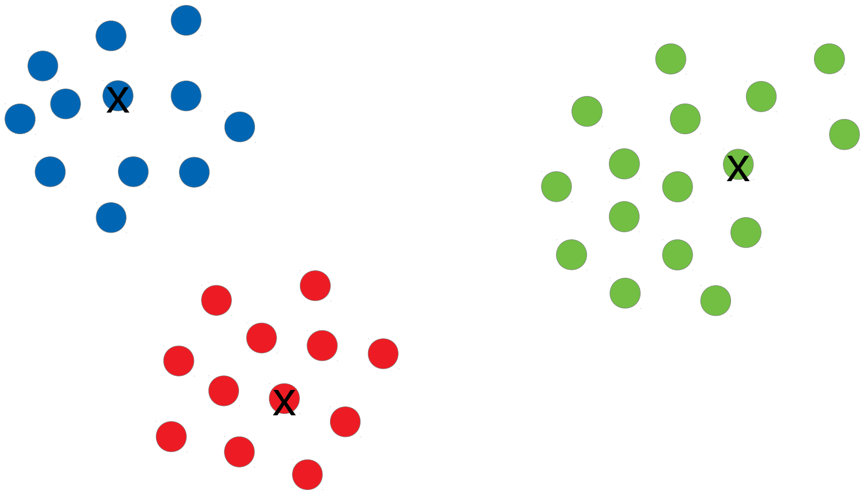
Step 1:



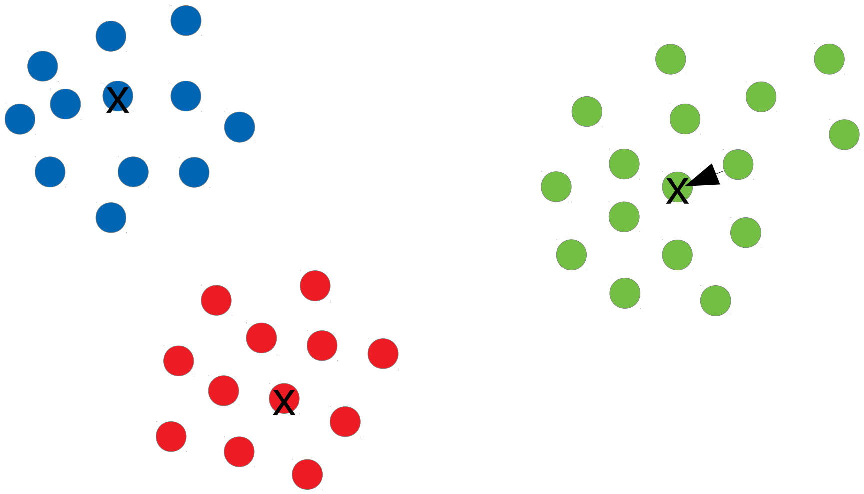
t=4

Clustering Algorithms: K-Means

Intuition:

$$\mu_i^{(t+1)} = \frac{1}{|S_i^{(t)}|} \sum_{x_j \in S_i^{(t)}} x_j$$

Step 2:

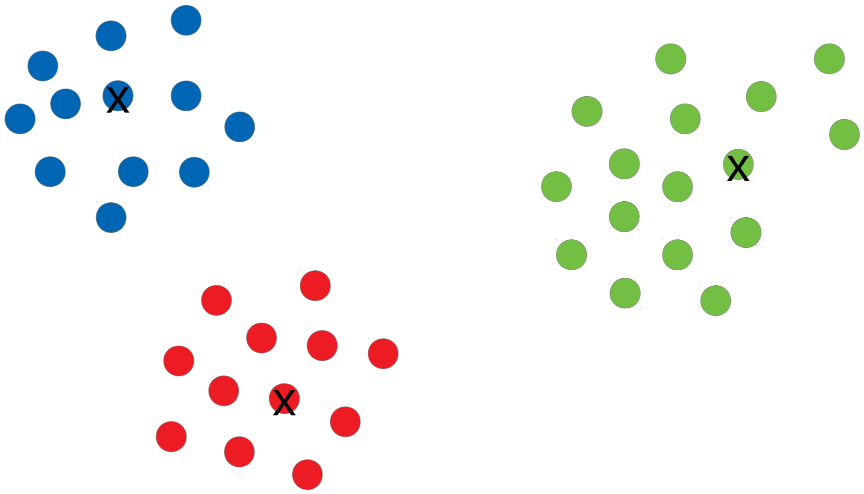


t=4

Clustering Algorithms: K-Means

Intuition: Convergence after fix t or fix means

Step 1:



t=5,6,7,...

Clustering Algorithms: K-Means

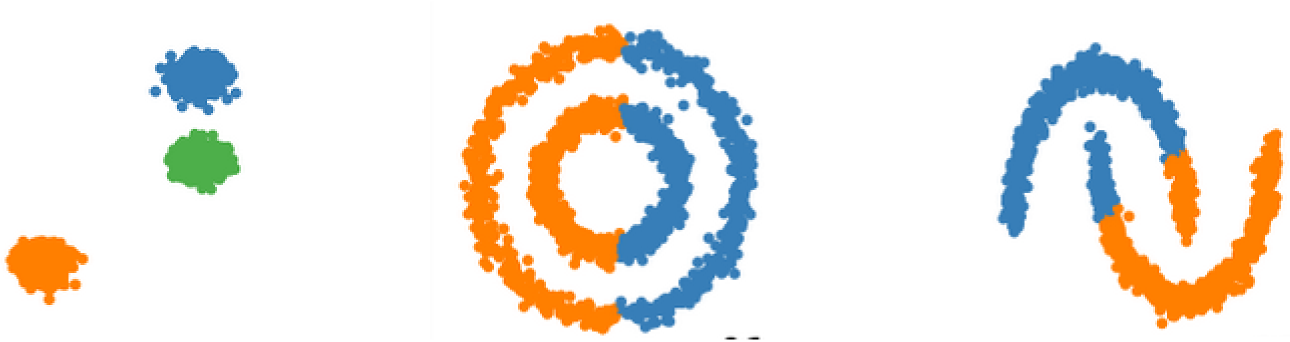
Evaluation:

- Very simple but effective clustering algorithm
- Advantages:
  - Easy to implement
  - Easy to parallelize

- Disadvantages
  - Need to know k in advance (or search for best k)
  - High complexity: HP-hard (exponential in data dimension)
  - Problem with non-blob shaped (non-convex) clusters

Clustering Algorithms: K-Means

Evaluation:



More practical examples in the Lab session….

Clustering Algorithms: DBSCAN

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Definition

Density-based spatial clustering of applications with noise (DBSCAN) is a density-based clustering ***non-parametric*** algorithm:

Given a set of points in some space, it groups together points that are closely packed together (points with many nearby neighbors), marking as outliers points that lie alone in low-density regions (whose nearest neighbors are too far away).

Clustering Algorithms: DBSCAN

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Given a set of points in some space, it groups together points that are closely packed together (points with many nearby neighbors), marking as outliers points that lie alone in low-density regions (whose nearest neighbors are too far away).

In contrast to K-Means, the number of clusters is not given

Clustering Algorithms: DBSCAN

Definitions in DBSCAN

Given a set of observations $(x_1, x_2, \ldots, x_n)$ we need:

Some distance function on the data: $d(x_i, x_j)$

Parameter: radius ε

Set of Neighbors: $\mathbb{N}(x_i)$

Parameter: Minimum number of Neighbors n_ε

Clustering Algorithms: DBSCAN

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Definitions in DBSCAN

Density at a data sample: number of neighbors in radius

$$\mathbb{d}(x_i) := |\mathbb{N}(x_i)| = |\{x_p : d(x_p, x_i) \leq \varepsilon\}|$$

Core samples: all samples with a density higher than a threshold

$$\{x_p : \mathbb{d}(x_p) \geq n_\varepsilon\}$$

Reachable samples: all samples with at least one neighbor

$$\{x_p : \mathbb{d}(x_p) \geq 1\}$$

Clustering Algorithms: DBSCAN

Definitions in DBSCAN

Outlier samples: All samples without neighbors

$$\{x_p : \mathbb{d}(x_p) = 0\}$$

Clustering Algorithms: DBSCAN

Basic Algorithm

Init: mark all samples as core, reachable or outlier
Remove outlier

For all core samples: choose next random core sample and recursively merge it's neighborhood with all neighbors that are also core samples. Increment Cluster ID.

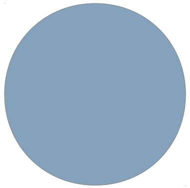
For all reachable samples: assign to closest cluster

Clustering Algorithms: DBSCAN

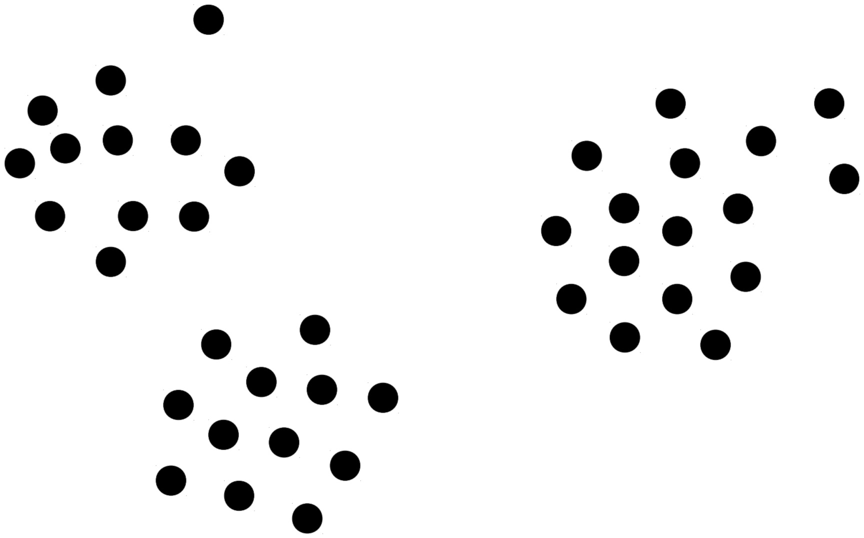
Intuition:

Init:

ε



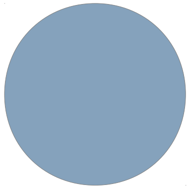
n_ε = 3



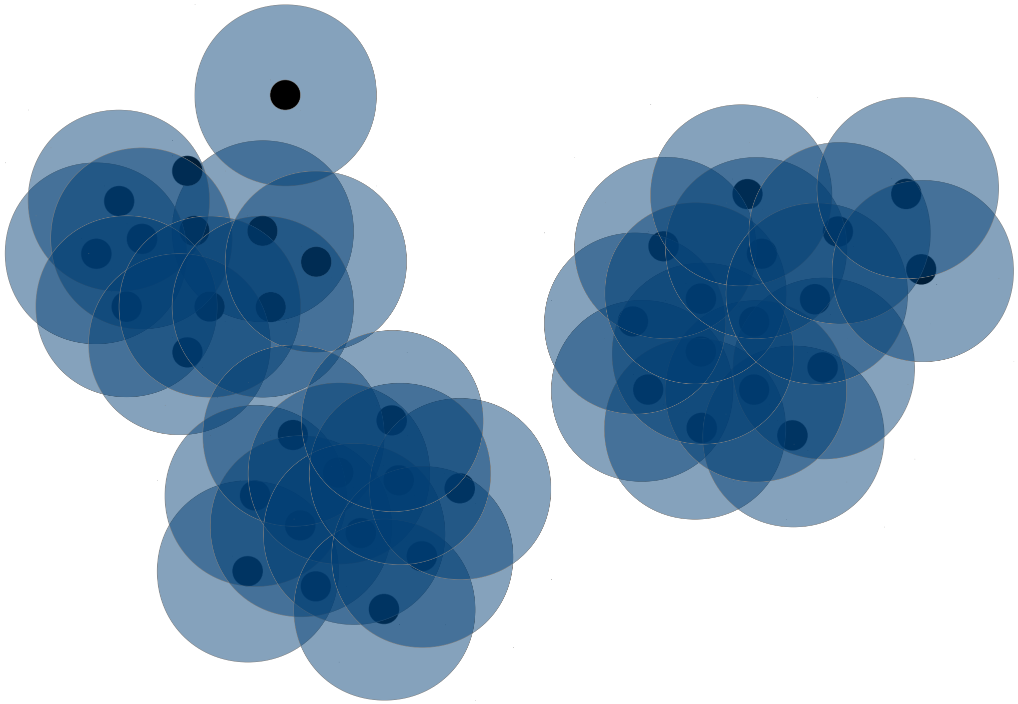
Clustering Algorithms: DBSCAN

Density:

Init:

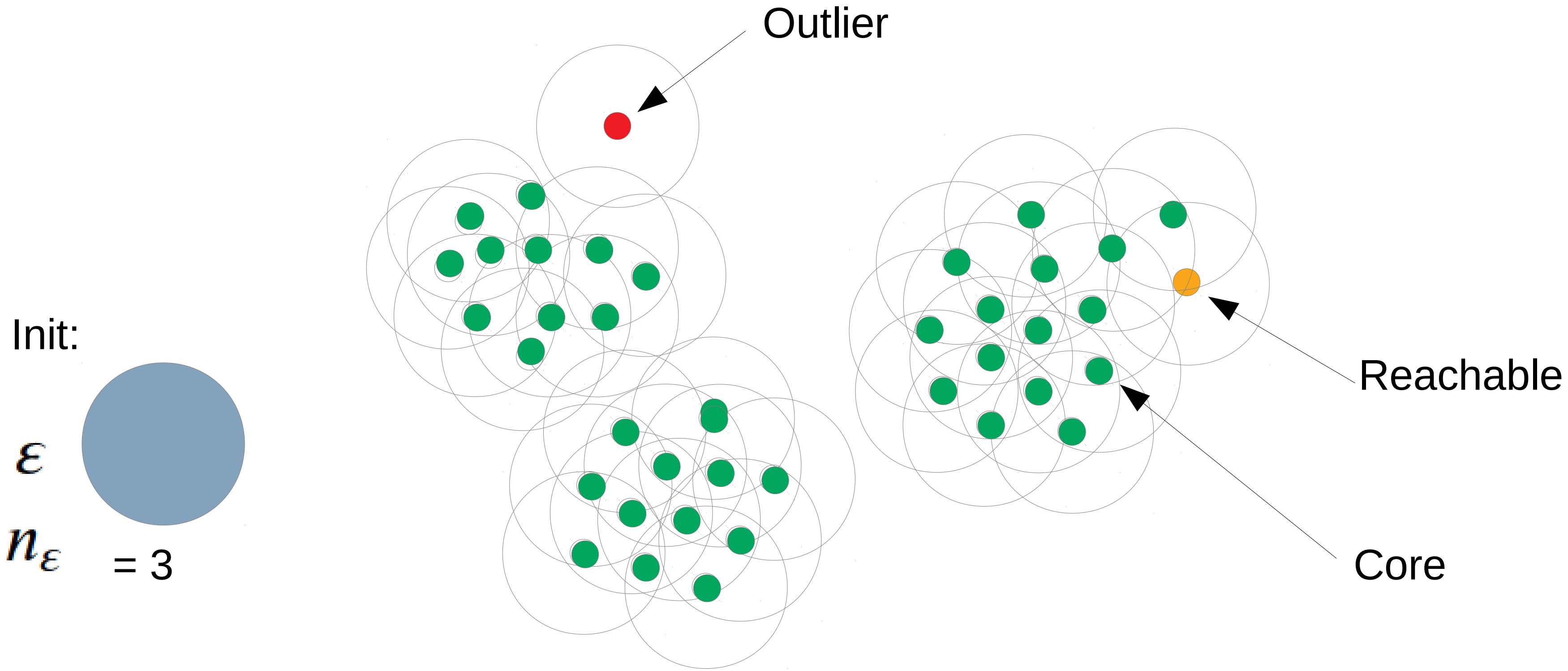
ε 

n_ε = 3



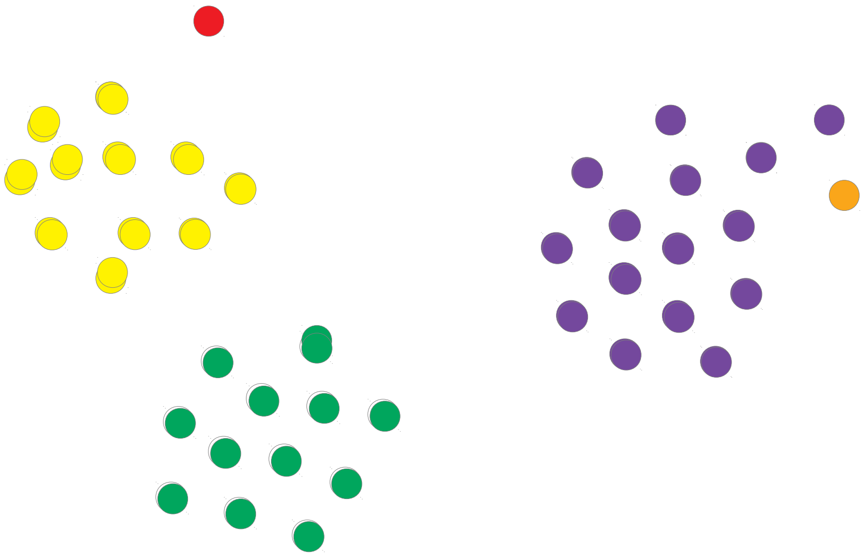
Clustering Algorithms: DBSCAN

Core – Reachable - Outlier:



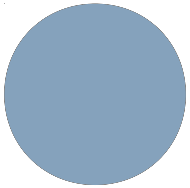
Clustering Algorithms: DBSCAN

Merge:



Init:

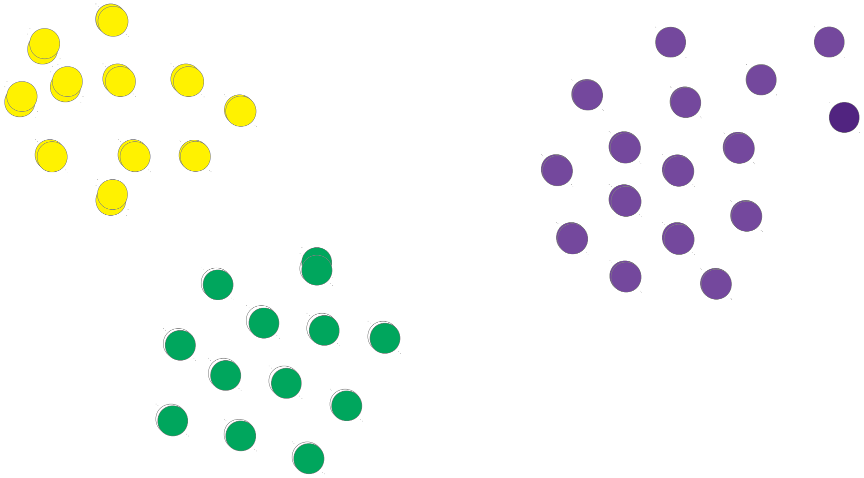
ε



$n_\varepsilon = 3$

Clustering Algorithms: DBSCAN

Final:



Clustering Algorithms: DBSCAN

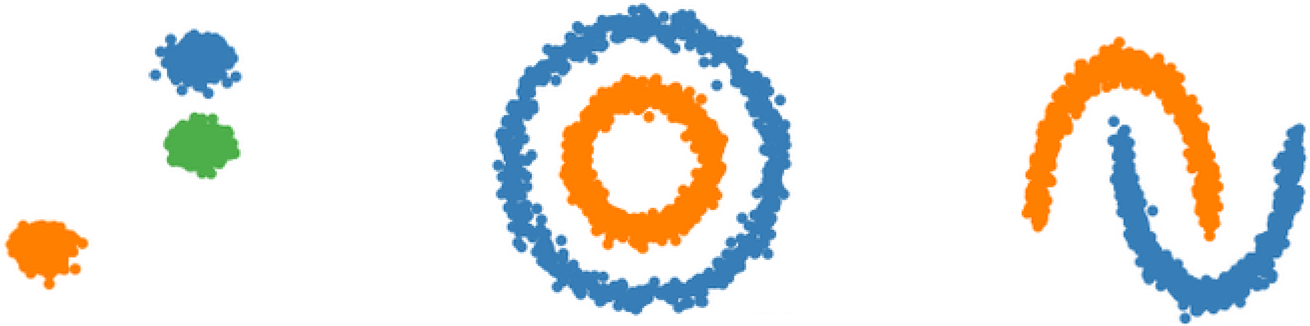
Evaluation:

- Very common Clustering Algorithm
- Advantages:
  - Does not need number of clusters
  - Works well for non convex clusters
  - Fast implementation possible (R-Trees)

- Disadvantages
  - Has two hyper-parameters to optimize
  - Fails on data with high variance in density
  - Not deterministic

Clustering Algorithms: DBSCAN

Evaluation:



More practical examples in the Lab session….

Clustering Algorithms: Evaluation

How to evaluate clustering:

- Visually → use dimension reduction techniques to visualize 2d or 3d

Clustering Algorithms: Evaluation

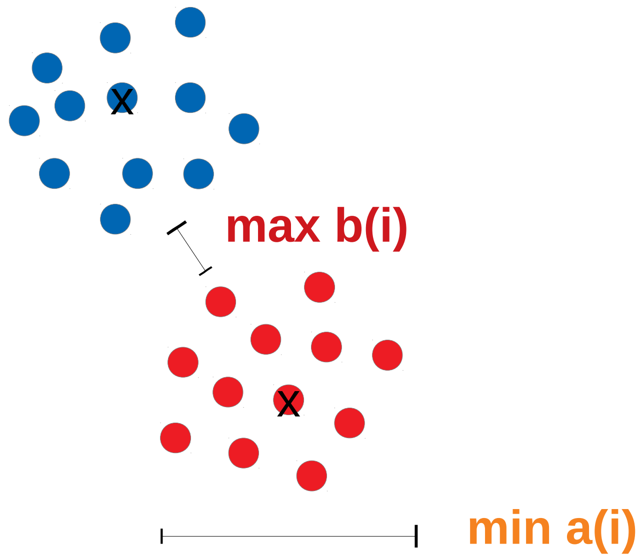
How to evaluate clustering:

- Visually → use dimension reduction techniques to visualize 2d or 3d
- **Quantitative quality measures (what is a good cluster?)**
  - **Low intra cluster variance**

$$a(i) = \frac{1}{|C_i| - 1} \sum_{j \in C_i, i \neq j} d(i,j)$$

  - **High extra cluster variance**

$$b(i) = \min_{i \neq j} \frac{1}{|C_j|} \sum_{j \in C_j} d(i,j)$$



For each data point $i \in C_i$ (data point i in the cluster C_i)

Clustering Algorithms: Evaluation

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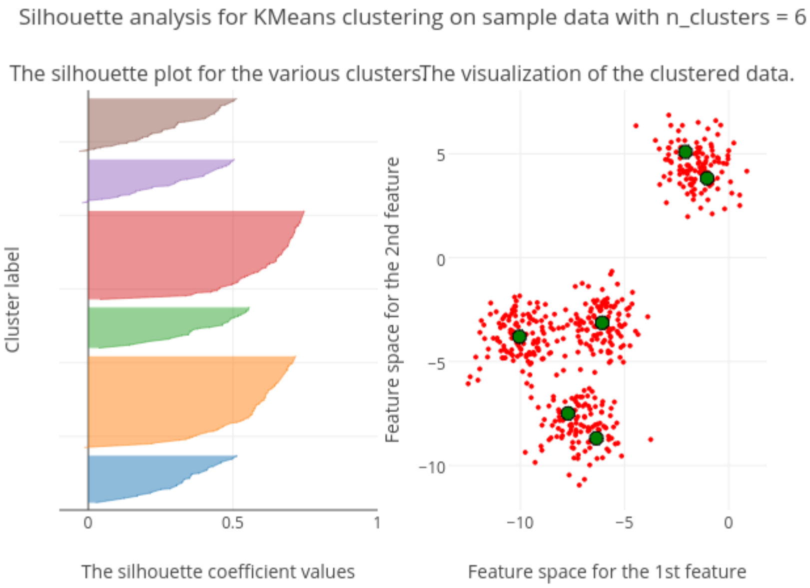
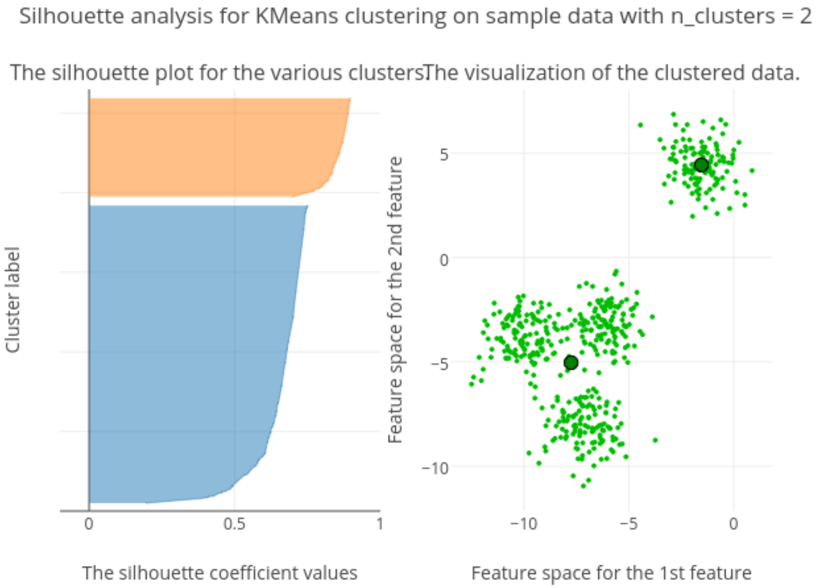
Silhouette Diagrams: finding the best number of clusters





[plots: https://plot.ly/scikit-learn/plot-kmeans-silhouette-analysis/]

Discussion

There are many more Clustering algorithms available…

… → lab session.