CIS 635 - Knowledge Discovery & Data Mining

Clustering Algorithms

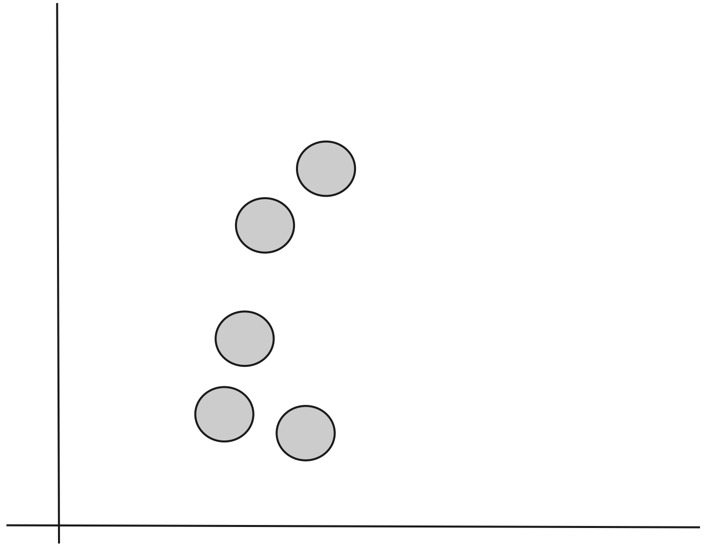
Clustering Algorithms

- **k-means**: Centroid Based
- **Hierarchical clustering**: Distance connectivity based
- **GMM**: Distribution based
- **DBSCAN**: Density Based

k-means Clustering

- Centroid based
- Only works for numeric data only
- Explicit k-centroid inputs (initialization)
- Iterative algorithm

k-means Clustering



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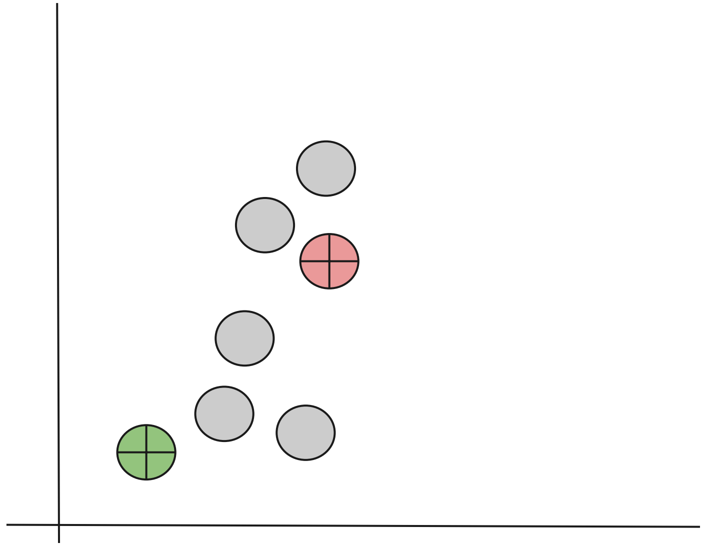
k-means Clustering



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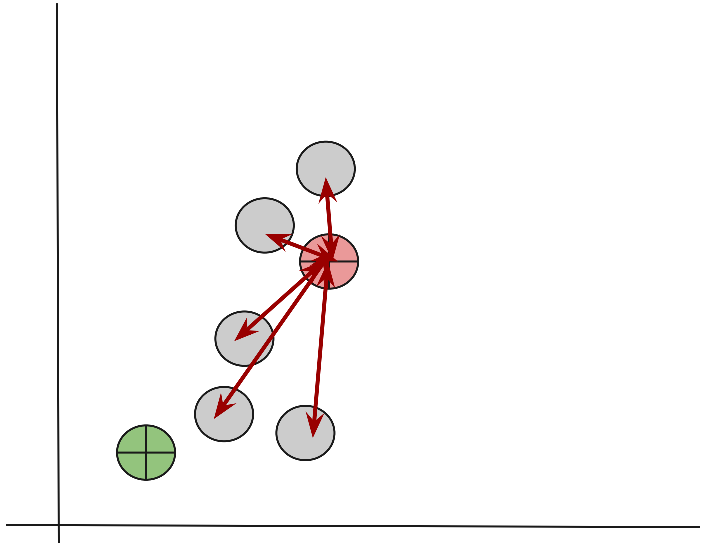
k-means Clustering



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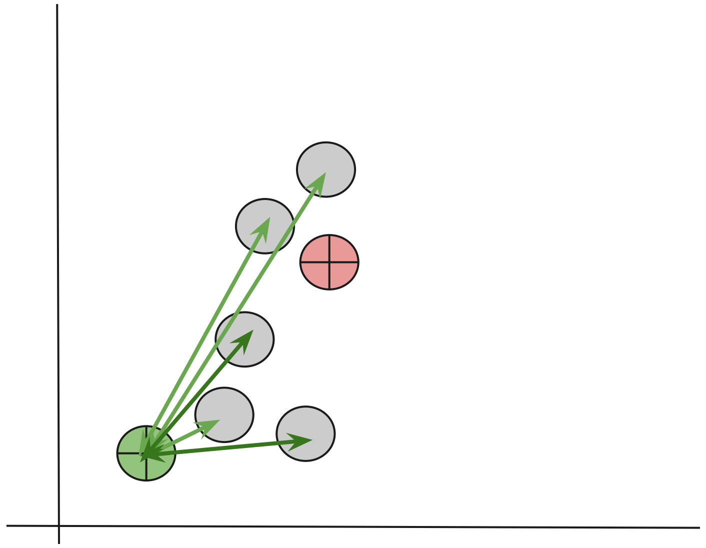
k-means Clustering



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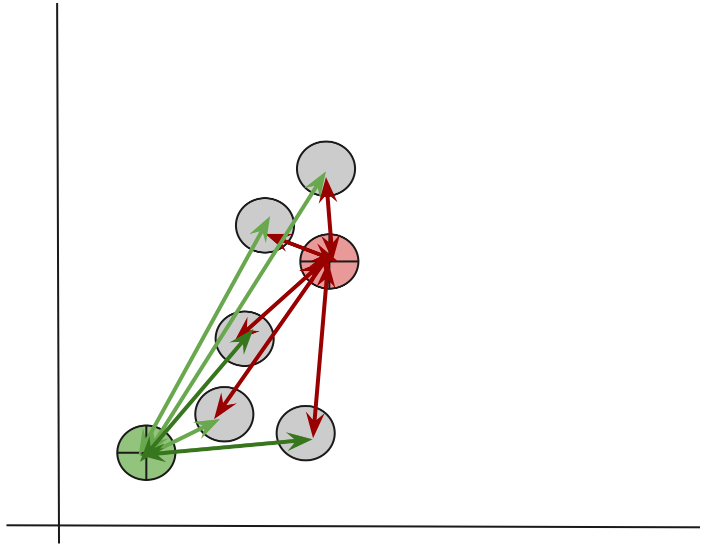

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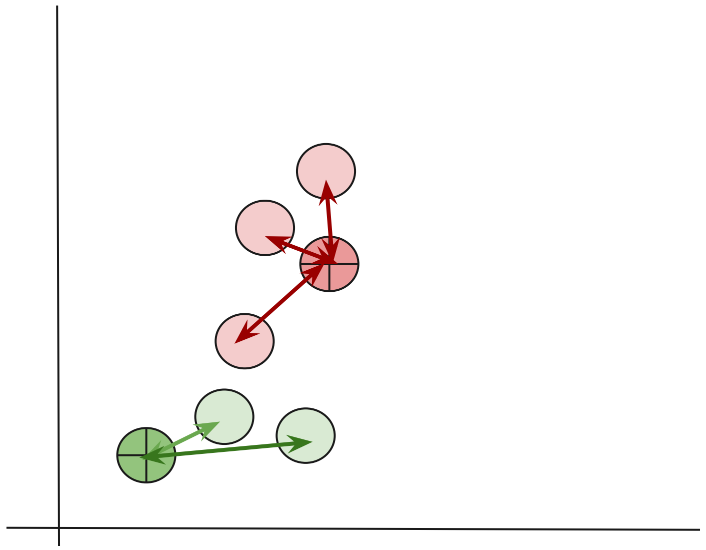

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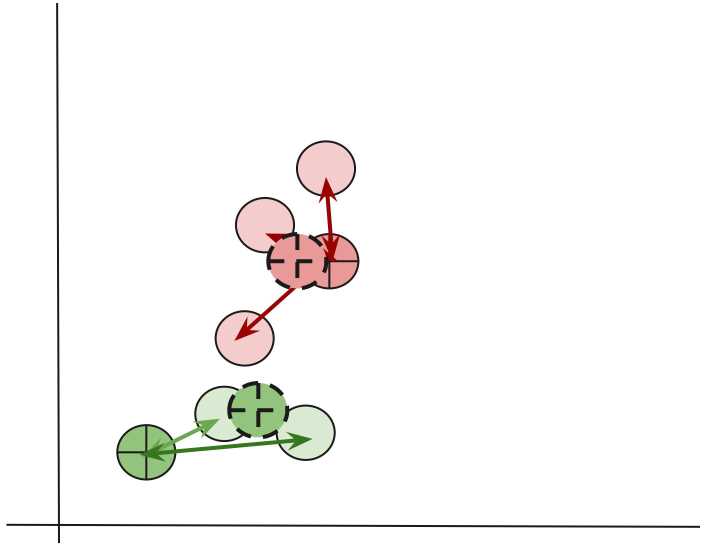
- **Assign cluster labels based on the distances measured.**

k-means Clustering



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- **Update the two means:**
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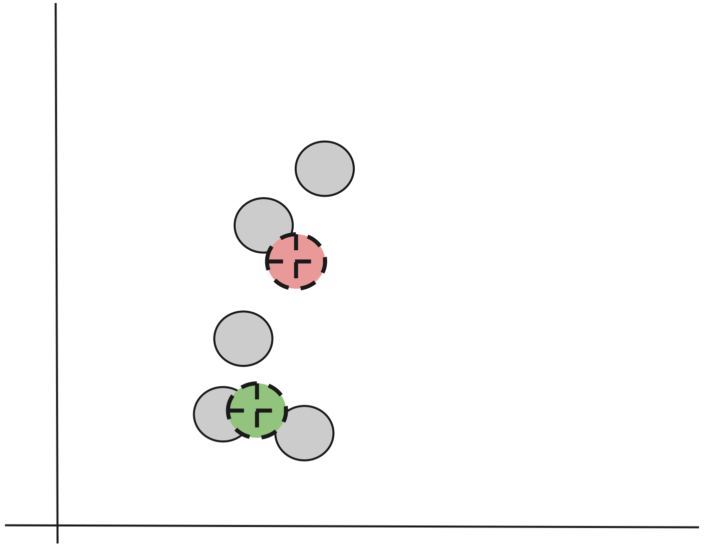
k-means Clustering



- 5 given data points of forms *(x_i, y_i)*: numeric
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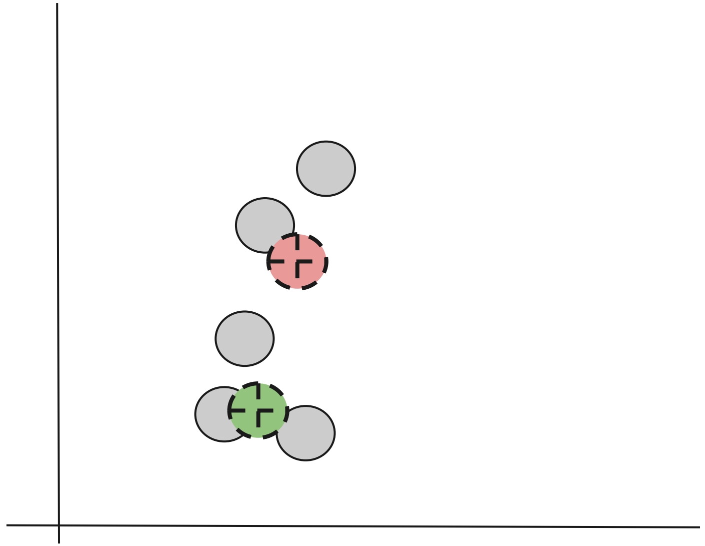
k-means Clustering



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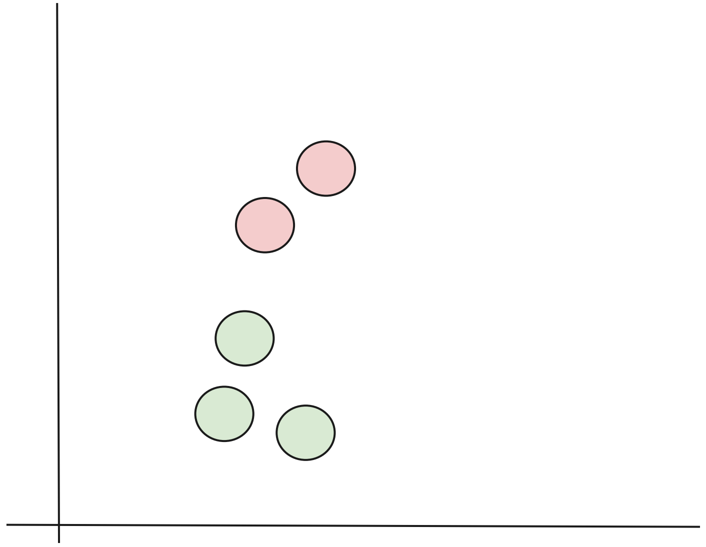
k-means Clustering



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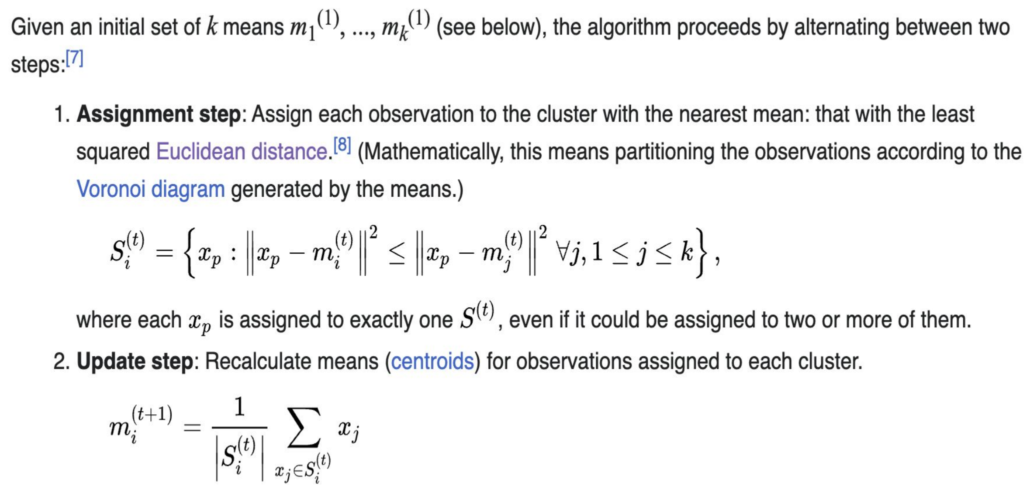
- Iterate until the means *(m_x, m_y)$_j$* don't move; or a predefined number of iterations are run
- **Likely the final cluster configuration**

k-means Clustering



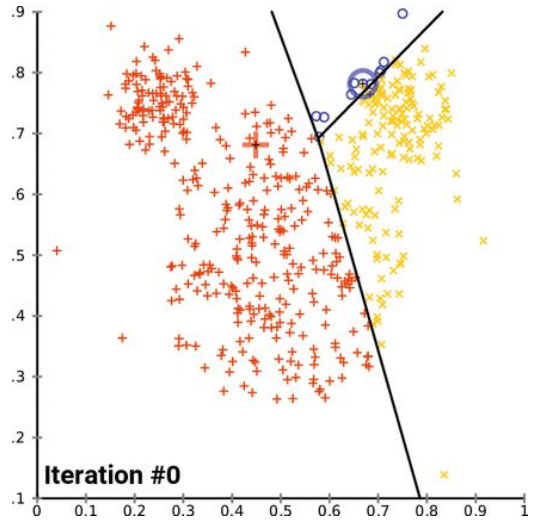
Given an initial set of k means $m_1{}^{(1)}$, ..., $m_k{}^{(1)}$ (see below), the algorithm proceeds by alternating between two steps:[7]

1. **Assignment step**: Assign each observation to the cluster with the nearest mean: that with the least squared Euclidean distance.[8] (Mathematically, this means partitioning the observations according to the Voronoi diagram generated by the means.)

   $$S_i^{(t)} = \left\{ x_p : \left\| x_p - m_i^{(t)} \right\|^2 \le \left\| x_p - m_j^{(t)} \right\|^2 \ \forall j, 1 \le j \le k \right\},$$

   where each x_p is assigned to exactly one $S^{(t)}$, even if it could be assigned to two or more of them.
2. **Update step**: Recalculate means (centroids) for observations assigned to each cluster.

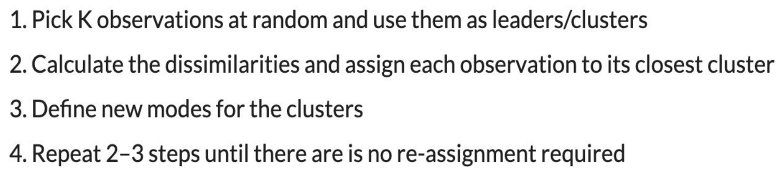
   $$m_i^{(t+1)} = \frac{1}{\left|S_i^{(t)}\right|} \sum_{x_j \in S_i^{(t)}} x_j$$



k-means [wiki]

k-modes is the categorical equivalent!

- Centroid based
- Only works for numeric data
- Explicit k-centroid inputs (initialization)
- Iterative algorithm
- Only

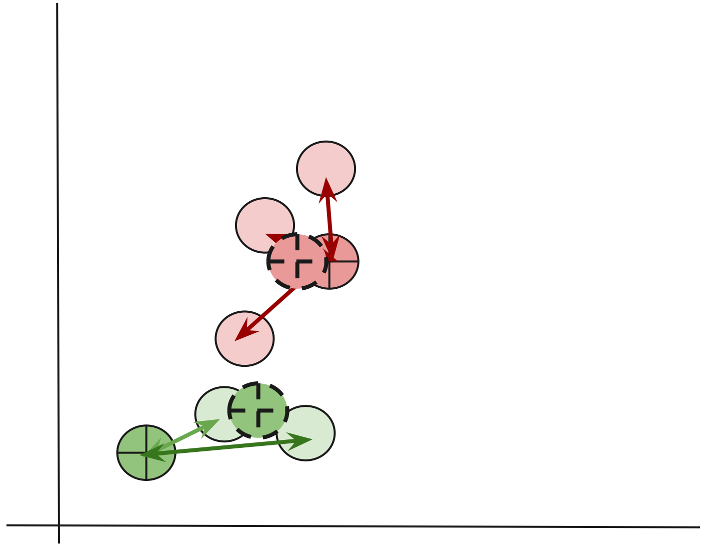


1. Pick K observations at random and use them as leaders/clusters
2. Calculate the dissimilarities and assign each observation to its closest cluster
3. Define new modes for the clusters
4. Repeat 2–3 steps until there are is no re-assignment required

- One simple metric: number of categorical value match
- Whiteboarding

[k-modes]

k-means Clustering



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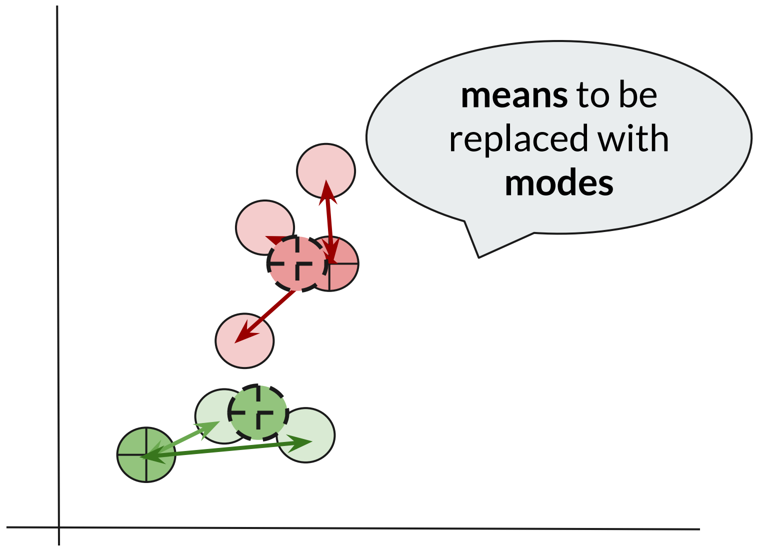
k-modes Clustering



- 5 given data points of forms (x_i, y_i): **categorical**
- For k = 2, the algorithm starts with two random (users can also provide based on their analysis/intuition) initials modes $(m_x, m_y)_j$ *where j = 1, .. k*
- Compares distance between the modes $(m_x, m_y)_j$ and all given (5) data points and for all *j*
- Assign cluster labels based on the distances measured.
- **Update the two modes:**
  - $m_x = 1/|x_i|$ **mode**(x_i)
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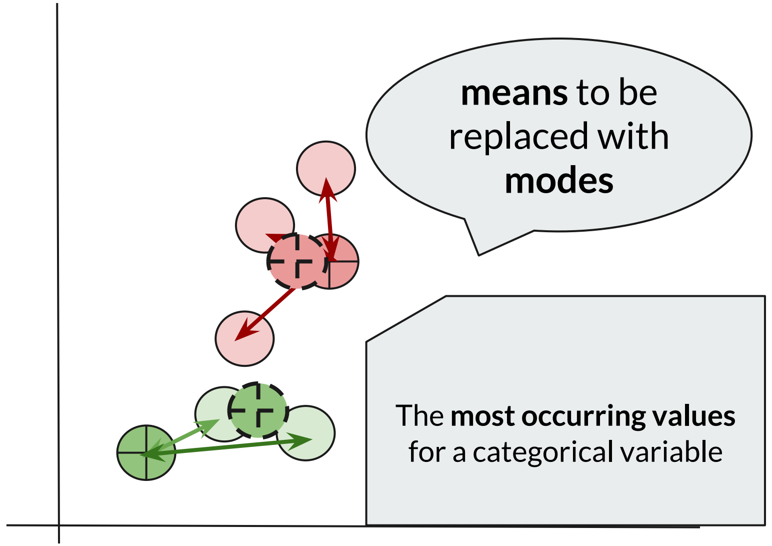
[k-modes]

k-modes Clustering


means to be replaced with **modes**
The **most occurring values** for a categorical variable

- 5 given data points of forms *(x_i, y_i)*: **categorical**
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  - **m_x = 1/|x_i| mode(x_i)**
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k-modes

How about when you have mixed data types?

- Either you have to convert data in one type
    - What could be the challenges?

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- Either you have to convert data in one type
  - What could be the challenges?
- Or, you have to have an algorithm that updates centroids

Clustering Algorithms

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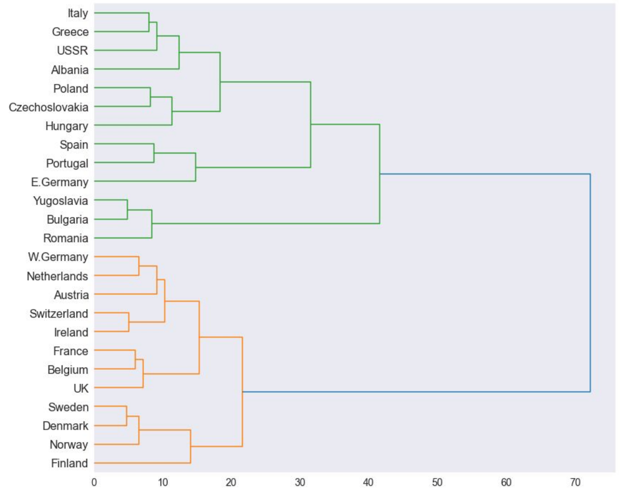
- **GMM**: Distribution based
- **DBSCAN**: Density Based

Hierarchical clustering

Agglomerative: This is a “bottom up” approach. Each observation starts as a new cluster, and pairs of clusters are merged as one moves up the hierarchy.

Divisive: This is a “top down” approach. All data starts as on cluster, and recursively splits into two/multiple clusters.

Grouping countries according to their protein consumption. (dendrogram graph below)



Gaussian Mixture Model (GMM)

$$X \sim \mathcal{N}(\mu, \sigma^2)$$

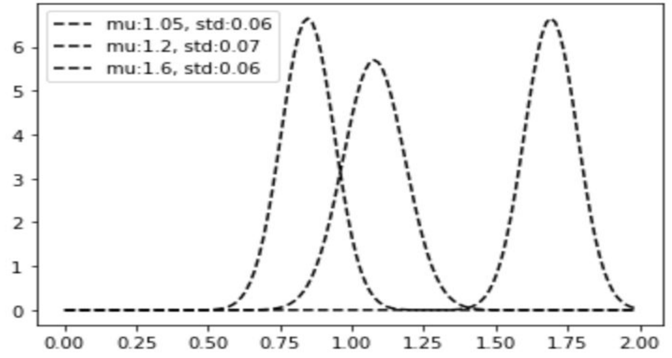
$$p(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

Basic idea from the model title itself:

- **Gaussian/Normal distribution**: distribution modeling some continuous variables such as: population height/weight in a certain region, yearly sales of a business etc.

An example problem

- Display the weight distribution of grade 5,6 and 10 students
- Choose an x (confusing between g 5 and 6) and explain through words



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- ***Mixture***: more than one object/component

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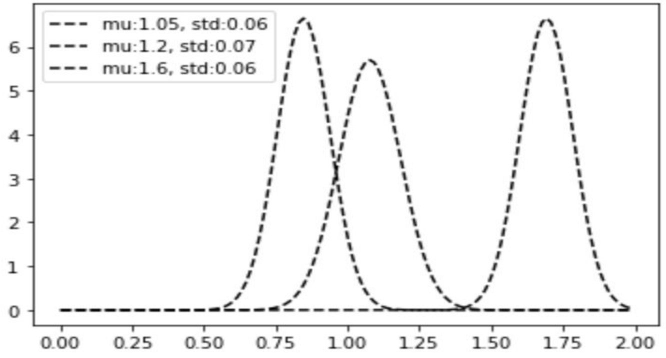
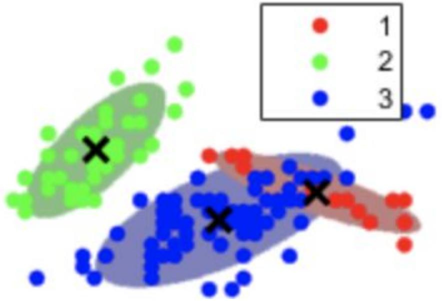


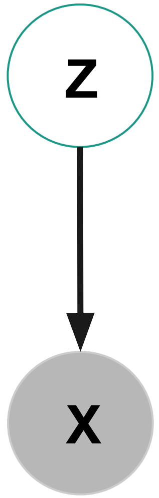
$$p(x) = \sum_{k=1}^{K} \pi_k \mathcal{N}(x|\mu_k,\, \sigma_k)$$

$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k).$$

Gaussian Mixture Model (GMM)

- Fig at the right shows the graphical model (B Net) of GMM
- X: feature vector; in our example case a vector with apples (size, color)
- Z: encoding of clusters (1-of-K is 1, rest are 0s), K is the number of clusters.
- Essentially GMM models(learns) the joint distribution (an example of what we call a generative model)





$$p(\mathbf{x}, \mathbf{z}) = p(\mathbf{z})p(\mathbf{x}|\mathbf{z})$$

$$p(\mathbf{x}) = \sum_{\mathbf{z}} p(\mathbf{z})p(\mathbf{x}|\mathbf{z}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

$$\boxed{0 \leqslant \pi_k \leqslant 1} \quad \boxed{\sum_{k=1}^{K} \pi_k = 1} \quad \boxed{p(\mathbf{z}) = \prod_{k=1}^{K} \pi_k^{z_k}.}$$

Model parameters(all *k* s)

$$\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}$$

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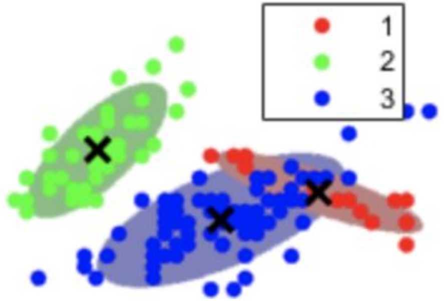
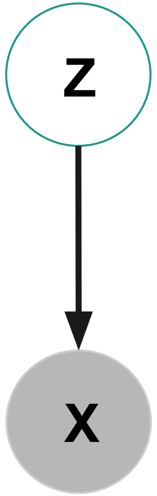


$$\begin{tikzcd} Z \arrow[d] \\ X \end{tikzcd}$$

Model parameters(all *k* s)

$$\pi, \mu, \Sigma$$

Gaussian Mixture Model (GMM)



- If given model parameters, using Bayes rule, we can estimate the class conditional probabilities for a given query X

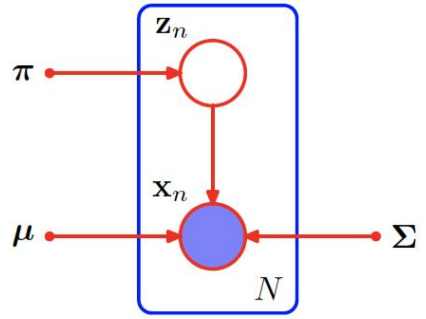
$$
\begin{aligned}
p(z_k = 1|\mathbf{x}) &= \frac{p(z_k = 1)p(\mathbf{x}|z_k = 1)}{\displaystyle\sum_{j=1}^{K} p(z_j = 1)p(\mathbf{x}|z_j = 1)} \\
&= \frac{\pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\displaystyle\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}.
\end{aligned}
$$

Maximum Likelihood Learning

- Start with random parameter initializations
- Optimize the following likelihood function for *N* data points

$$\ln p(\mathbf{X}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{n=1}^{N} \ln \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right\}$$

$$\log p(X) = \log(p(Z)p(X|Z))$$
$$= \log p(Z) + \log p(X|Z)$$

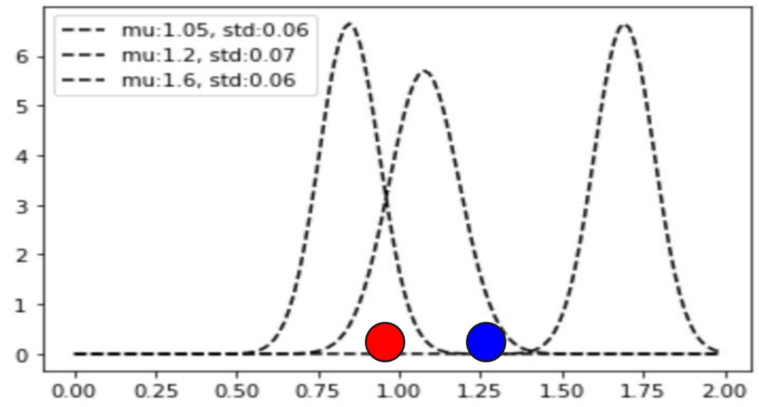


- Some popular techniques:
  - Expectation Maximization algorithm
  - We can also use gradient based optimization techniques

Why do we need GMM ?

- For clustering data points (like other methods - k-means, hierarchical clustering)
- Soft clustering: cluster assignment probability scores, ***p(Z|X)***
- It offers us a probability distribution over the (features & clusters) space, and this can be used as a part of a larger/complex modeling tasks, ***P(X, Z)***

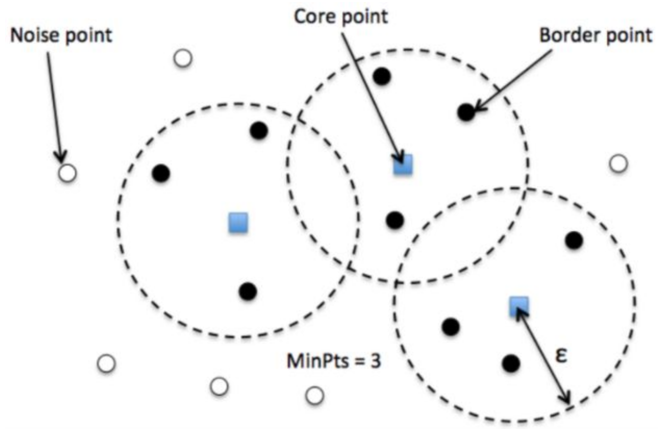
Gmm 3 components



DBSCAN

- Density-Based Spatial Clustering of Applications with Noise
- Two parameters:
  - **minPts**: The minimum number of points (a threshold) clustered together to be considered dense.
  - **eps** (ε): A distance measure that will be used to locate the points in the neighborhood of any point.
- The algorithm proceeds by arbitrarily picking up a point in the dataset.
- If there are at least **'minPoint'** points within a **radius of 'ε'** to the point then we consider all these points to be part of the same cluster.
- The clusters are then expanded by recursively repeating the neighborhood calculation for each neighboring point

Model details with visual demonstration



"The idea that a cluster in data space is a **contiguous region** of **high point density**, separated from other such clusters by contiguous regions of **low point density**."

DBSCAN

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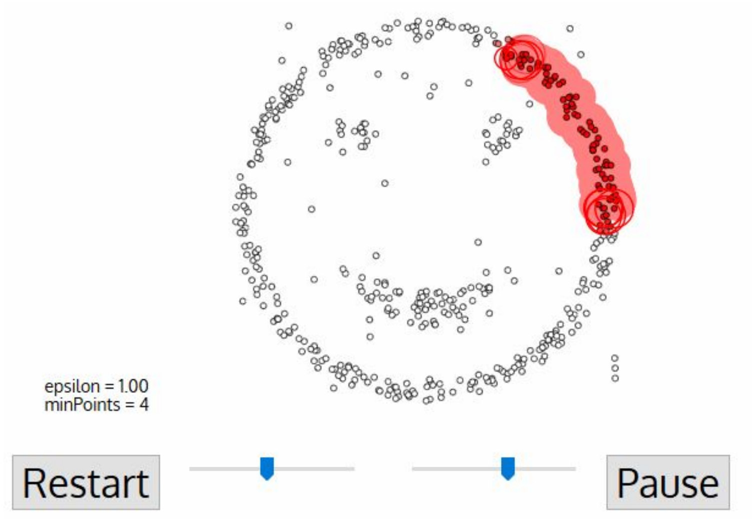
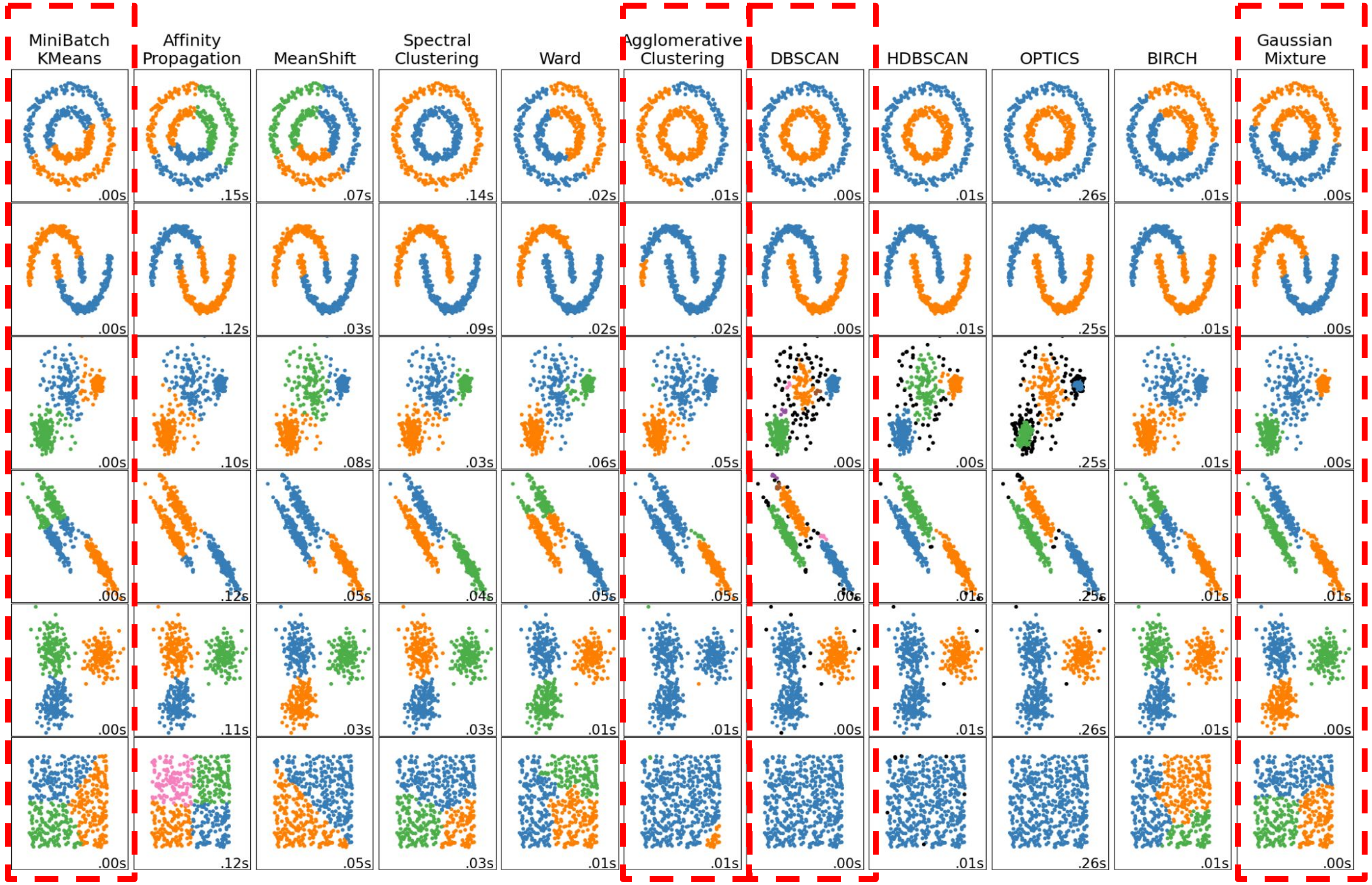

epsilon = 1.00
minPoints = 4

Reference

sklearn



MiniBatch KMeans
Affinity Propagation
MeanShift
Spectral Clustering
Ward
Agglomerative Clustering
DBSCAN
HDBSCAN
OPTICS
BIRCH
Gaussian Mixture
.00s
.15s
.07s
.14s
.02s
.01s
.00s
.01s
.26s
.01s
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sklearn packages

Clustering: sklearn

Clustering: sklearn (API reference)