MÁSTER EN DATA SCIENCE

Clustering

Machine Learning I

Felipe Alonso-Atienza

Universidad Rey Juan Carlos

About me

- Senior Expert Data Scientist @BBVA
  - Scientific Committee
  - AM-GW: portfolio optimization
  - PDF parsing
  - Churn and sales prediction
  - (Robust) customer segmentation

- (Part-time) Associate professor at @ETSIT-URJC
  - Statistical signal processing and machine learning with application to cardiac electrophysiology

Machine learning taxonomy

- Supervised Learning (labeled data)
  - Classification and Regression
- Unsupervised Learning (unlabeled data)
  - Dimensionality reduction: PCA, SVD, …
  - Mani-fold learning: isomap, t-sne, u-map, embedding using autoencoders, …
  - Clustering: K-means, hierarchical, mixture of gaussians, DBSCAN, HDBSCAN, spectral …
- Reinforcement Learning

Other taxonomies

- Parametric vs non-parametric
  - Logistic regression vs KNN classifier
  - Scalability vs flexibility

- Discriminative vs generative
  - Logistic regression vs Naïve Bayes
  - Discriminant border vs pdf fitting
  - p(y|x) vs p(y,x)

Outline

1. What is clustering?
2. K-means
3. Hierarchical
4. DBSCAN
5. Mixture of gaussians
6. Spectral Clustering

What's clustering

- Grouping unlabeled examples
  - It is the task of partitioning the dataset into groups, called **clusters**
  - Points within a single cluster are very similar and points in different clusters are different
  - Clustering algorithms assign (or predict) a number to each data point, indicating which cluster a particular point belongs to

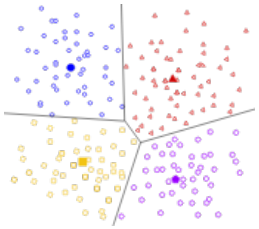
Uses of Clustering

- Market segmentation
- Group items by some features: docs, pictures, music, search results
- Anomaly detection
- Infer missing data
- Data compression
- Privacy: userID vs clusterID

Types of Clustering

- For an exhaustive list, see this paper.

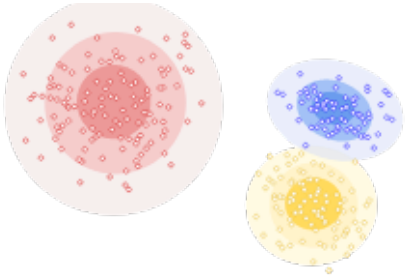
1. Centroid-based: k-means



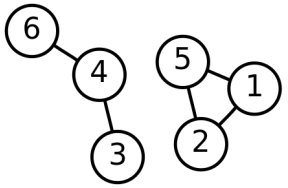
2. Connectivity-based: hierarchical

3. Density-based: DBSCAN

4. Distribution-based: mixture of gaussians



5. Graph-based: spectral clustering



Outline

1. What is clustering?
2. K-means
3. Hierarchical
4. DBSCAN
5. Mixture of gaussians
6. Spectral Clustering

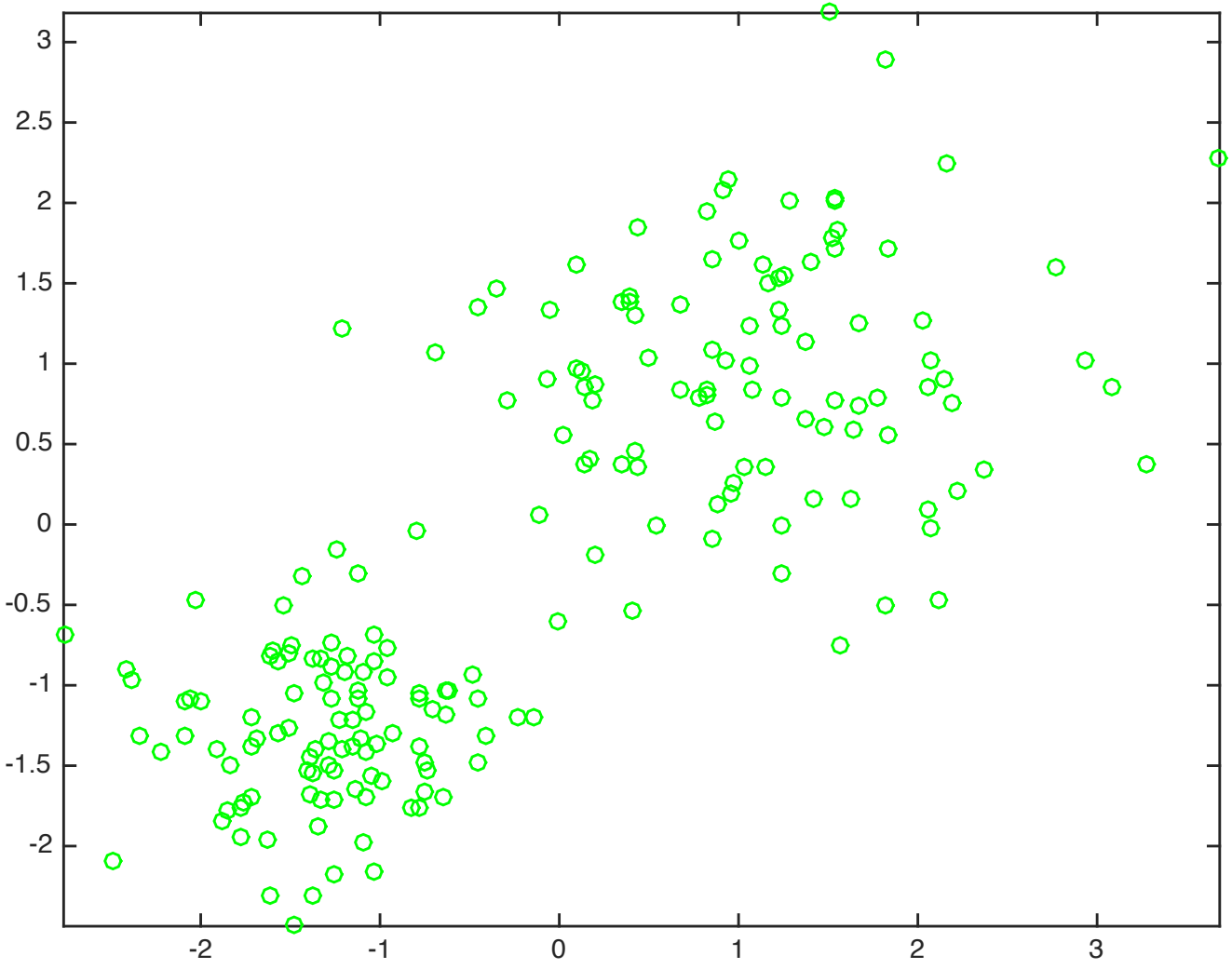
K-means

- One of the simplest and most commonly used clustering algorithms

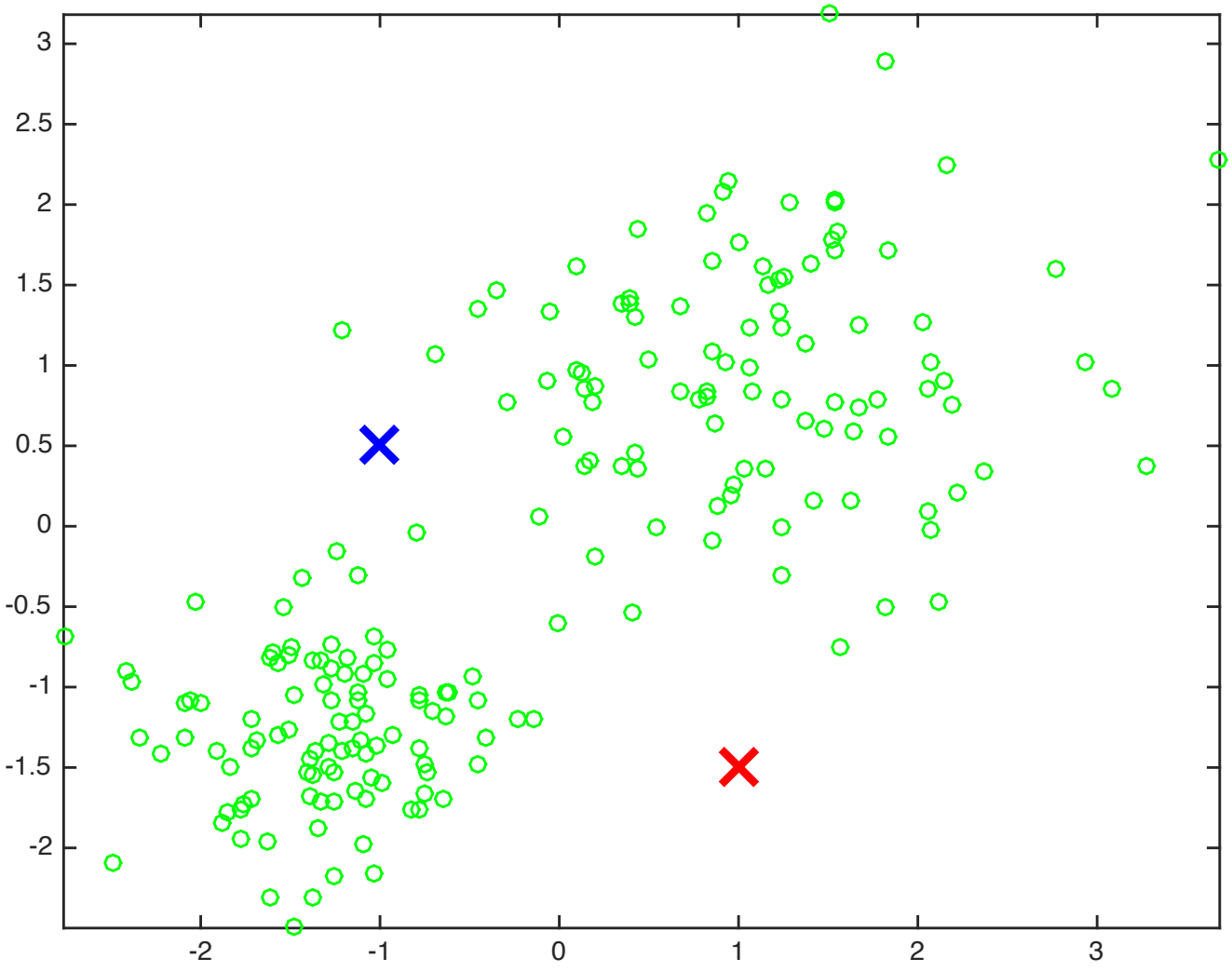
- The algorithm alternates between two steps:
  1. Assigning each data point to the closest cluster center, and then
  2. Setting each cluster center as the mean of the data points that are assigned to it.

- The algorithm is finished when the assignment of instances to clusters no longer changes

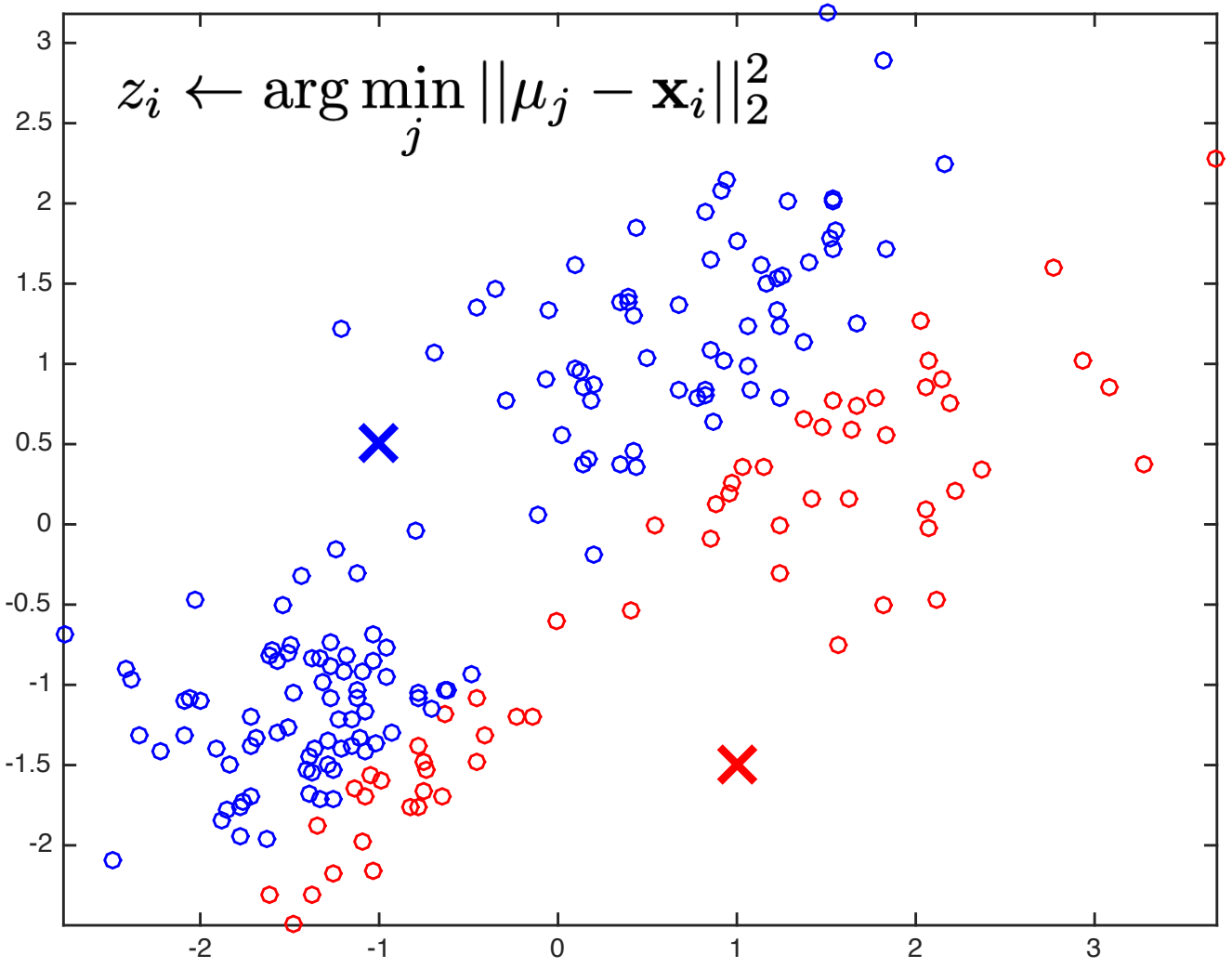
K-means



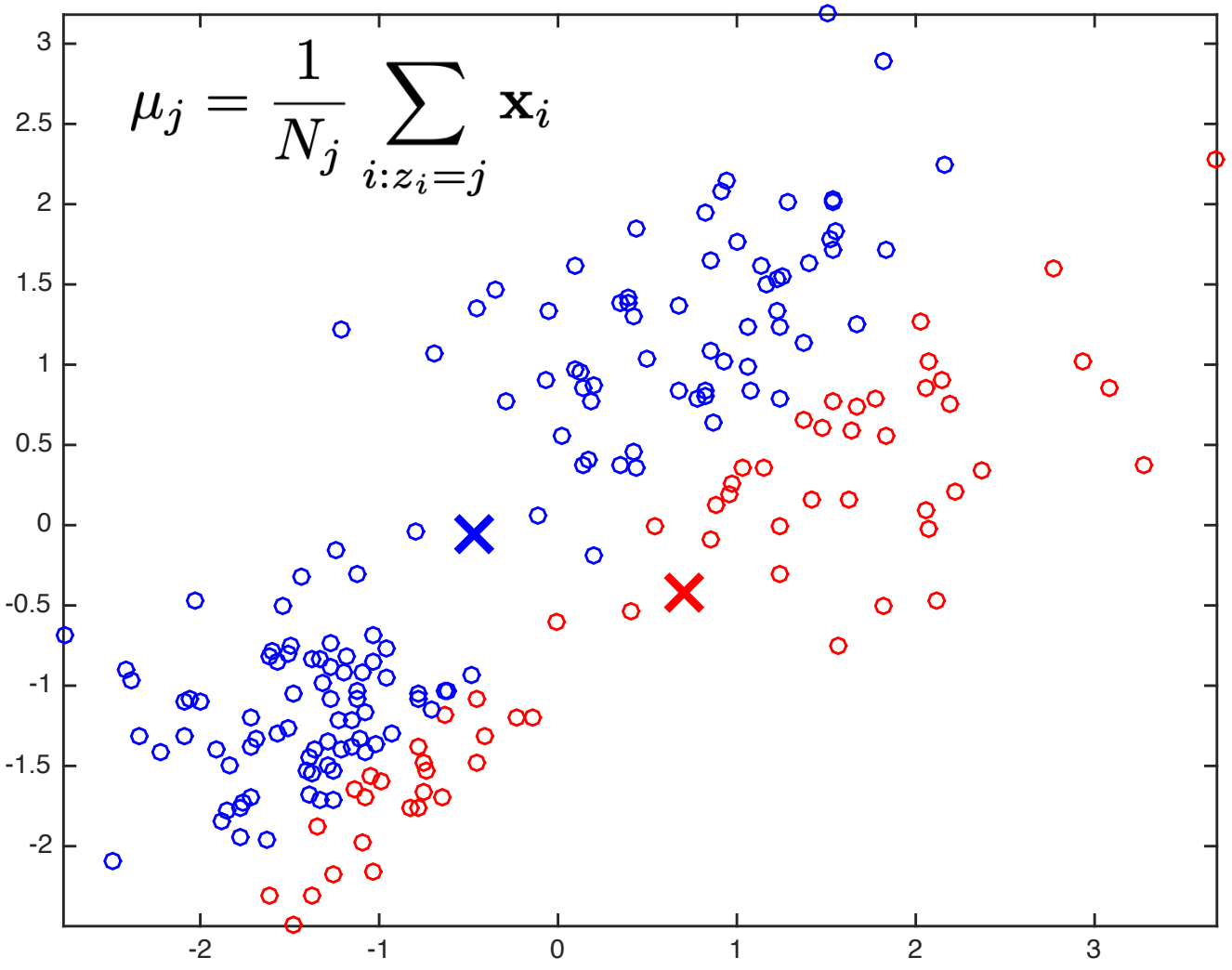
K-means: initialize cluster centers μ_k



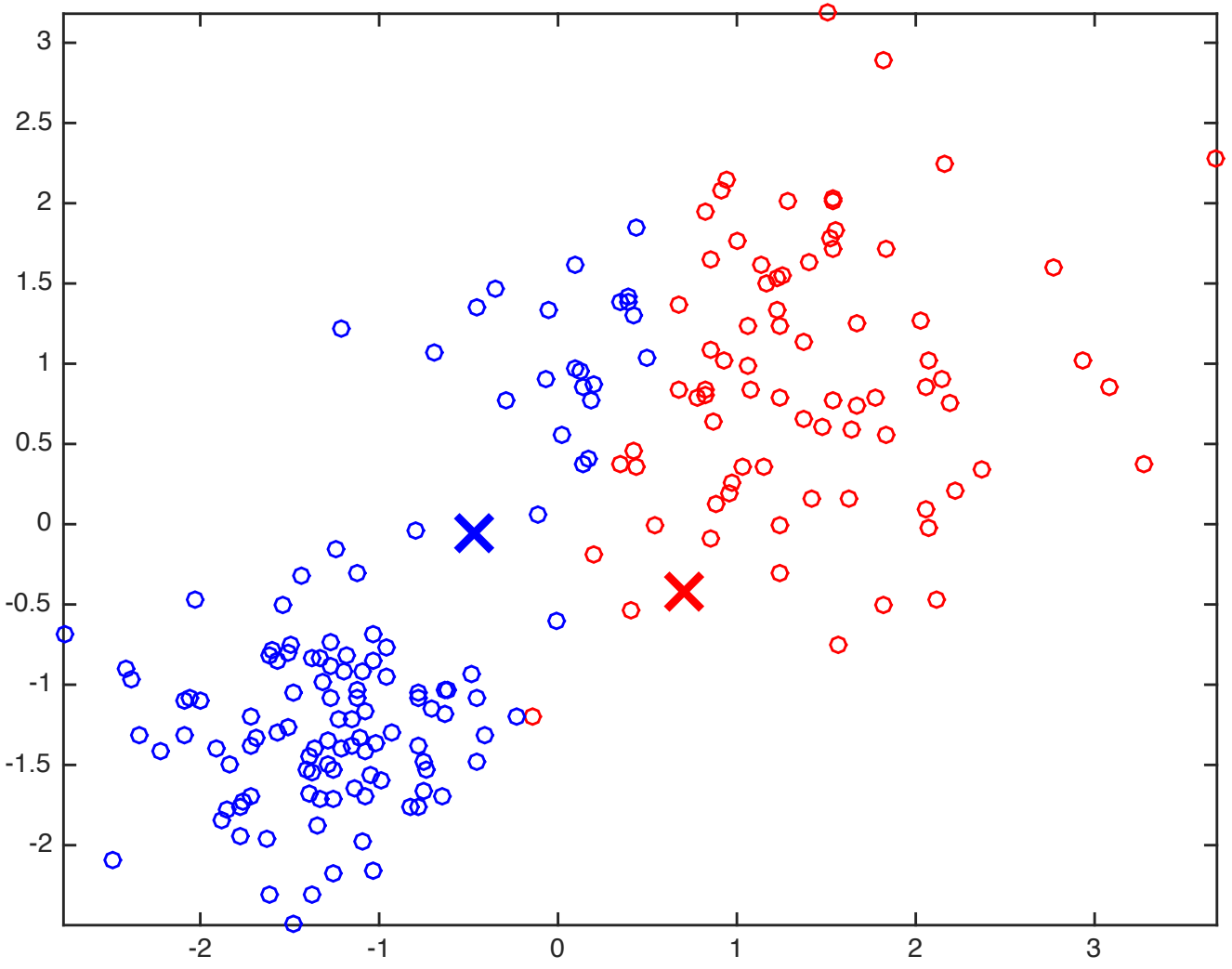
K-means: assign observations to cluster center



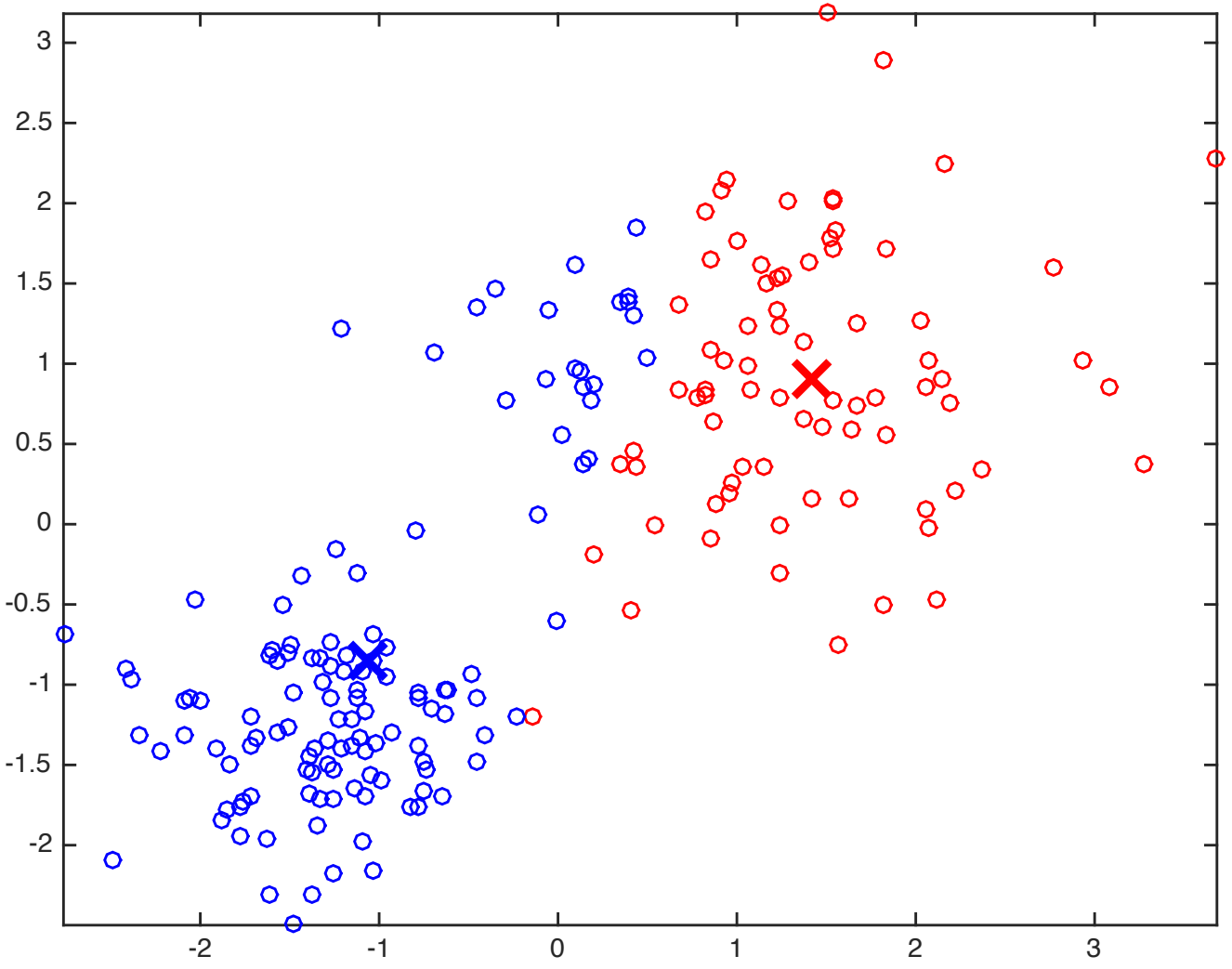
K-means: recompute centroids



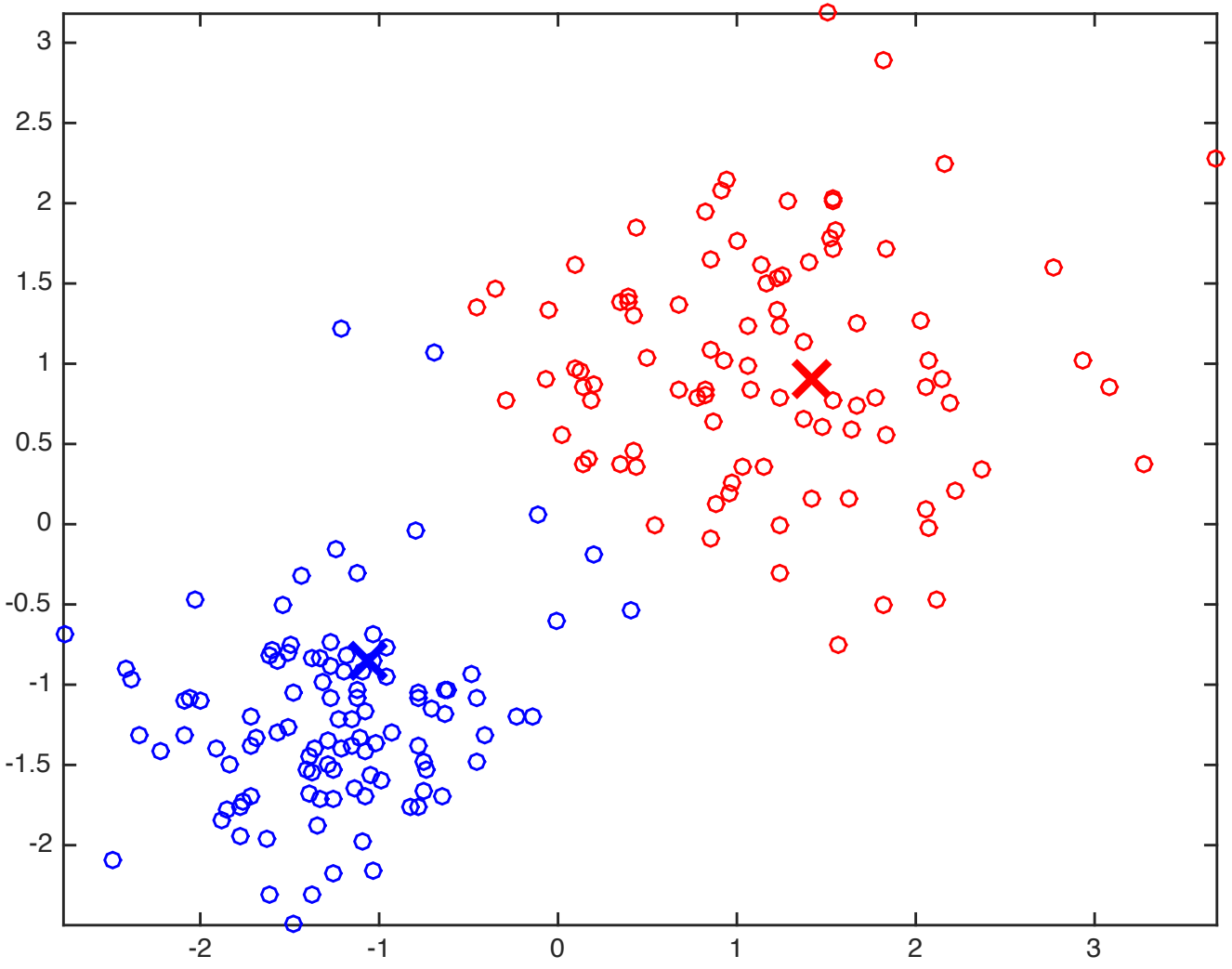
K-means: assign observations to cluster center



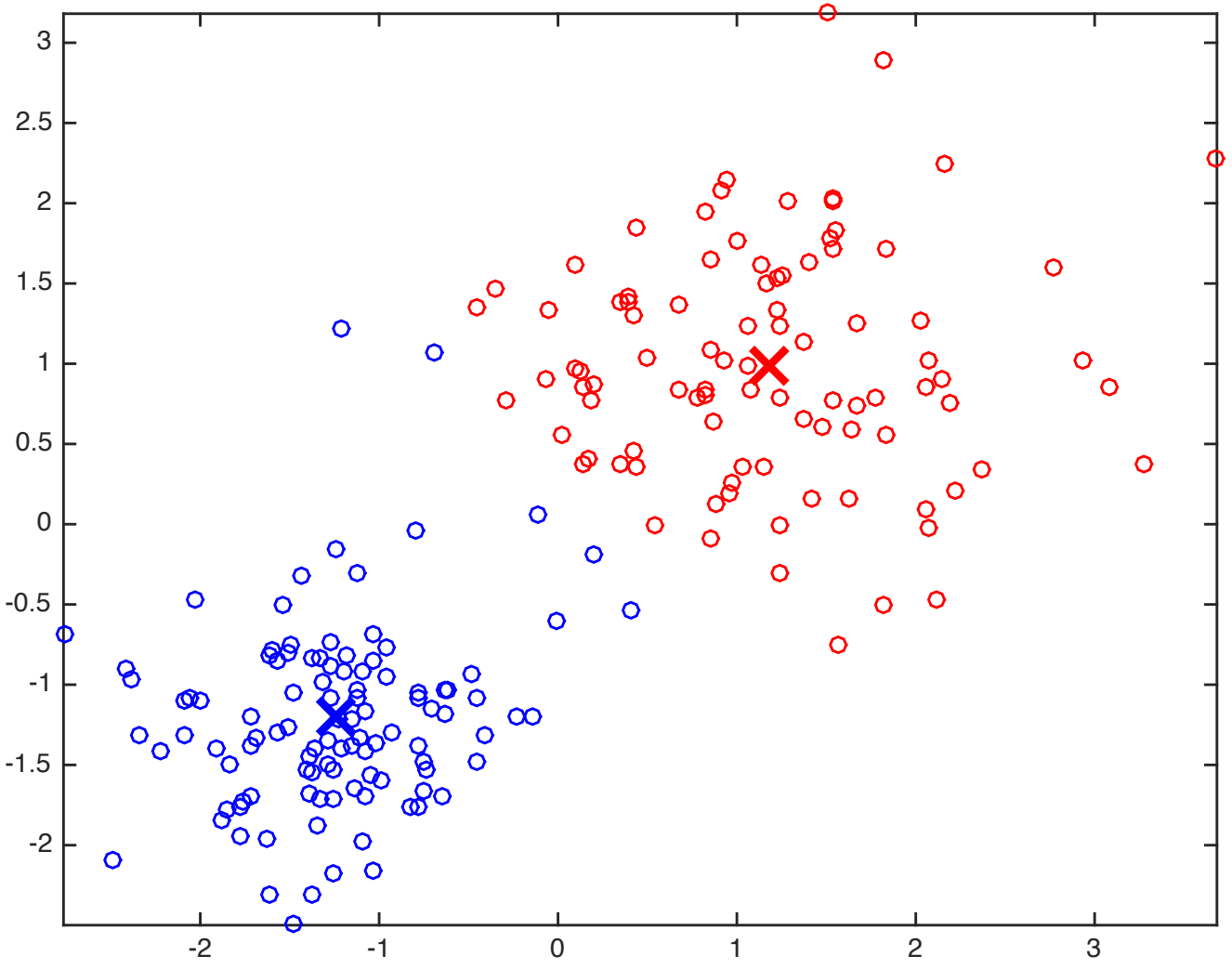
K-means: recompute centroids



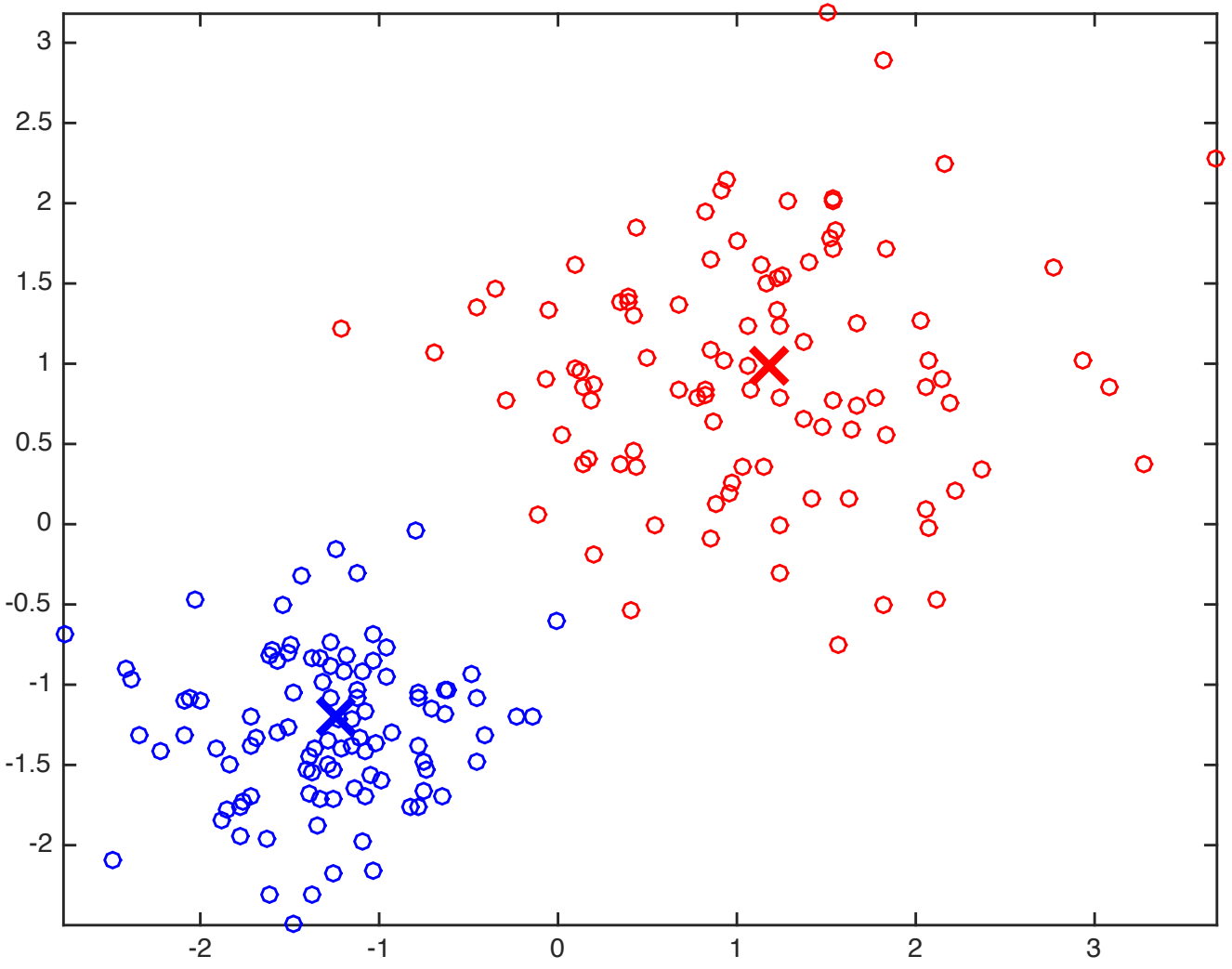
K-means: assign observations to cluster center



K-means: recompute centroids



K-means: assign observations to cluster center



K-means in action

https://github.com/FelipeURJC/clustering

K-means recap

- OKs
  - Simple and scalable (large data sets)
  - Adapts to new examples (predict)

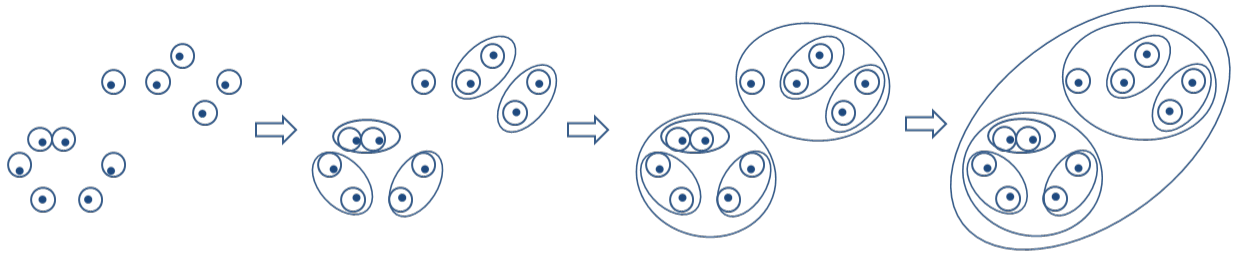
- KOs:
  - Choosing k manually.
  - Highly dependent on the initialization of the centroids
    - Computation is often done several times, with different initializations
    - K-means++
  - Scaling with number of dimensions: as the number of dimensions increases, a distance-based similarity measure converges to a constant value between any given examples.
  - Centroids can be dragged by outliers

Outline

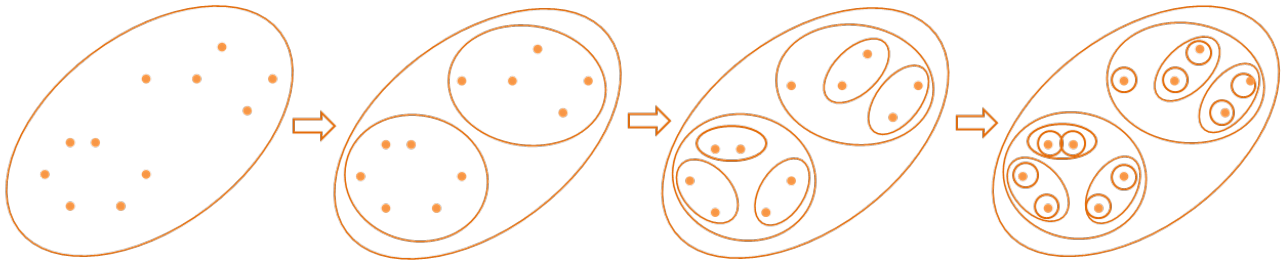
1. What is clustering?
2. K-means
3. **Hierarchical**
4. DBSCAN
5. Mixture of gaussians
6. Spectral Clustering

Hierarchical clustering

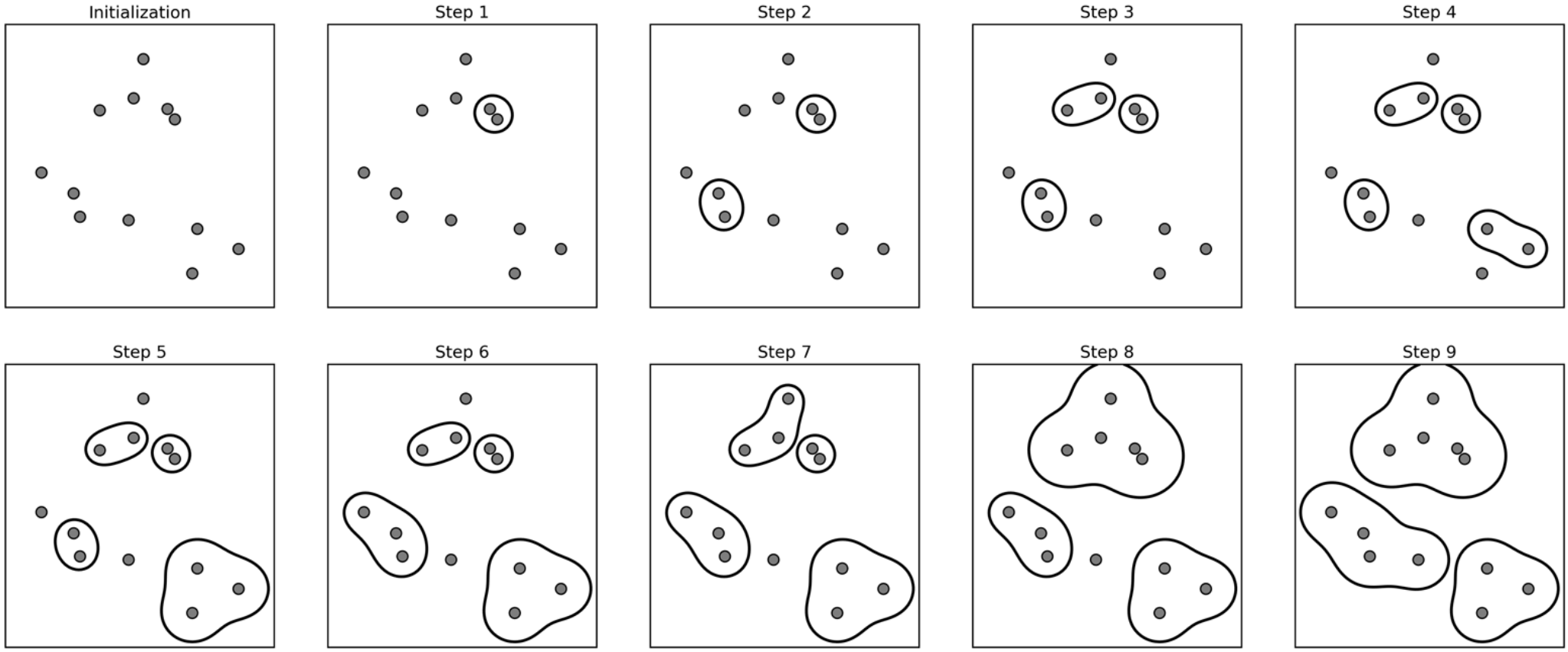
- General family of clustering algorithms that build nested clusters by merging or splitting them successively:
  - Agglomerative (bottom-up): each observation starts in its own cluster, and pairs of **most similar clusters are merged** as one moves up the hierarchy.



  - Divisive (top-down) all observations start in one cluster, and splits are performed recursively as one moves down the hierarchy (not in sklearn)



Agglomerative clustering



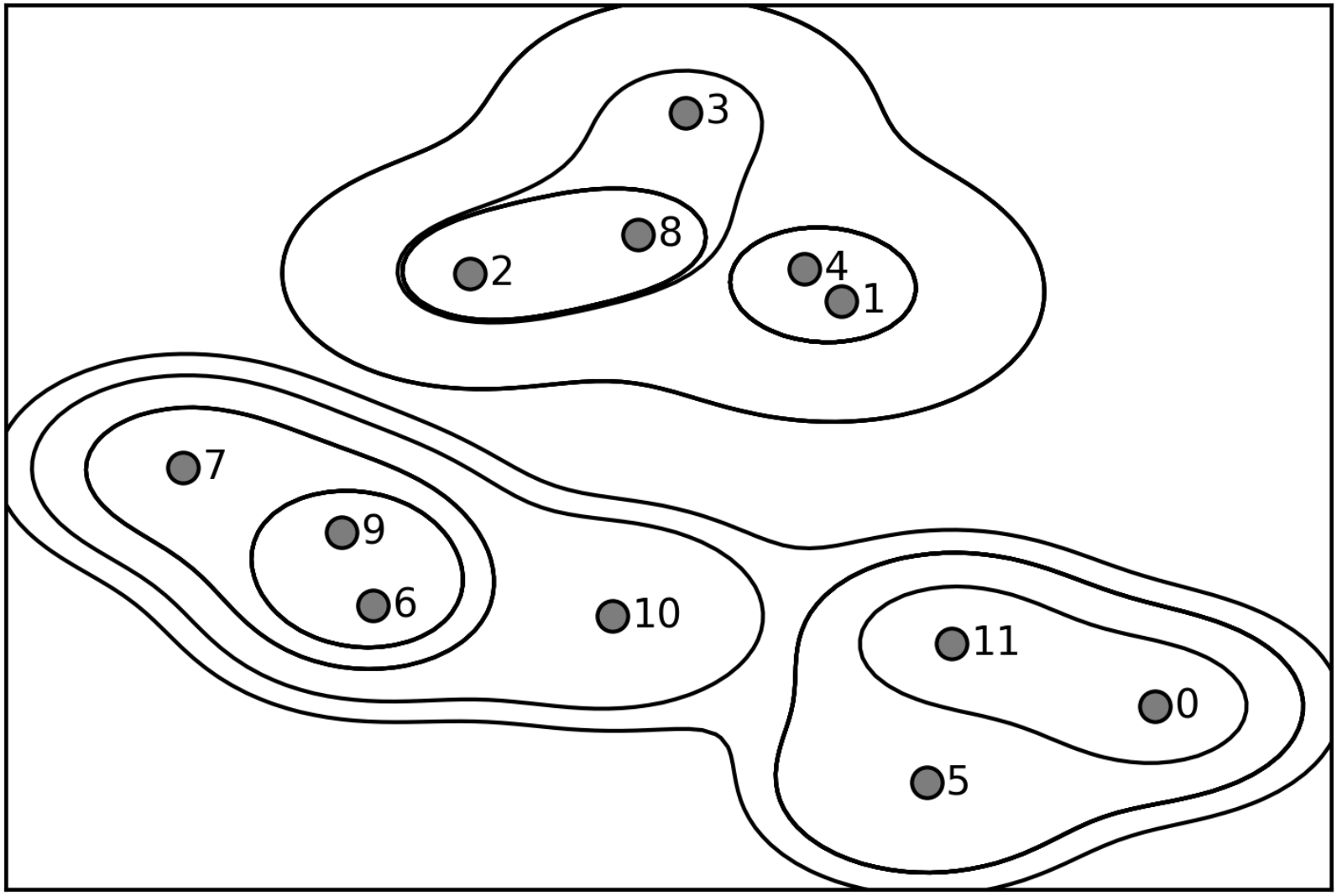
https://github.com/amueller/introduction_to_ml_with_python/blob/master/03-unsupervised-learning.ipynb

Agglomerative clustering

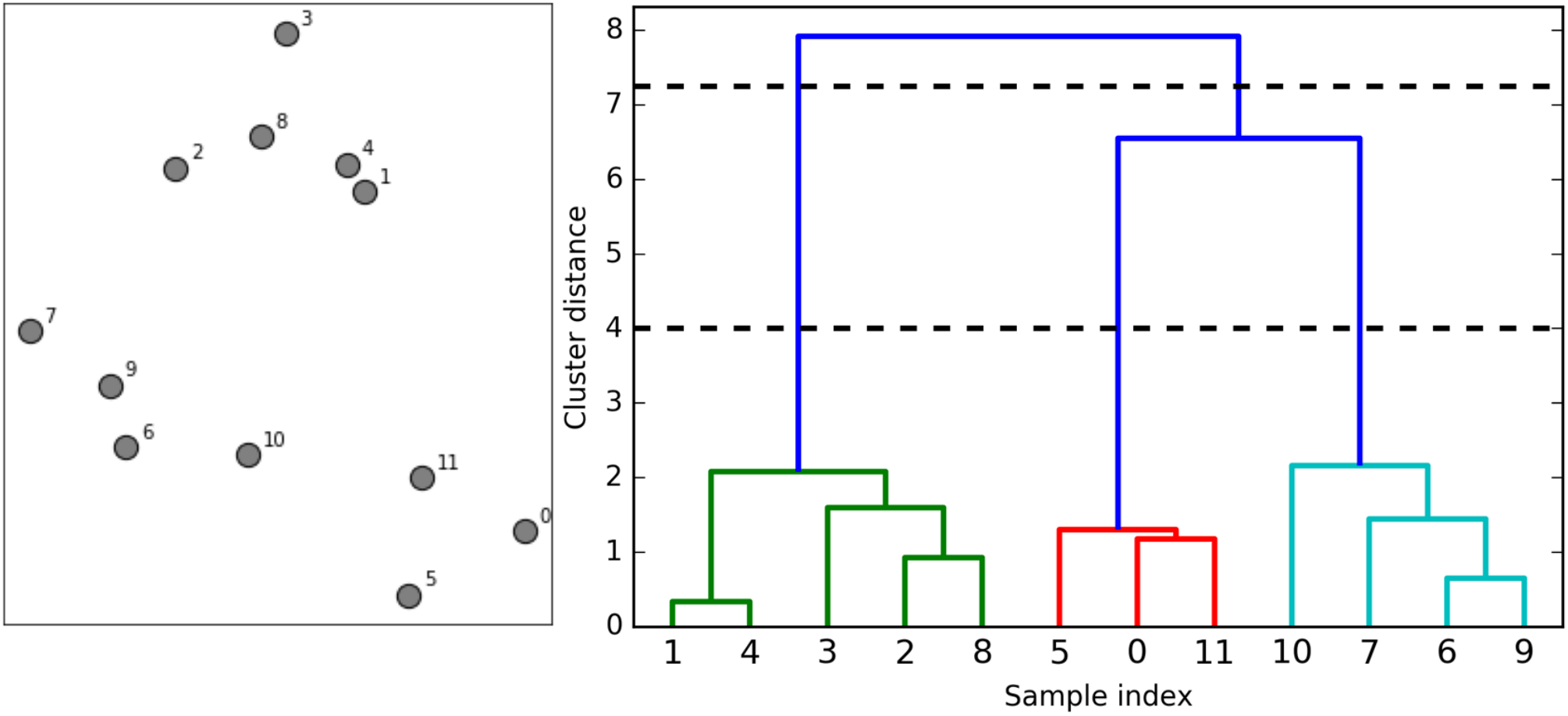
- There are several *linkage criteria* that specify how exactly the "**most similar cluster**" is measured.

- This measure is always defined between two existing clusters. :
  - Ward linkage minimizes the sum of squared differences within all clusters.
  - Maximum or complete linkage minimizes the maximum distance between observations of pairs of clusters.
  - Average linkage minimizes the average of the distances between all observations of pairs of clusters.
  - Single linkage minimizes the distance between the closest observations of pairs of clusters.

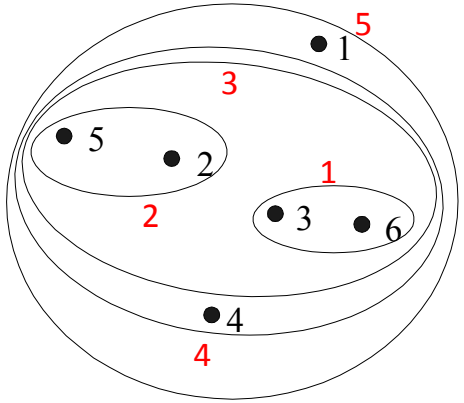
Visualizing agglomerative clustering



Dendrogram

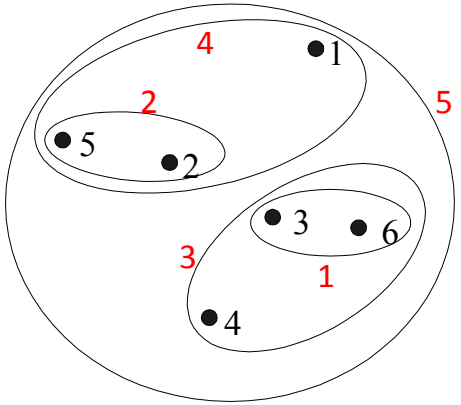

3
8
2
4
1
7
9
6
10
11
0
5
Cluster distance
0
1
2
3
4
5
6
7
8
1 4 3 2 8 5 0 11 10 7 6 9
Sample index

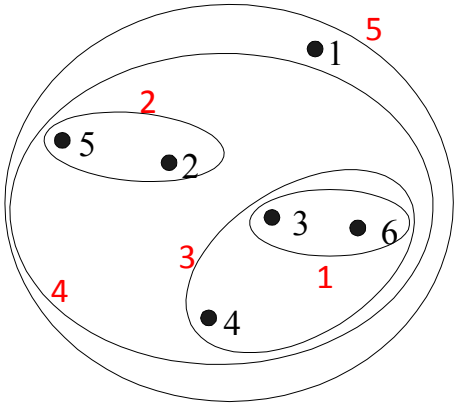
Agglomerative clustering in action



MIN

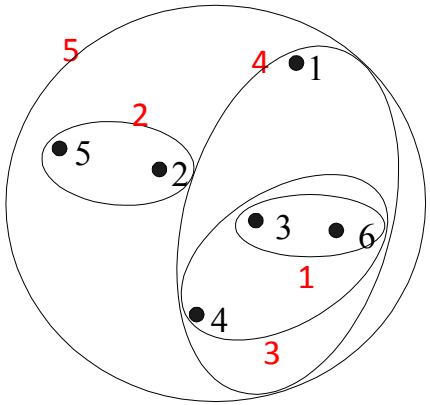
MAX





Group Average

Ward's Method



https://github.com/FelipeURJC/clustering

Agglomerative clustering recap

- OKs
  - Do not have to assume any particular number of clusters
  - They may correspond to meaningful taxonomies (e.g. shopping websites)

- KOs:
  - Does not adapt to new examples (predict)
  - Partitioning rather than clustering the data, and depending on the linkage the following problems might occur:
    - Sensitivity to noise and outliers
    - Difficulty handling different sized clusters and irregular/complex shapes
    - Breaking large clusters

Outline

1. What is clustering?
2. K-means
3. Hierarchical
4. DBSCAN
5. Mixture of gaussians
6. Spectral Clustering

DBSCAN

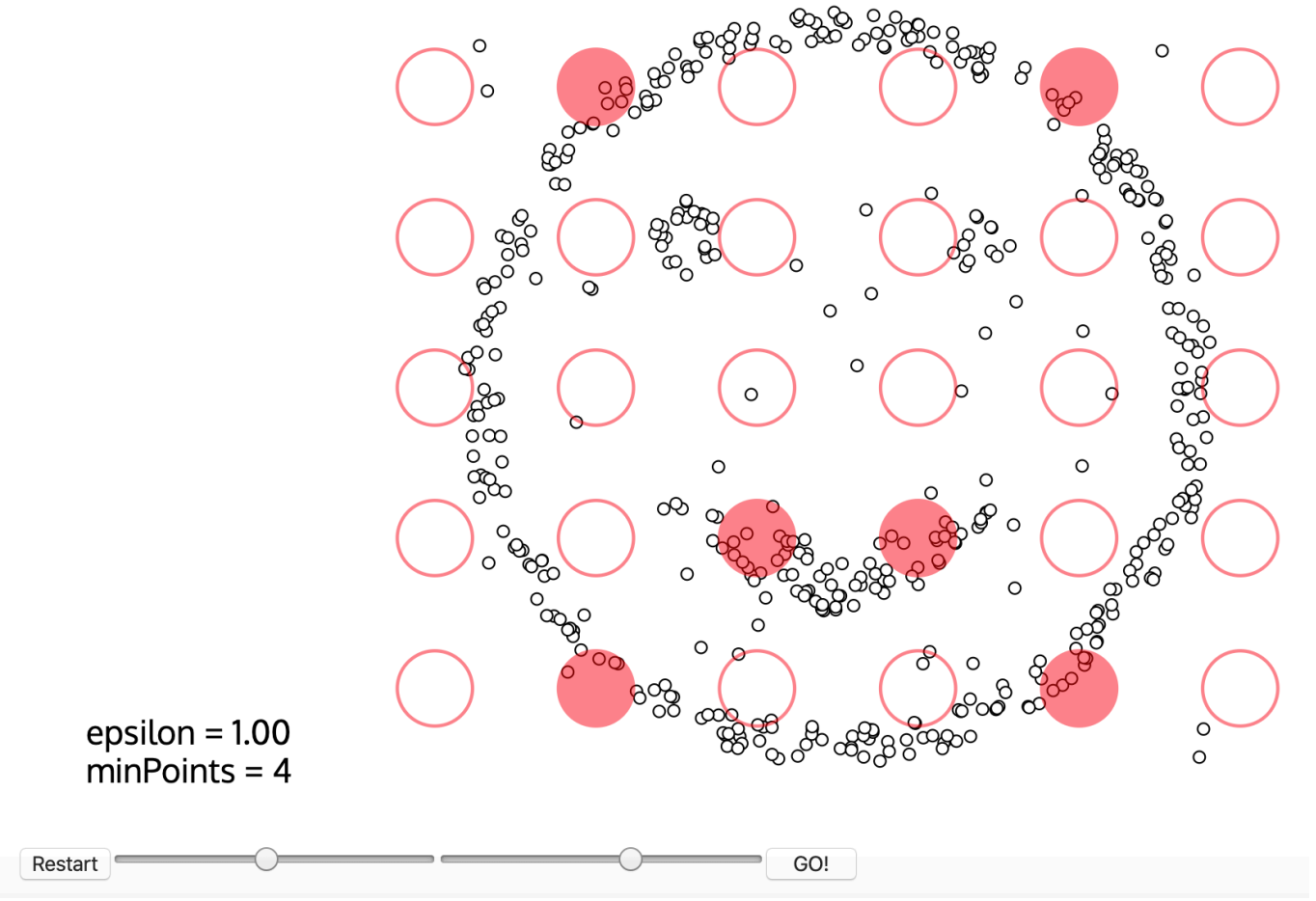
- Stands for "density-based spatial clustering of applications with noise"
- Main features:
  - It does not require the user to set the number of clusters a priori
  - It can capture clusters of complex shapes
  - It can identify points that are not part of any cluster
  - It is somewhat slower than agglomerative clustering and k-means, but still scales to relatively large datasets
- The idea behind DBSCAN is that clusters form dense regions of data, separated by regions that are relatively empty

DBSCAN algorithm

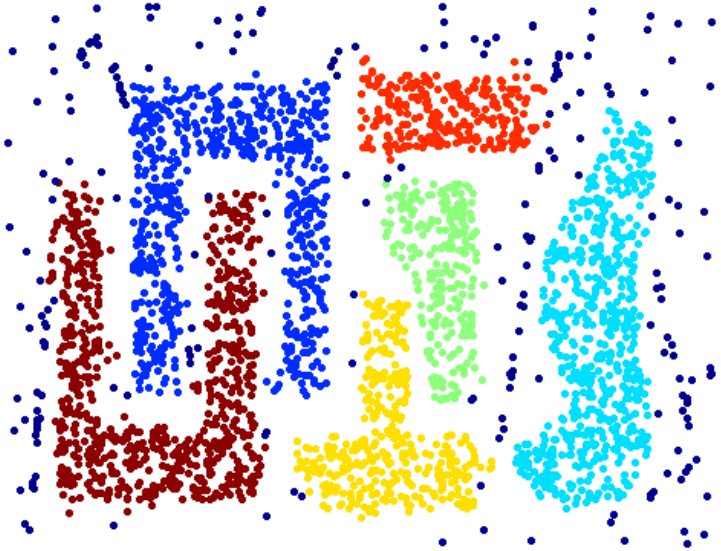
1. The algorithm works by picking an arbitrary point to start with
2. It then finds all points with distance **`eps`** or less from that point
3. If there are less than **`min_samples`** points within distance **`eps`** of the starting point
   - this point is labeled as **`noise`**, meaning that it doesn't belong to any cluster
4. If there are more than **`min_samples`** points within a distance of eps
   - the point is labeled as **`core sample`** and assigned a new cluster label
5. Then, all neighbors (within eps) of the point are visited
6. If they have not been assigned a cluster yet, they are assigned the new cluster label that was just created.
7. If they are **`core samples`**, their neighbors are visited in turn, and so on. The cluster grows until there are no more core samples within distance **`eps`** of the cluster.
8. Then another point that hasn't yet been visited is picked, and the same procedure is repeated.

DBSCAN algorithm

- Better if we visualize how it works



DBSCAN in action



https://github.com/FelipeURJC/clustering

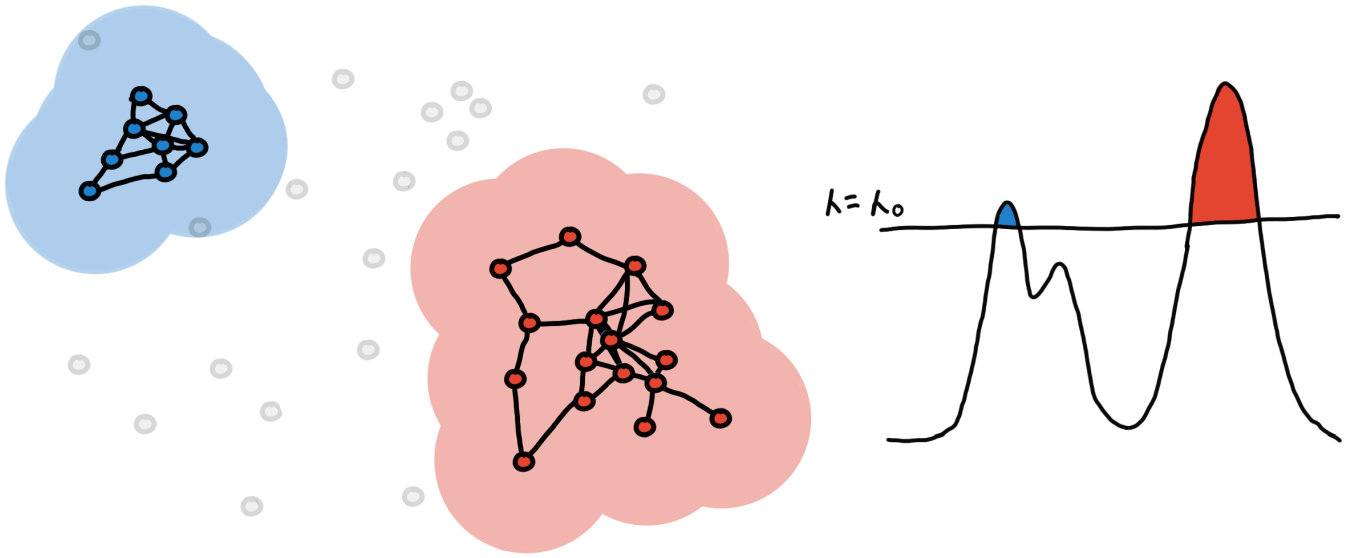
DBSCAN recap

- OKs (already mentioned)
  - Resistant to Noise
  - Can handle clusters of different shapes and sizes

- KOs:
  - Does not adapt to new examples (predict)
  - Cannot handle varying densities
  - Sensitive to parameters: hard to determine the correct set of parameters

Extra: HDBSCAN

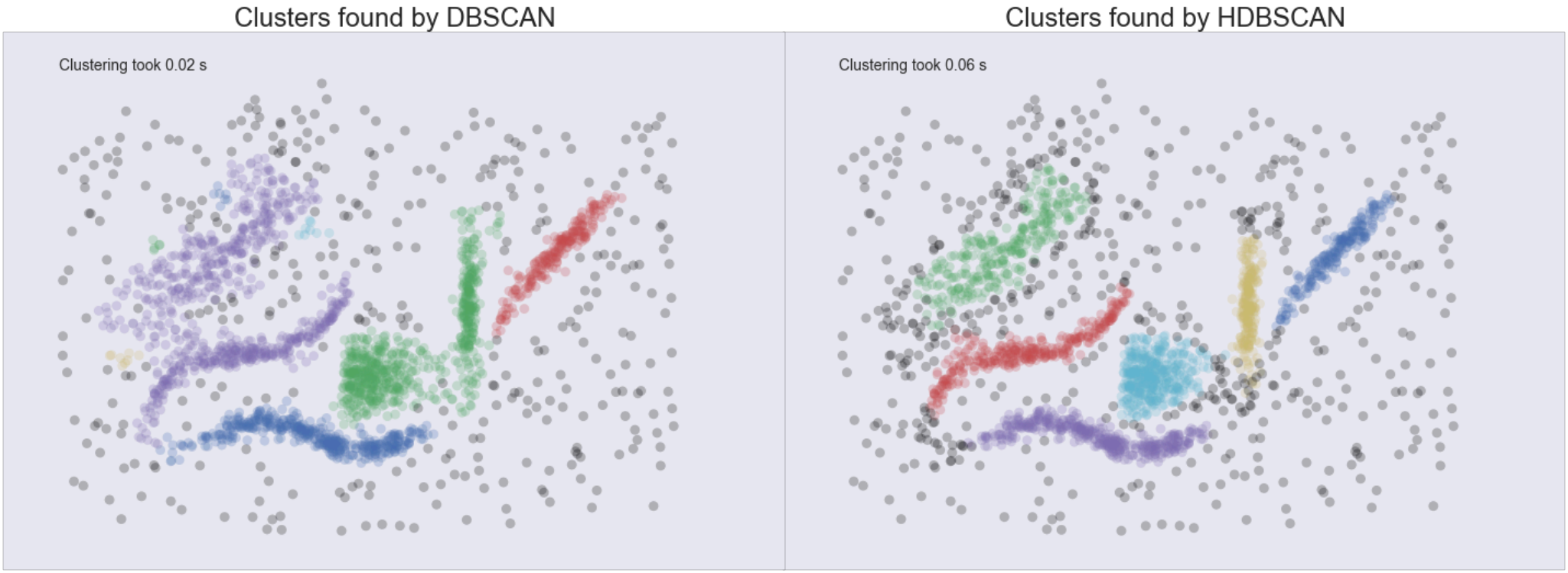
- It stands for Hierarchical DBSCAN
- It looks for regions of the data that are denser than the surrounding space



https://github.com/scikit-learn-contrib/hdbscan

HDBSCAN

- Comparison to DBSCAN



https://nbviewer.jupyter.org/github/scikit-learn-contrib/hdbscan/blob/master/notebooks/Comparing%20Clustering%20Algorithms.ipynb

Outline

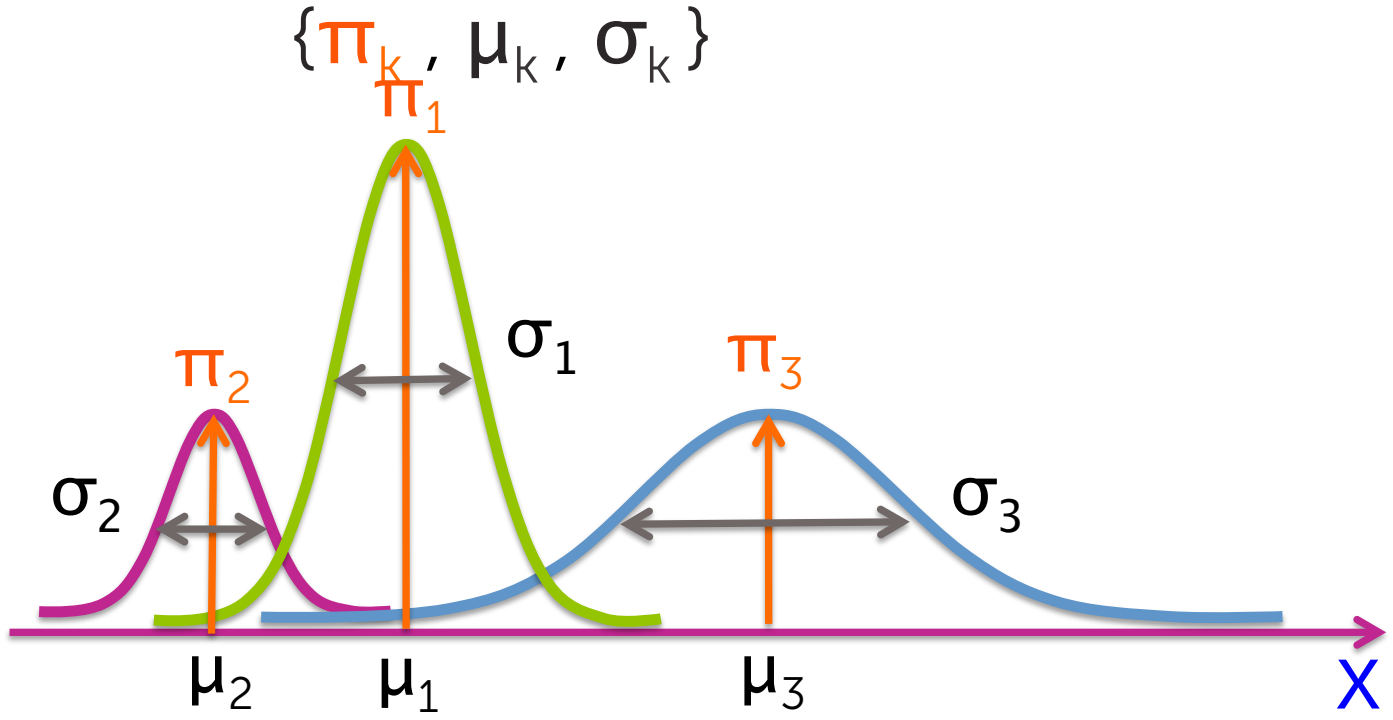
1. What is clustering?
2. K-means
3. Hierarchical
4. DBSCAN
5. Mixture of gaussians
6. Spectral Clustering

Mixture of gaussians

- It is a **probabilistic model**
  - Hard vs. soft clustering
    - Hard clustering: every point belongs to exactly one cluster
    - Soft clustering: **every point belongs to several clusters with certain degrees**
      - e.g. 54% chance document is world news, 45% science, 1% sports, and 0% entertainment
  - Probabilistic clustering
    - Each cluster is mathematically represented by a parametric distribution
    - The entire data set is modeled by a mixture of these distributions

Mixture of gaussians

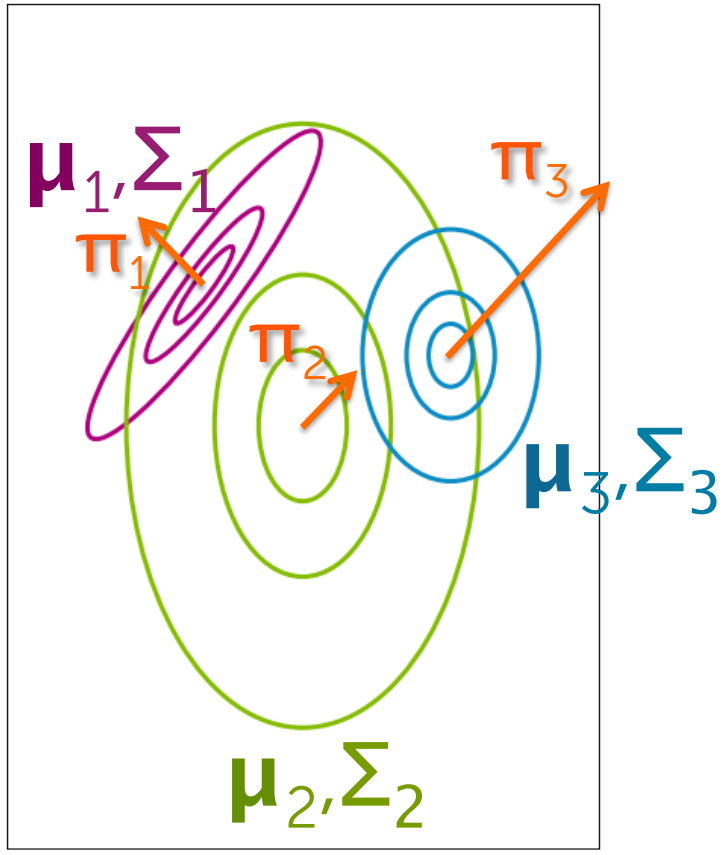
- It is a **probabilistic model** that assumes all the data points are generated from a mixture of a finite number of Gaussian distributions with unknown parameters (need to be estimated)



Mixture of gaussians

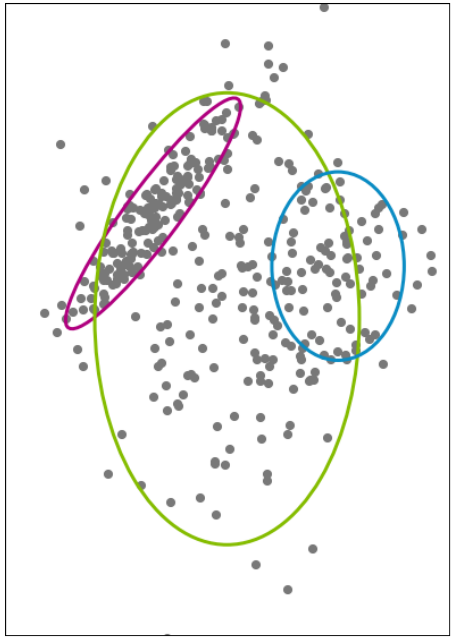
- Each mixture component represents a unique cluster specified by

$$\{\pi_k , \boldsymbol{\mu}_k , \Sigma_k\}$$



Expectation maximization (EM)

- E-step: for given parameter values we can compute the expected values of the **responsibilities**



Responsibility cluster k takes for observation i

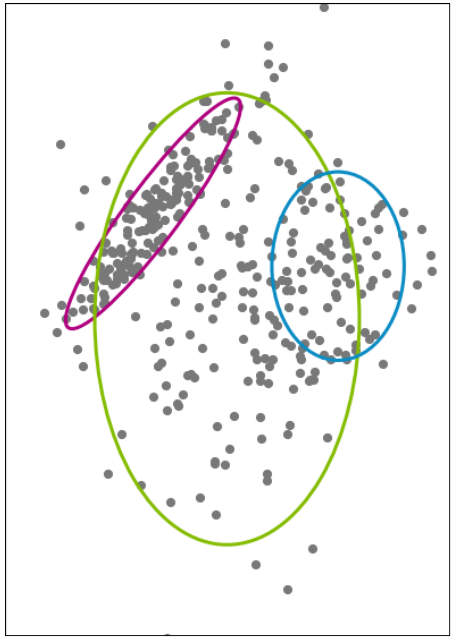
$$r_{ik} = \pi_k \; N(x_i \mid \mu_k, \Sigma_k)$$

Initial probability of being from cluster k

How likely is the observed value $\mathbf{x}_i$ under this cluster assignment?

Expectation maximization (EM)

- E-step: for given parameter values we can compute the expected values of the **responsibilities**



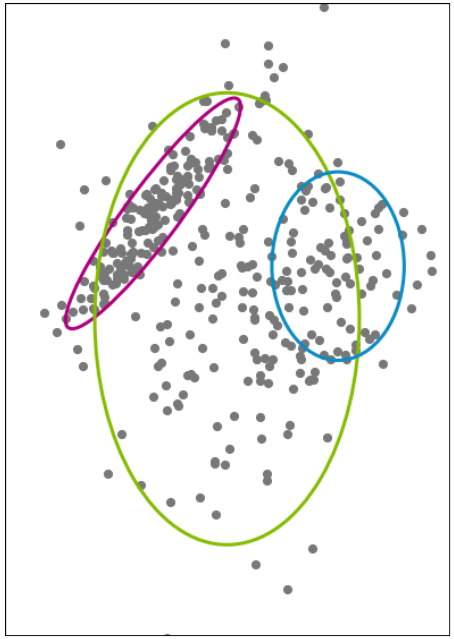
Responsibility cluster k takes for observation i

$$r_{ik} = \frac{\pi_k \; N(x_i \mid \mu_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j N(x_i \mid \mu_j, \Sigma_j)}$$

Normalized over all possible cluster assignments

Expectation maximization (EM)

- M-step: maximize the expected complete log likelihood.
  - Update parameters



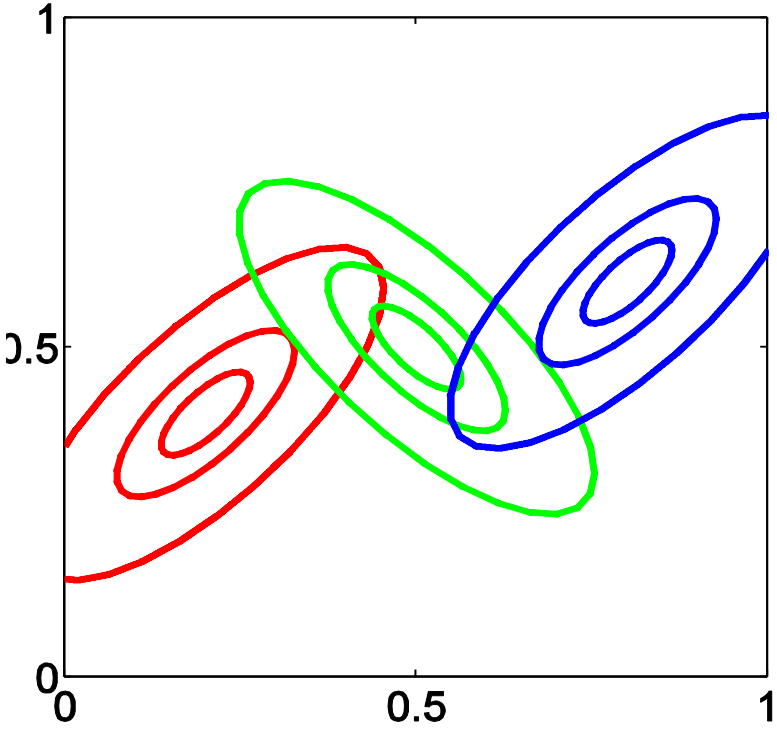
$$\pi_k = \frac{\sum_i r_{ik}}{n} \qquad \mu_k = \frac{\sum_i r_{ik} x_i}{\sum_i r_{ik}}$$

$$\Sigma_k = \frac{\sum_i r_{ik}(x_i - \mu_k)(x_i - \mu_k)^T}{\sum_i r_{ik}}$$

Expectation maximization (EM)

- Iterate E-step and M-step until the log likelihood of data does not increase any more.
  - Converge to local optimal
  - Need to restart algorithm with different initial guess of parameters (as in K-means)

Mixture of gaussians in action



https://github.com/FelipeURJC/clustering

Mixture of gaussians recap

- OKs:
  - Give probabilistic cluster assignments
  - Have probabilistic interpretation
  - Can handle clusters with varying sizes, variance etc.

- KOs:
  - Gaussian distribution assumption
  - log likelihood can have many local minima and multiple restars are required (like k-means)
  - Overfitting issues

Outline

1. What is clustering?
2. K-means
3. Hierarchical
4. DBSCAN
5. Mixture of gaussians
6. Spectral Clustering

Spectral clustering

- Graph-based method that clusters data using eigenvectors (spectral decomposition) of matrices derived from the distance between points

- Similarity graphs: given a set of points X = {x_1, x_2,… , x_n} with pairwise similarities s_{ij} or pairwise distances d_{ij}, transform them into a graph:
  - **Ɛ-neighborhood graph**: we connect all points whose pairwise distances are smaller than Ɛ
  - **K-nn graph**: connect x_i with x_j if x_j is among k-nn of x_i
  - **Fully connected** (or affinity matrix A)

$$s_{ij} = s(x_i, x_j) = A_{ij} = \begin{cases} \exp\left(-||x_i - x_j||^2/2\sigma^2\right), & \text{if } i \neq j \\ 0, & \text{if } i = j \end{cases}$$

Spectral clustering: algorithm

- Graph Laplacian: $L = D - A$
  - *D* diagonal matrix whose (*i*,*i*)-element is the sum of A's *i*-th row

Normalized spectral clustering according to Ng, Jordan, and Weiss (2002)

Input: Similarity matrix $S \in \mathbb{R}^{n \times n}$, number k of clusters to construct.

- Construct a similarity graph by one of the ways described in Section 2. Let W be its weighted adjacency matrix.
- Compute the normalized Laplacian L_{sym}.
- **Compute the first k eigenvectors $u_1, \ldots, u_k$ of L_{sym}.**
- Let $U \in \mathbb{R}^{n \times k}$ be the matrix containing the vectors $u_1, \ldots, u_k$ as columns.
- **Form the matrix $T \in \mathbb{R}^{n \times k}$ from U by normalizing the rows to norm 1,** that is set $t_{ij} = u_{ij} / (\sum_k u_{ik}^2)^{1/2}$.
- For $i = 1, \ldots, n$, let $y_i \in \mathbb{R}^k$ be the vector corresponding to the i-th row of T.
- Cluster the points $(y_i)_{i=1,\ldots,n}$ with the k-means algorithm into clusters $C_1, \ldots, C_k$.

Output: Clusters $A_1, \ldots, A_k$ with $A_i = \{j | \, y_j \in C_i\}$.

https://papers.nips.cc/paper/2092-on-spectral-clustering-analysis-and-an-algorithm.pdf

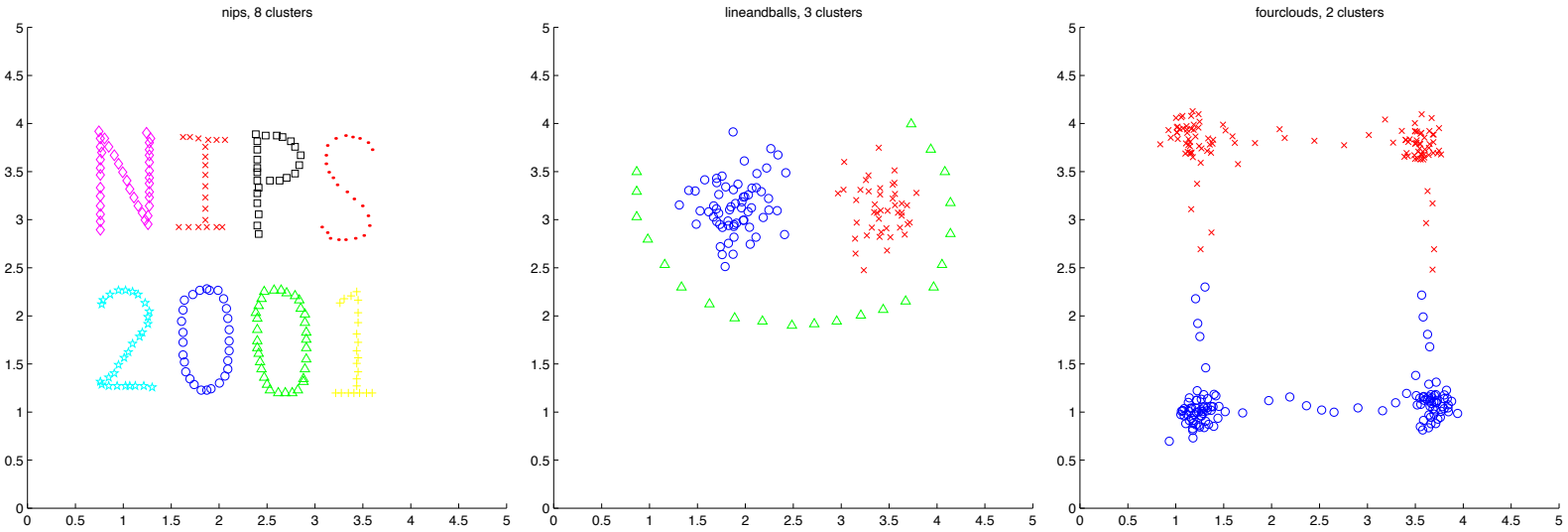
https://citeseerx.ist.psu.edu/viewdoc/download;jsessionid=D95EF48A1E4714D5C6865E945D6E3B57?doi=10.1.1.165.9323&rep=rep1&type=pdf

Spectral clustering: intuition

- **Spectral clustering** avoids the curse of dimensionality by adding a pre-clustering step to your algorithm
  - Curse of dimensionality: as the number of dimensions increases, a distance-based similarity measure converges to a constant value between any given examples

- Other possibilities
  - Reduce the dimensionality of feature data by using PCA
  - Reduce the dimensionality of feature data by using embeddings

Spectral clustering in action



https://github.com/FelipeURJC/clustering

Spectral clustering recap

- OKs:
  - Clustering formulated as a graph cut problem
  - More stable and scalable than K-means (manifold learning)

- KOs:
  - Those inherited from K-means:
    - Number of clusters
    - Noise and outliers

References

- D. Xu, Y. Tian, "A comprenhensive survey of clustering algorithms", Ann. Data. Sci. 2015.
- A. Ng, M. Jordan, and Y. Weiss, "On spectral clustering: Analysis and an algorithm," NIPS-2001
- U. Von Luxburg, "A tutorial on spectral clustering," MPI for Biological Cybernetics, TR-149, 2006.
- A. Müller, S. Guido,"Introduction to machine learning with Python", O'Reilly Media 2016
- AA Patel, "Hands-on unsupervised learning with Python", O'Reilly Media 2019