Clustering

Organizing data points into **similar groups**

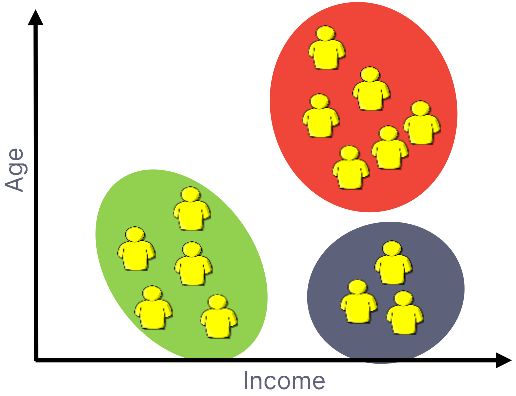
Faculty of Mathematics and Computer Science, University of Bucharest
and
Sparktech Software

Academic Year 2018/2019, 1st Semester

Reminder – Unsupervised Learning

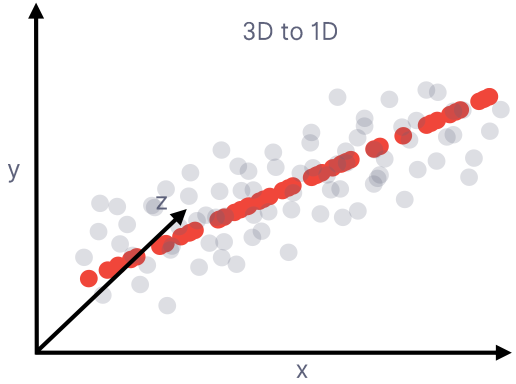
- Unlike *Supervised Learning*, there is no expected label in the training phase.
- We are trying to **discover structure** in the data.

Clustering
Grouping *similar* items



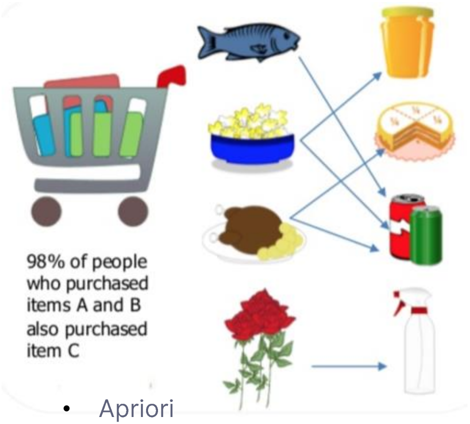
- K-means
- DBSCAN
- Hierarchical Clustering

Dimensionality Reduction
Reducing the number of features



- Principal Component Analysis (PCA)
- T-SNE
- Self-organizing Maps (SOMs)

Association Rule Mining
Finding frequent patterns and correlations



- Apriori
- FP-growth

Clustering

- **Clustering** of **Cluster Analysis** 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* to each other than to objects in other groups.

- There are several types of models:
    - *Centroid-based* – Each cluster is represented by a prototype point (a “center”) (e.g. K-means)
    - *Density-based* – Clusters a considered denser regions of space. (e.g. DBSCAN)
    - *Hierarchical models* – There is a hierarchical relationship between clusters.
    - *Distribution models* – Clusters are modeled using statistical distributions. (e.g. GMM)
    - *Graph-based* – Clusters are considered cliques in a graph (e.g. HCS)
    - *Others*

- Based on the relation between objects and clusters:
    - *Hard-clustering* (or *Partitioning*) – One point can only be in one cluster.
    - *Soft-clustering* (*or Fuzzy-clustering*) – A point can have a degree of membership in multiple clusters.

K-Means

Centroid-based partitioning into a **fixed** number of clusters

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K-means

- **K-means** is a clustering algorithm which aims to *partition* the data points into a *fixed* number of clusters *k*.
- It is a *centroid-based* method, which means that each cluster is represented by a *prototype point* (called a **centroid**) and every point is assigned to the cluster with the *closest* centroid.
- The goal is to find a clustering which minimizes the **within-cluster sum of squares** (i.e. *variance* of clusters).
- K-means uses an iterative method and it converges to a *local optimum*.
    - Finding the global optimum is *NP-hard*

K-means Algorithm

```
initialization:
    - select k random cluster centers
repeat:
    “assignment” step:
        - assign each point to the cluster of the nearest center
    “update” step:
        - move the cluster centers to the mean point of each cluster
```

K-means Algorithm

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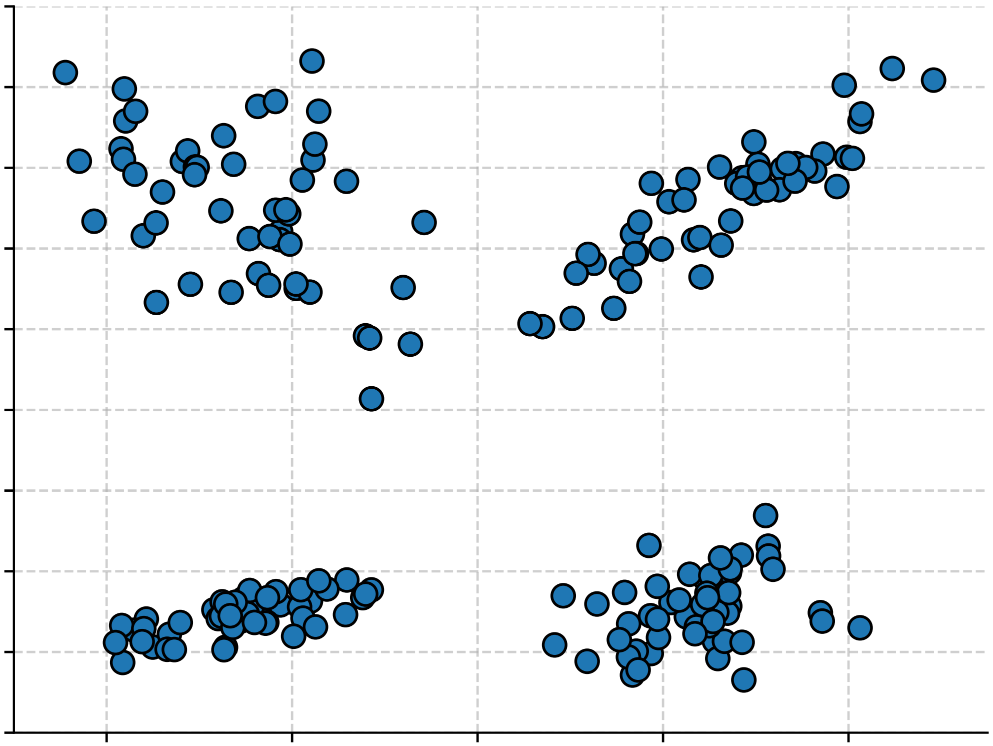
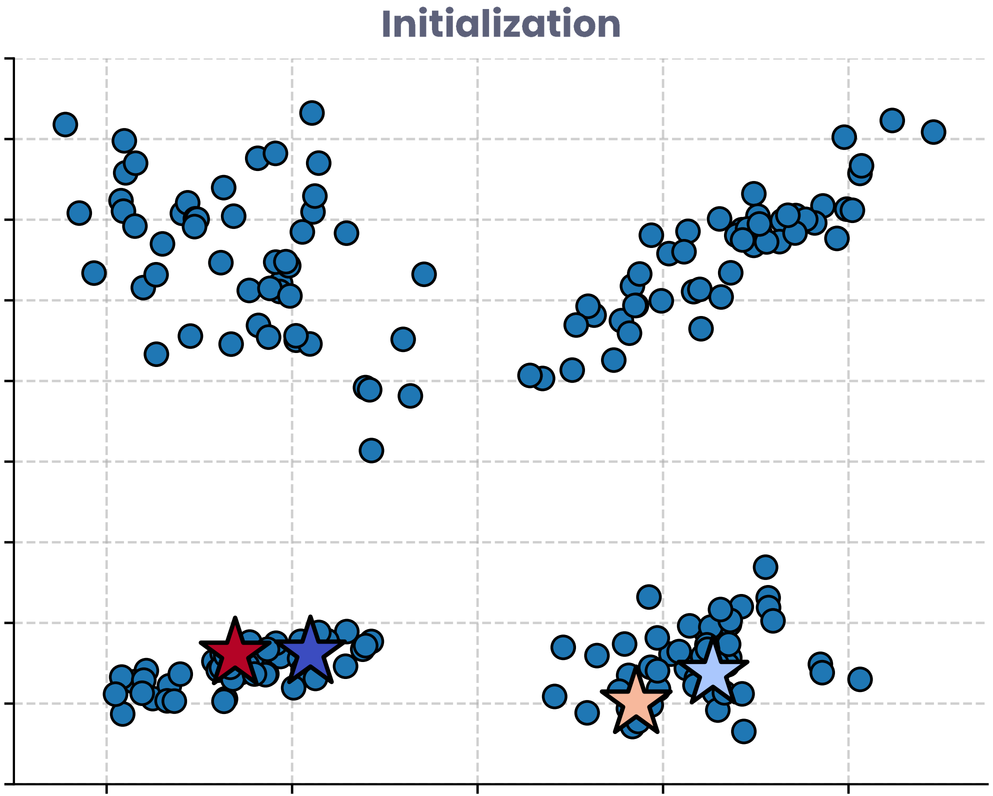
K-means is an instance of the *Expectation-Maximization (EM)* algorithm

K-means Algorithm



K-means Algorithm

- Choose $k = 4$ random cluster centers.



K-means Algorithm

- Choose $k = 4$ random cluster centers.
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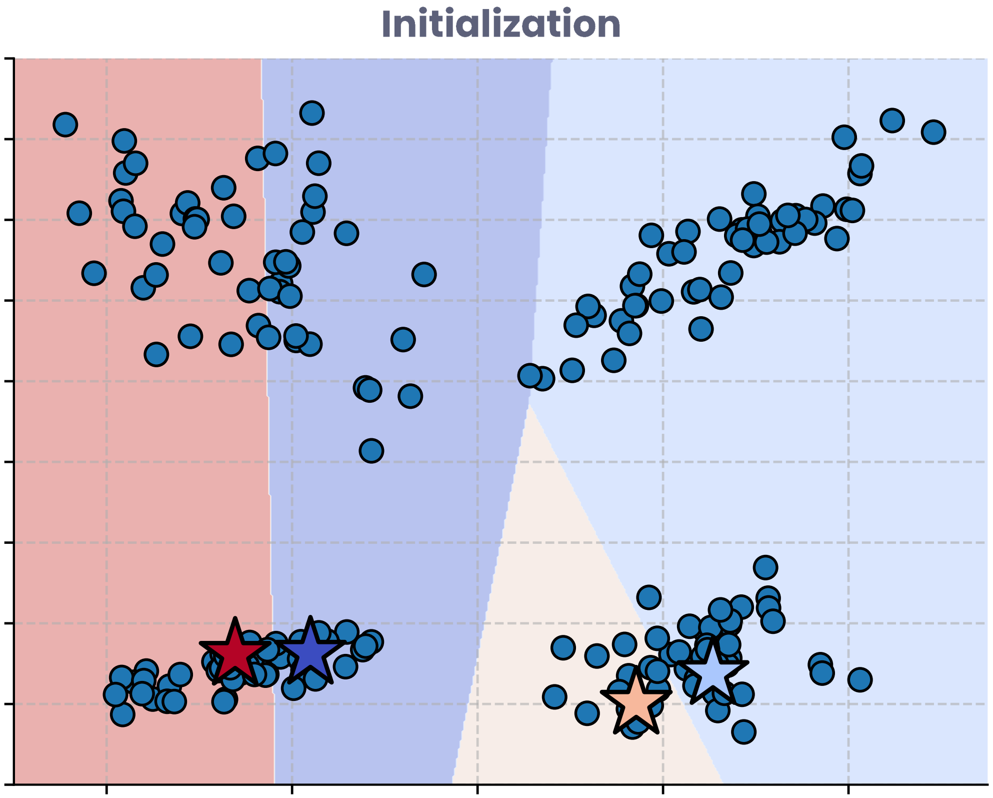

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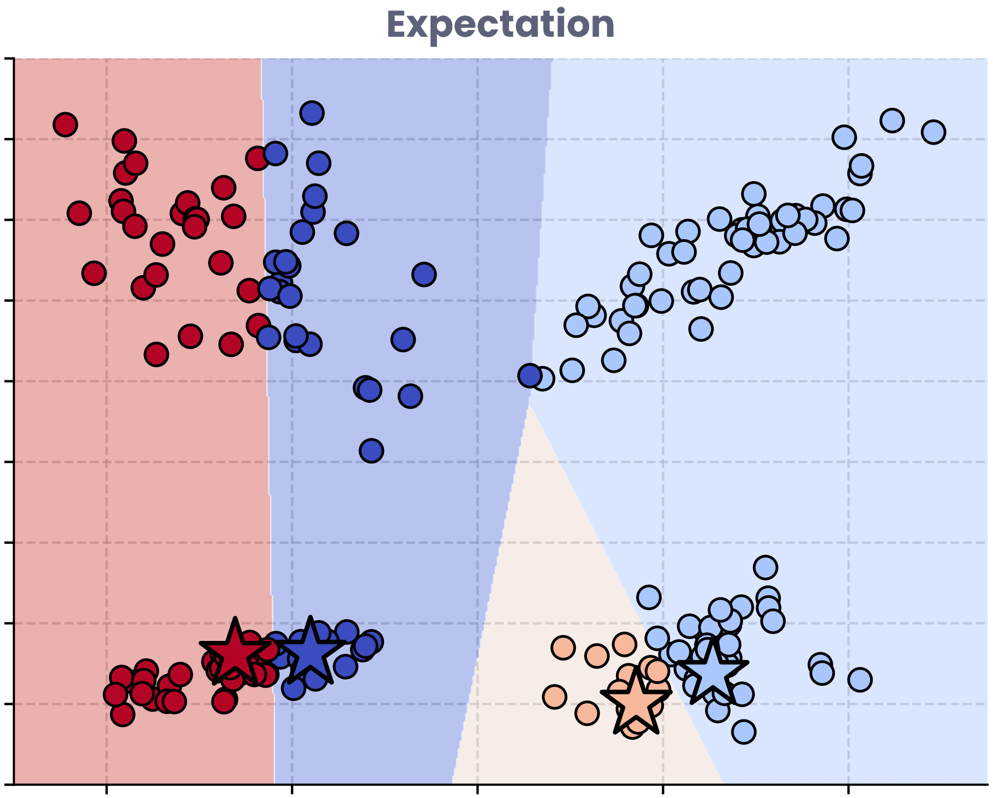

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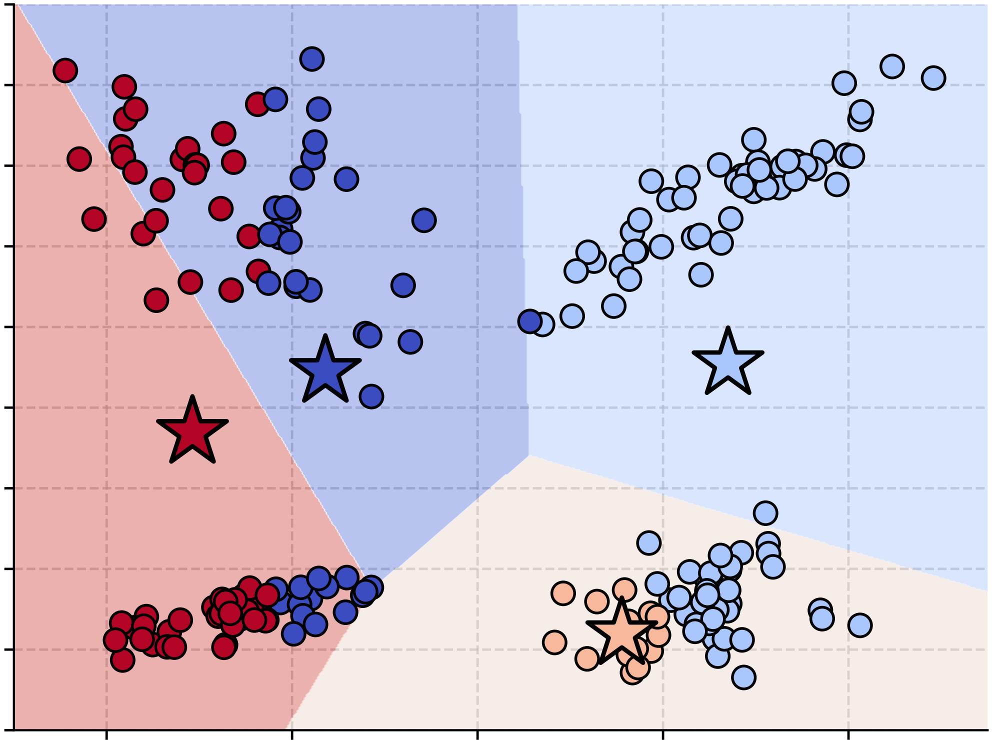
Maximization



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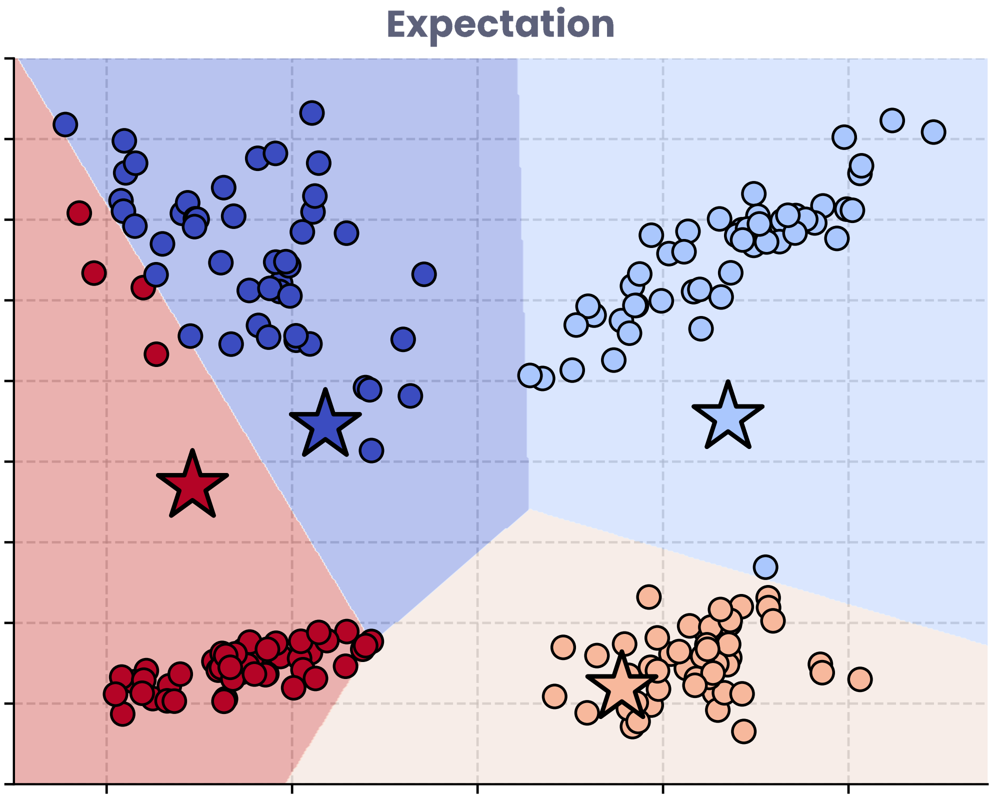

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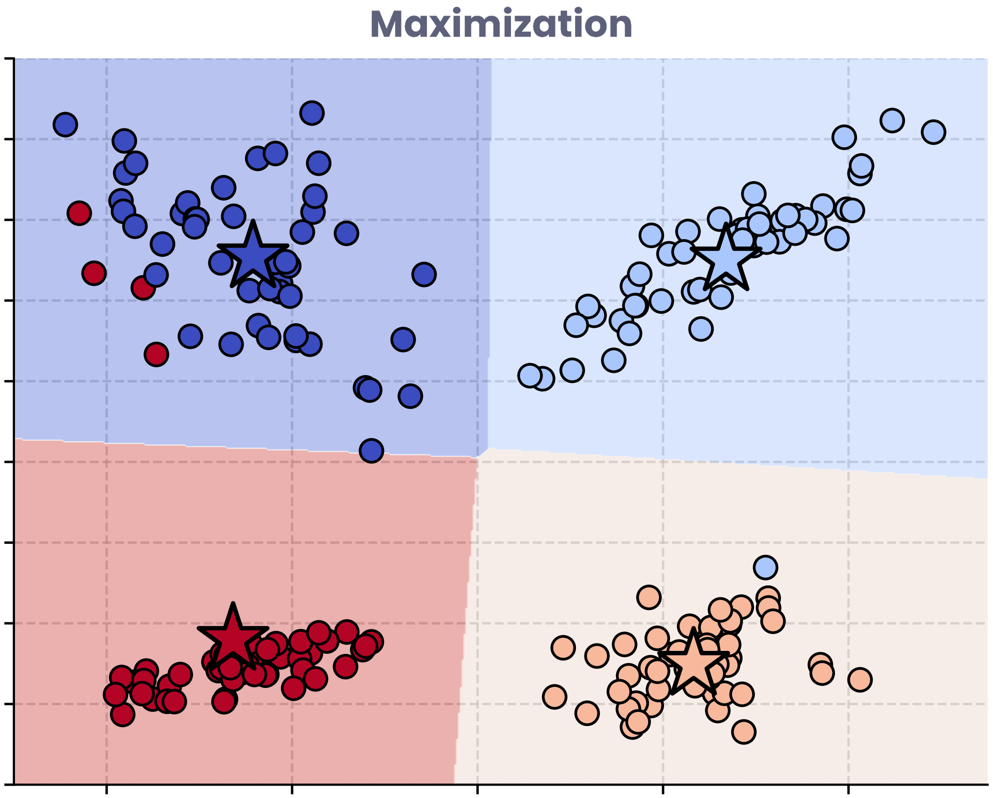

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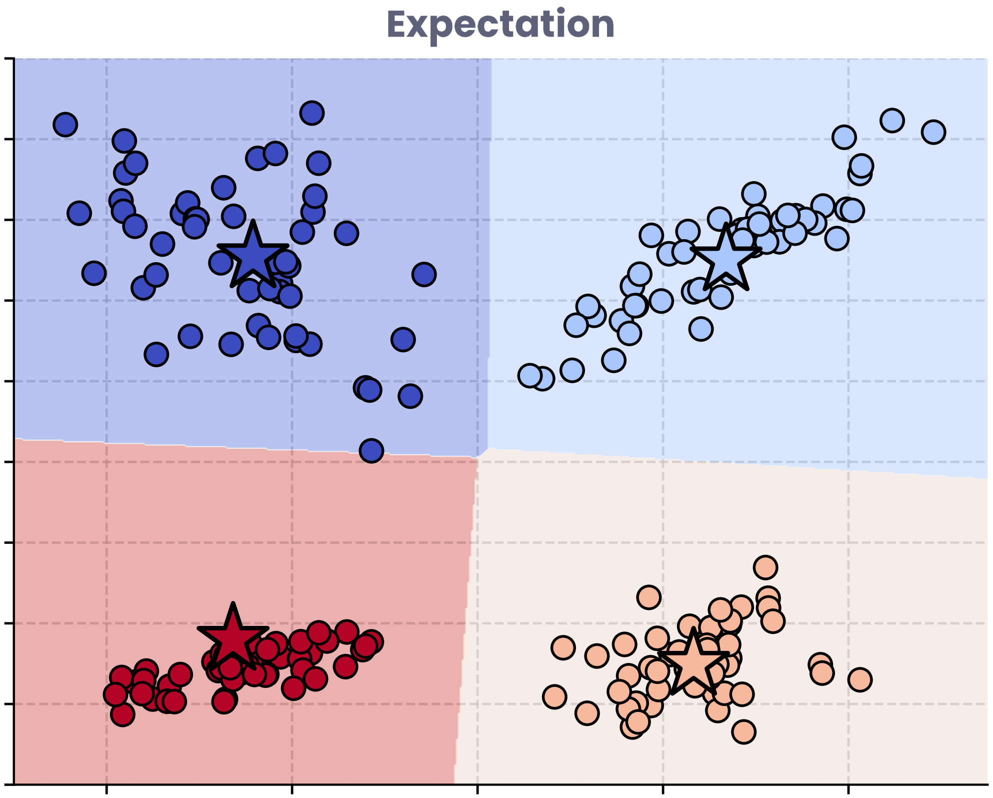

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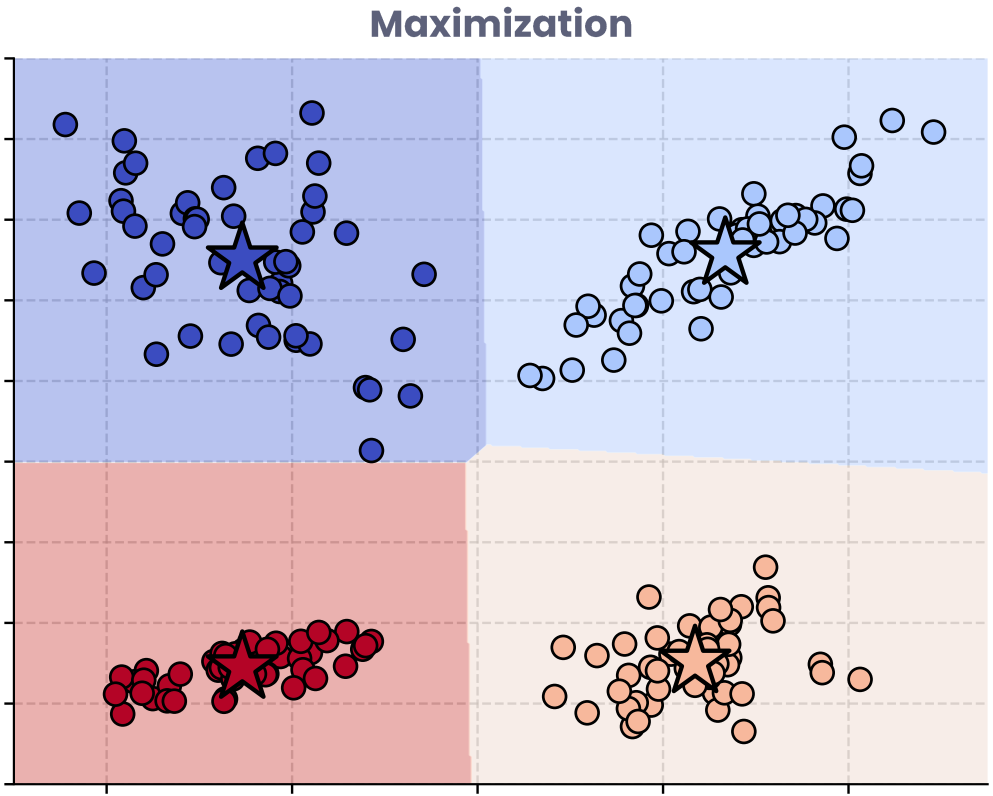

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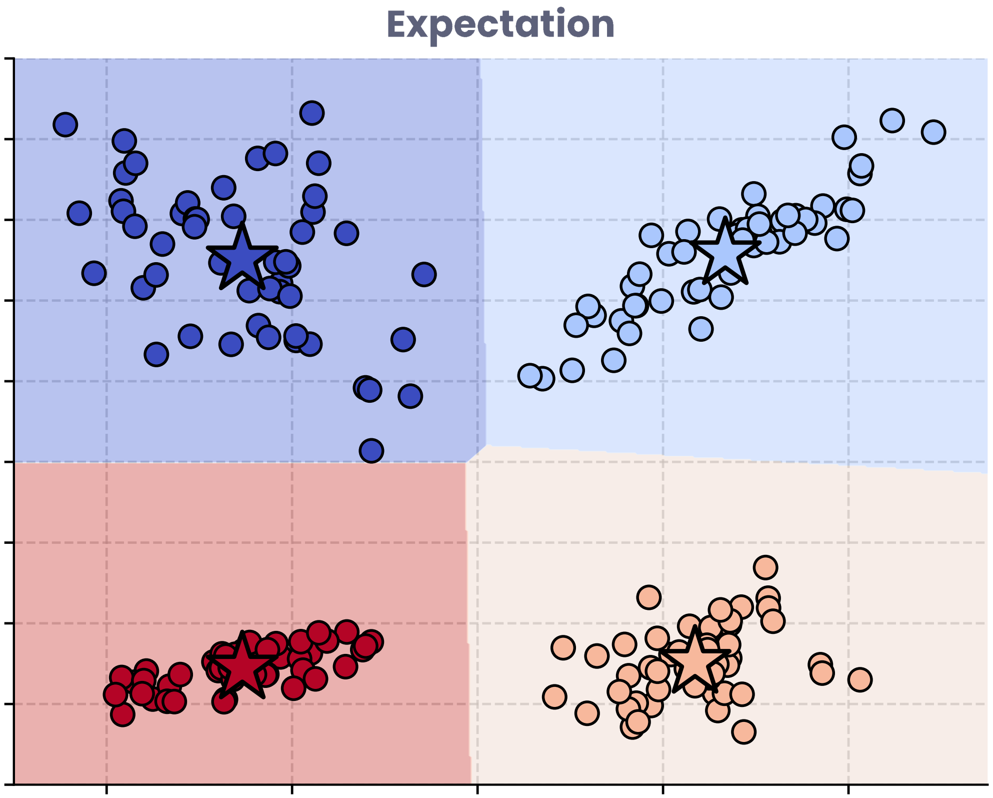

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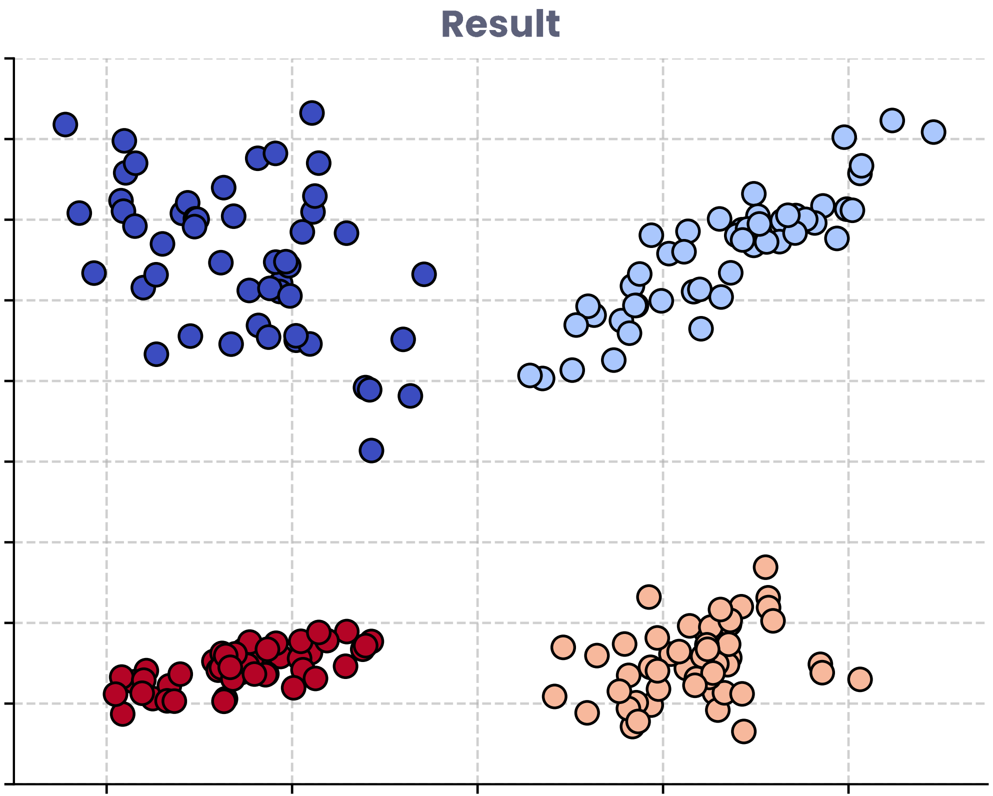
- Move each centroid to the true mean of its cluster (“Maximization”).
- **Assignment did not change anything, so stop.**



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$$\boldsymbol{J} = \sum_{\boldsymbol{j}=\boldsymbol{1}}^{\boldsymbol{k}} \sum_{\vec{\boldsymbol{x}} \in \boldsymbol{C}_{\boldsymbol{j}}} \left\| \vec{\boldsymbol{x}} - \vec{\boldsymbol{\mu}}^{(j)} \right\|^{\boldsymbol{2}}$$

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Where:

- $z_{ij} = \begin{cases} 1 & \text{if } \vec{x}^{(i)} \in C_j \\ 0 & \text{otherwise} \end{cases}$
- $\vec{\mu}^{(j)} \in \mathbb{R}^n$ is the centroid of cluster C_j

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- **Goal:** Minimize J with respect to z_{ij} and $\vec{\mu}^{(j)}$

Finding the global optimum is NP-hard

Algorithm (2)

```
initialization:
    - choose random values for μ⃗^(j), for all j ∈ {1,2,…,k}
repeat:
    “expectation” step:
        - minimize J w.r.t. z_ij, keeping μ⃗^(j) fixed
    “maximization” step:
        - minimize J w.r.t. μ⃗^(j), keeping z_ij fixed
```

Algorithm (2)

- "**Expectation**" step:

Minimize

$$J = \sum_{i=1}^{m} \sum_{j=1}^{k} z_{ij} \left\| \vec{x}^{(i)} - \vec{\mu}^{(j)} \right\|^2$$

With respect to z_{ij}, keeping $\vec{\mu}^{(j)}$ fixed.

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- There must be only one $z_{ij} = 1, \forall i$ (i.e. $\vec{x}^{(i)}$ must be in only one cluster).

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  - To minimize J, we must set $z_{ij^*} \coloneqq \begin{cases} 1 & \text{if } j^* = \mathrm{argmin}_{\mathrm{j}} \left\| \vec{x}^{(i)} - \vec{\mu}^{(j)} \right\| \\ 0 & \text{otherwise} \end{cases}$

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- In other words, **we set $\vec{\mu}^{(j)}$ to the mean of all points in $\boldsymbol{C}_j$**

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This is for one particular $\vec{\mu}^{(j)}$, we do it for all j

Parameters and Evaluation

How to choose k?

- Number of clusters *k* is a *hyperparameter*. How do we get a good k?

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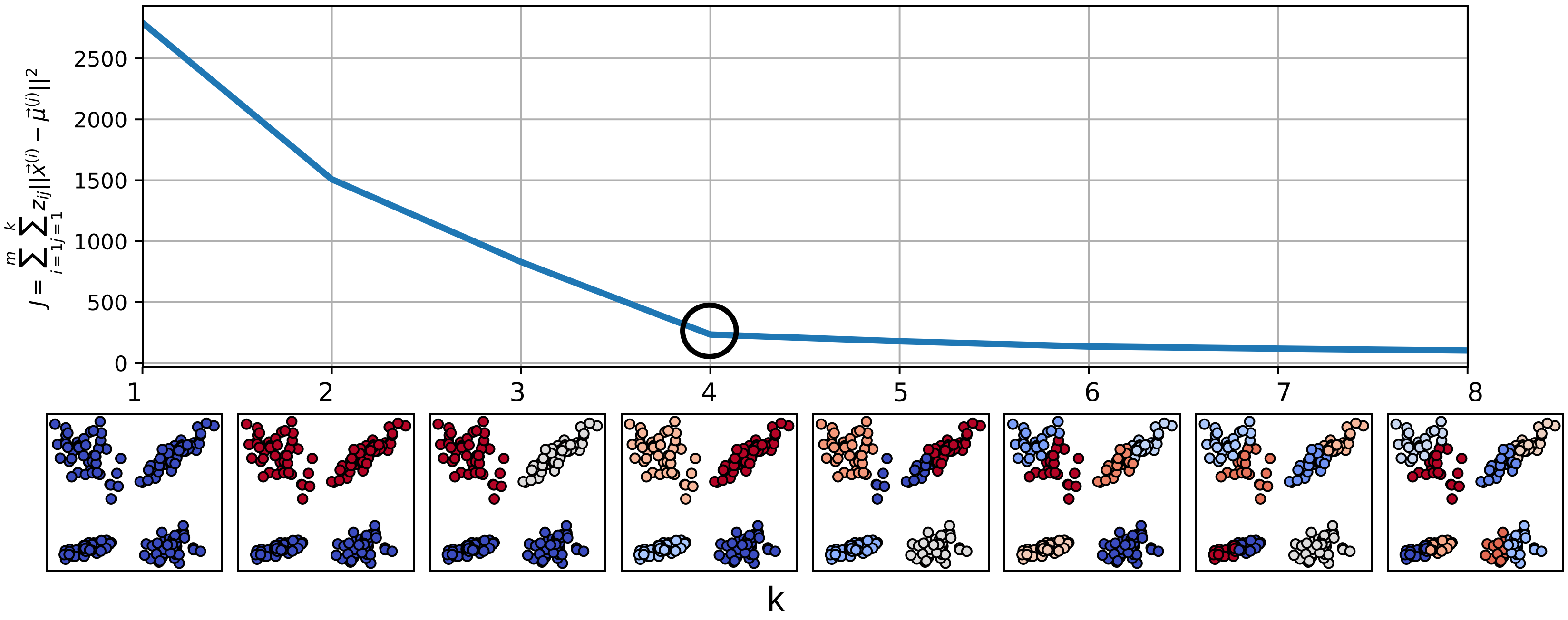
- Number of clusters *k* is a *hyperparameter*. How do we get a good k?
- **Elbow method**
  - Start with a small *k* value and increase it until adding another cluster does not result in a much lower *distortion value*.
  - In other words, the new cluster does not explain much more of the *variance* in the data.
- **Silhouette Coefficient**
  - A measure of how *tight* each cluster is and how *far apart* cluster are from one another.
  - Choose a *k* value which results in a clustering with a large silhouette coefficient.

The Elbow Method

- Choose *k* such that adding another cluster wouldn't *explain much more of the variance* in the data (i.e. does not give a much lower distortion value):



Silhouette Coefficient

- Measures the *tightness of clusters* and *separation between clusters*:

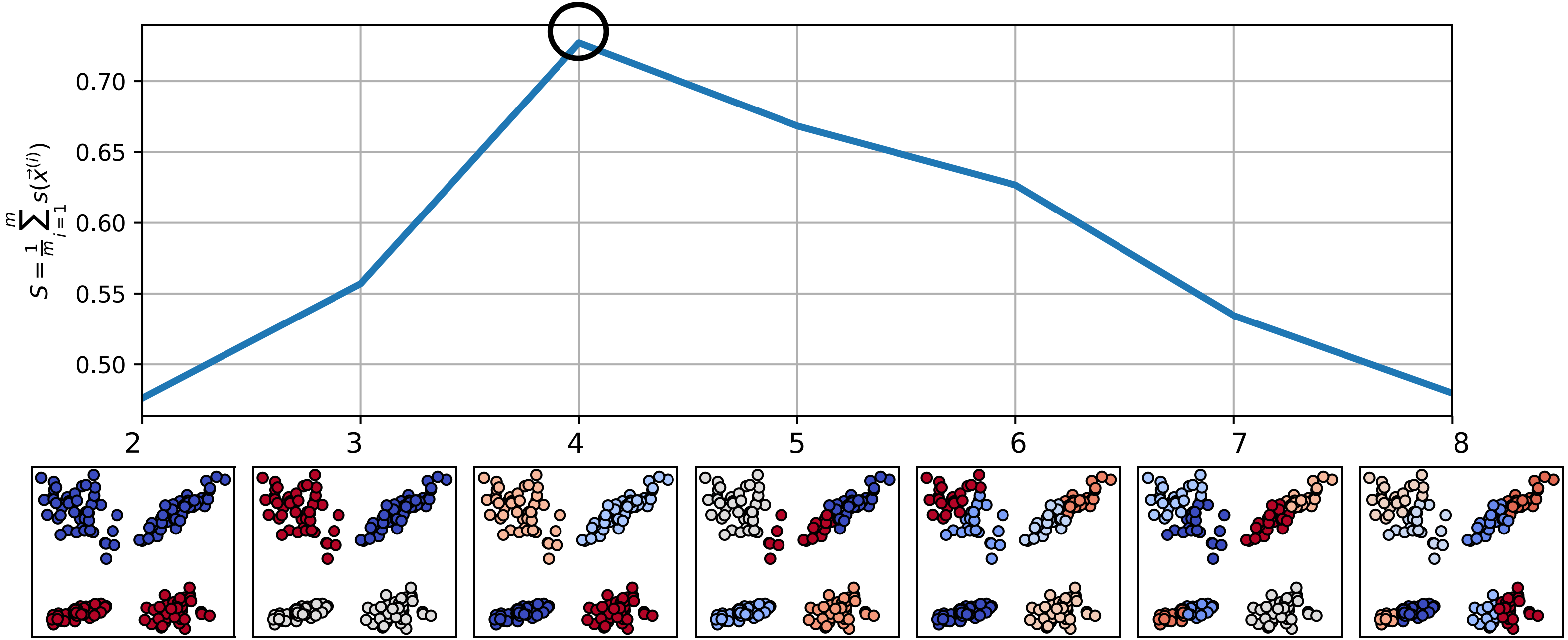
$$s\left(\vec{x}^{(i)}\right) = \frac{b\left(\vec{x}^{(i)}\right) - a\left(\vec{x}^{(i)}\right)}{\max\left(a\left(\vec{x}^{(i)}\right), b\left(\vec{x}^{(i)}\right)\right)}$$

Where:

- $a\left(\vec{x}^{(i)}\right)$ – average distance between $\vec{x}^{(i)}$ and all other points in the same cluster
- $b\left(\vec{x}^{(i)}\right)$ – lowest average distance to all points in any other cluster
  - The average distance to the closest “neighboring” cluster.

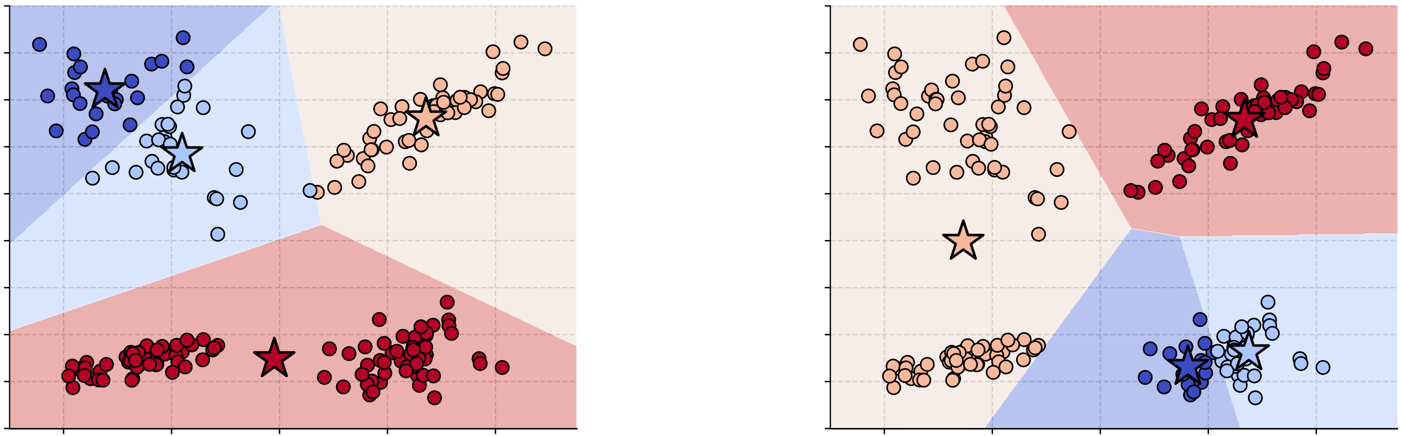
Silhouette Coefficient

- Choose *k* which gives the highest mean silhouette:



Local minima

- K-means can get stuck in *local minima*.
- Both of the following states are stable (further iterations will not change anything):



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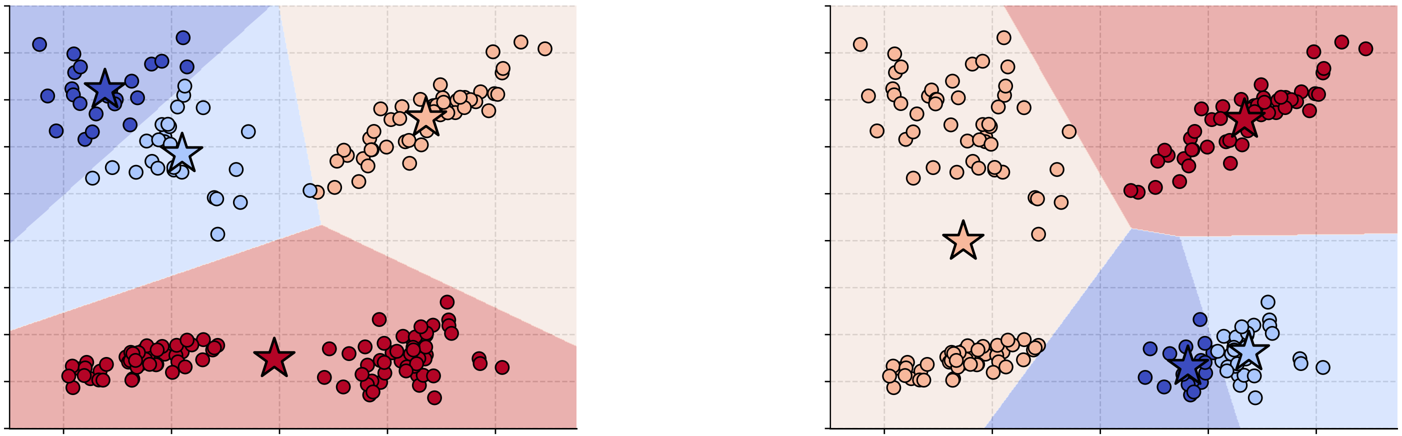

- Possible solutions:
    - Run the algorithm multiple times and pick the result with the *lowest distortion* (or *highest silhouette*)
    - Use a better initialization method.

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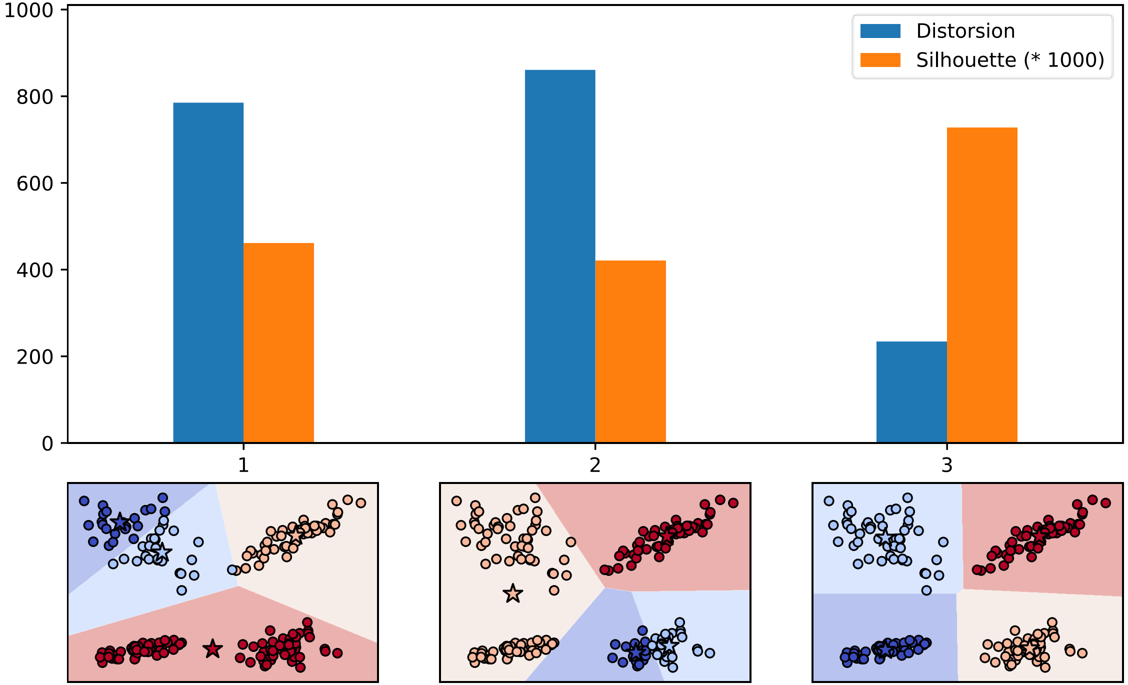


Local minima

- Use a better initialization method:
    - *“k-means++: the advantages of careful seeding”*, Arthur, D., Vassilvitskii, S., 2007.

choose first center uniformly at random from the data points

repeat until all k centers have been chosen:

  - compute $D\left(\vec{x}^{(i)}\right)$, the distance from $\vec{x}^{(i)}$ to the nearest chosen center

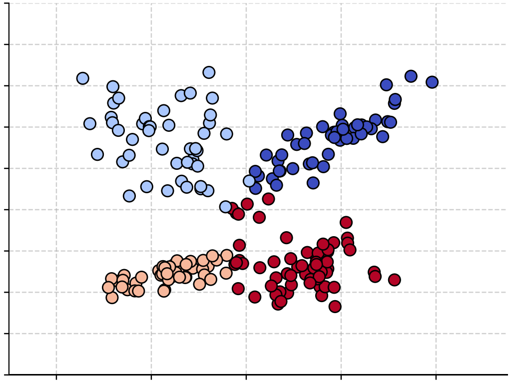
  - choose a new center at random with probability $P\left(\vec{x}^{(i)}\right) \sim D\left(\vec{x}^{(i)}\right)^2$

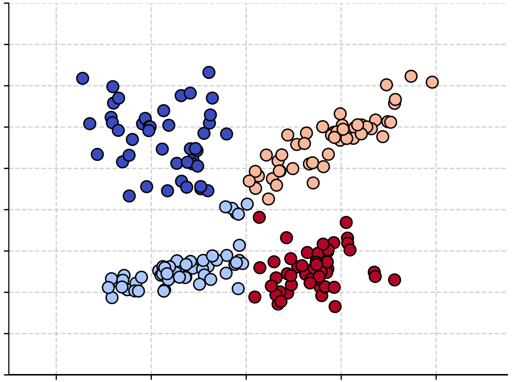
run standard k-means algorithm

-
    - The idea is to try to spread out the initial cluster centers.

Comparing clusterings

- How similar are these two clusterings?





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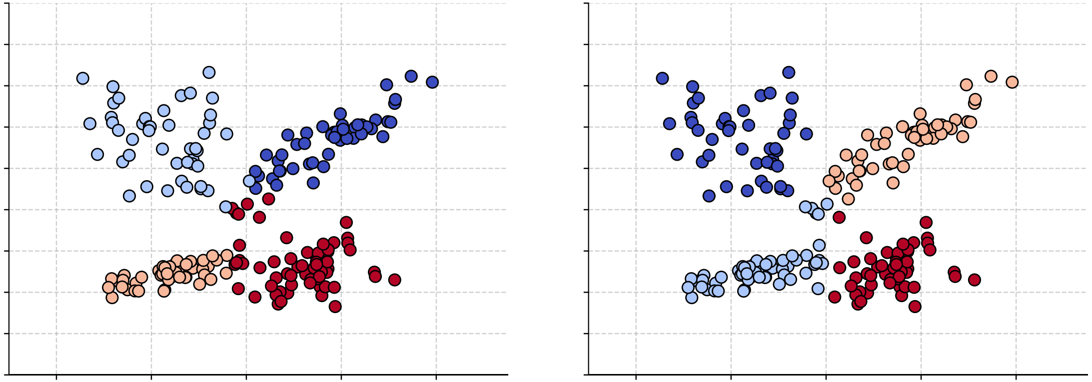

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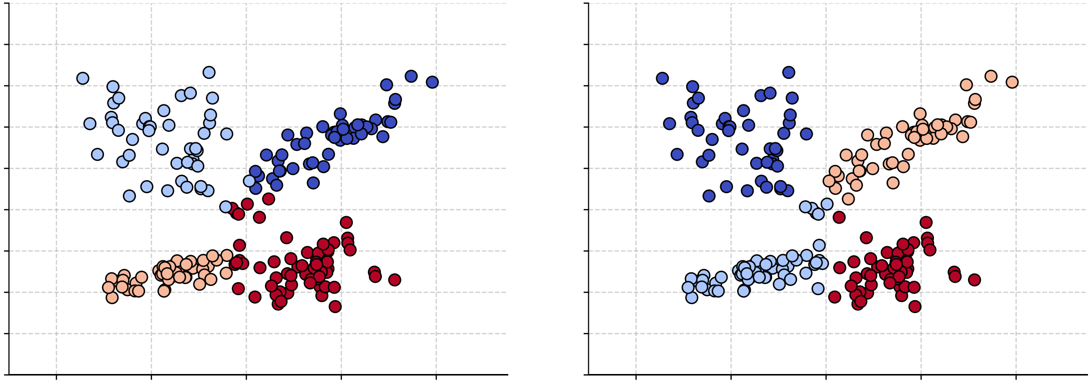


- **Rand Index** measures how often two clustering agree in terms of grouping points:

$$R = \frac{a + b}{n(n-1)/2}$$

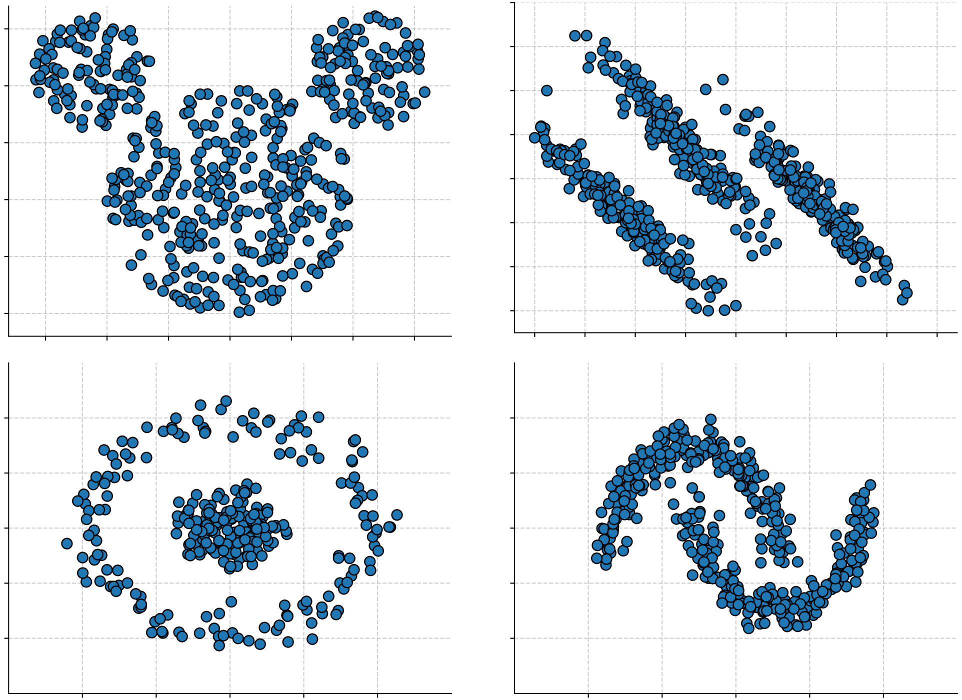
  - a is the number of pairs of points which are in the same cluster in both clusterings.
  - b is the number of pairs of points which are in different clusters in both clusterings.

The actual "label" assigned to each cluster (represented here by color) doesn't matter, only the grouping of points matters.

Adjusted Rand Index is a form of Rand index which also take into account that clusterings might agree by chance.

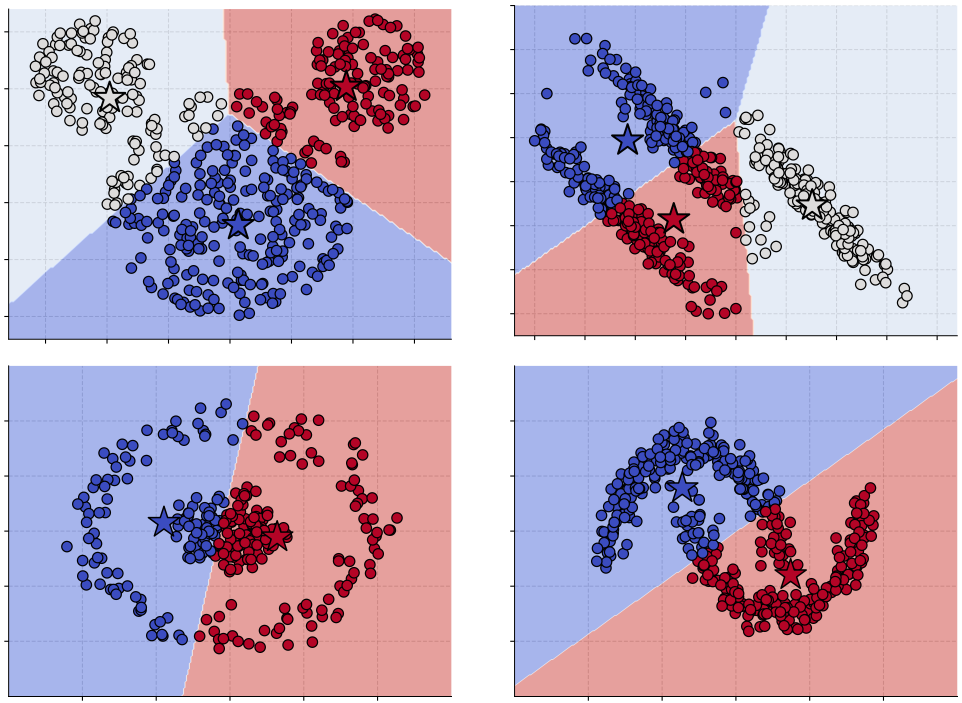
K-means Limitations

- How will K-means handle these datasets?



K-means Limitations

- How will K-means handle these datasets?
- Not so good…
  - K-means only produces *convex clusters*.
  - It doesn't handle *non-spherical clusters* very well.
  - It tends to produce *clusters of equals sizes*.



K-means Variations

Soft K-means

- K-means "*expectation*" step: $z_{ij^*} \coloneqq \begin{cases} 1 & \text{if } j^* = \mathrm{argmin}_j \left\| \vec{x}^{(i)} - \vec{\mu}^{(j)} \right\| \\ 0 & \text{otherwise} \end{cases}$ (i.e. assign point $\vec{x}^{(i)}$ to the cluster with the closest centroid)
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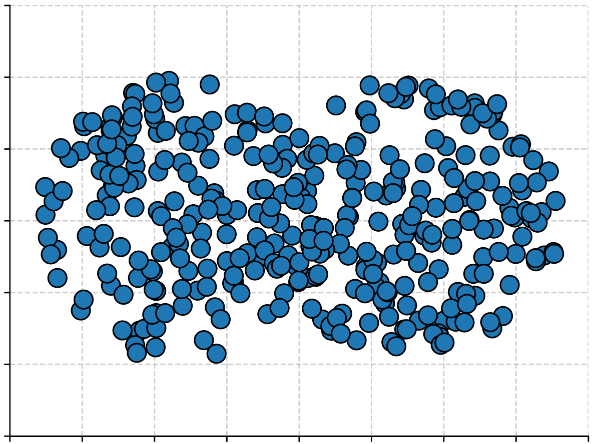

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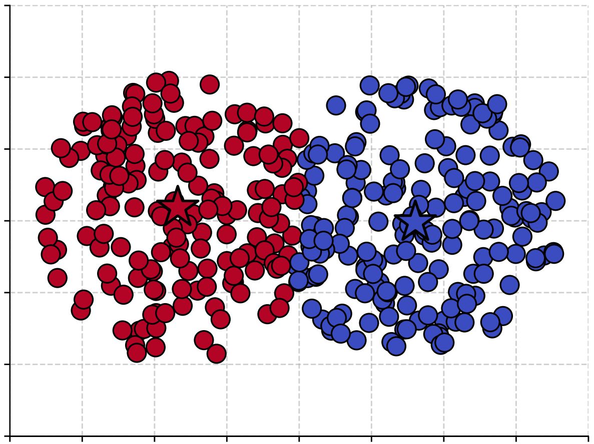

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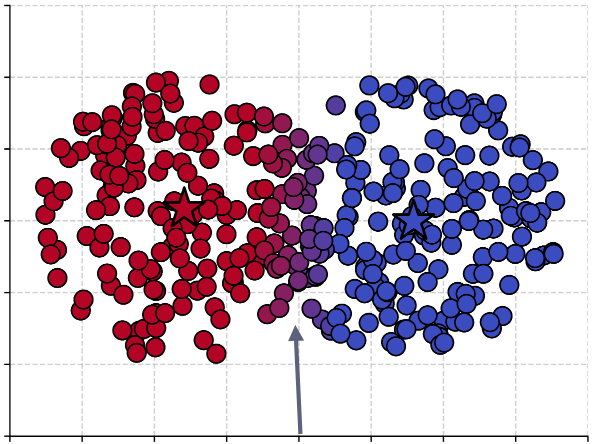
- With *hard-clustering*, the assignment in such regions will mostly be due to chance from random initialization.
- **Soft K-means** redefines the "expectation" step such that $z_{ij} \in \mathbb{R}$ is the *degree of membership* of $\vec{x}^{(i)}$ to cluster C_j :

$$z_{ij^*} \coloneqq \frac{e^{-\beta \left\| \vec{x}^{(i)} - \vec{\mu}^{(j^*)} \right\|}}{\sum_j e^{-\beta \left\| \vec{x}^{(i)} - \vec{\mu}^{(j)} \right\|}}$$

Expectation

$$\vec{\mu}^{(j)} = \frac{\sum_i z_{ij} \vec{x}^{(i)}}{\sum_i z_{ij}}$$

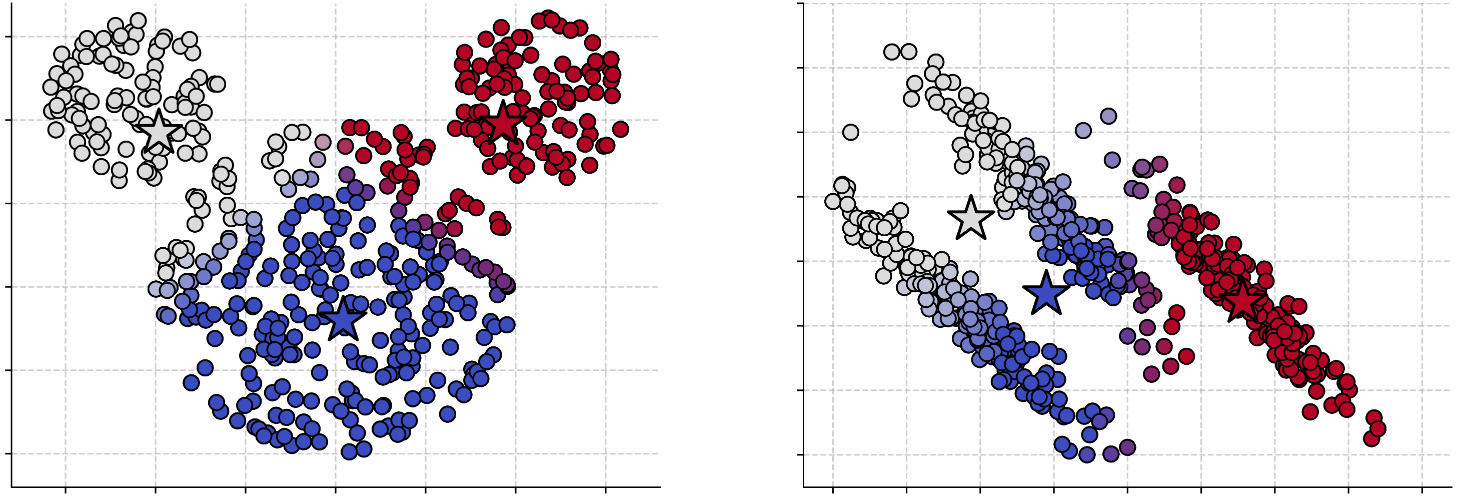
Maximization



Points in this area have ~0.5 membership in both clusters.

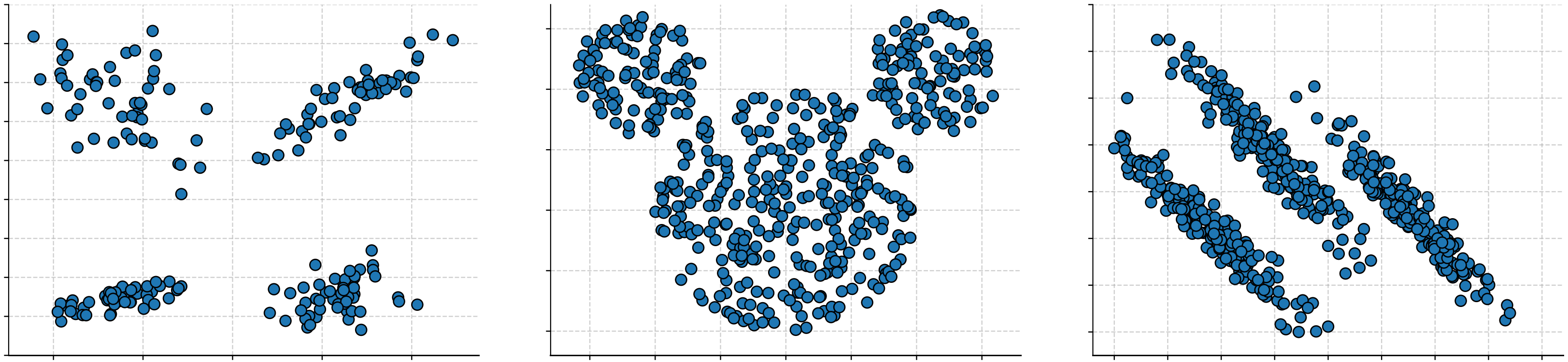
Soft K-means

- Soft K-means does not solve the unequal-size and non-spherical clusters issues.



Gaussian Mixture Models

- **GMMs** are *probabilistic models* which assumes that data points are generated by a mixture of *normal distributions* (a.k.a. *Gaussians*).
- A *expectation-maximization* algorithm can be used to fit the Gaussians by maximizing the *likelihood* of data.



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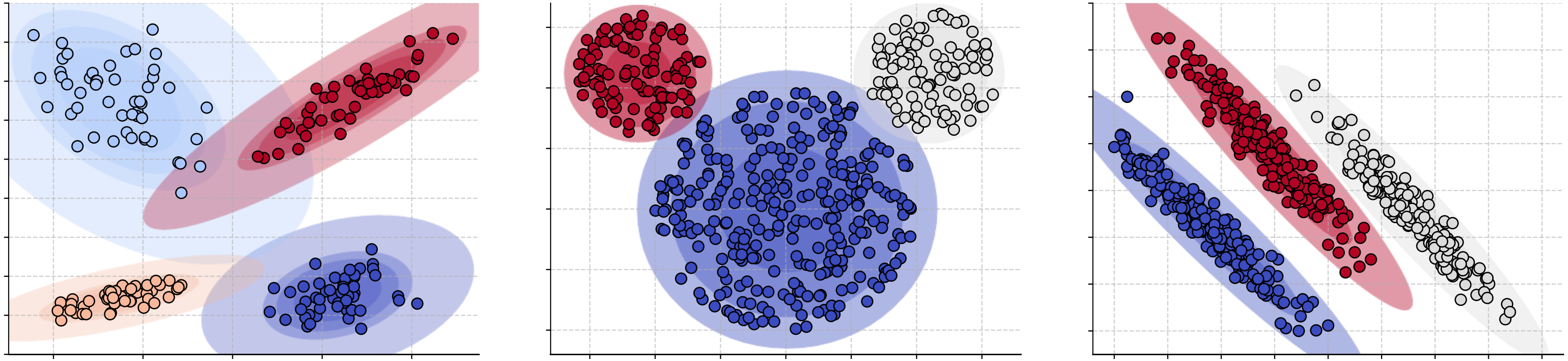

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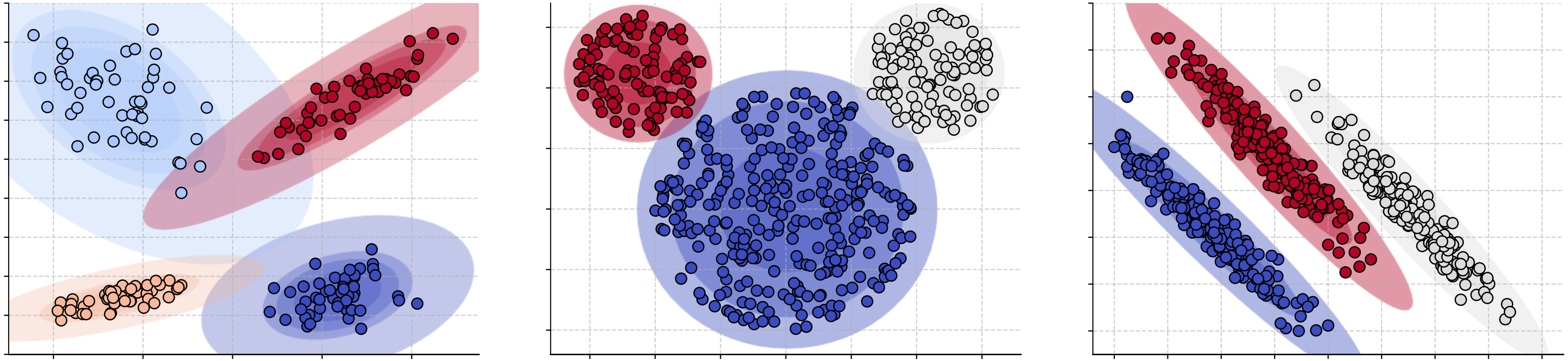

- It can be viewed as an extension of *Soft K-means* in which each cluster has both a *mean* and a *covariance matrix* (which gives the non-spherical shape).

Getting rid of centroids

- **Expectation** step means setting $z_{i\,j^*} = \begin{cases} 1 & \text{if } j^* = \mathrm{argmin_j} \left\| \vec{x}^{(i)} - \vec{\mu}^{(j)} \right\| \\ 0 & \text{otherwise} \end{cases}$

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Norm of a vector is the square root of the dot product with itself.

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*We can use a **kernel function.***

Kernel K-means

- Assign each point to a random cluster.
- Repeat until no change occurs:

$$z_{ij^*} \coloneqq \begin{cases} 1 & \text{if } j^* = \text{argmin}_j \left(-2\frac{1}{|C_j|}\sum_{\vec{x}' \in C_j} K(\vec{x}^{(i)}, \vec{x}') + \frac{1}{|C_j|^2}\sum_{\vec{x}' \in C_j}\sum_{\vec{x}'' \in C_j} K(\vec{x}', \vec{x}'') \right) \\ 0 & \text{otherwise} \end{cases}$$

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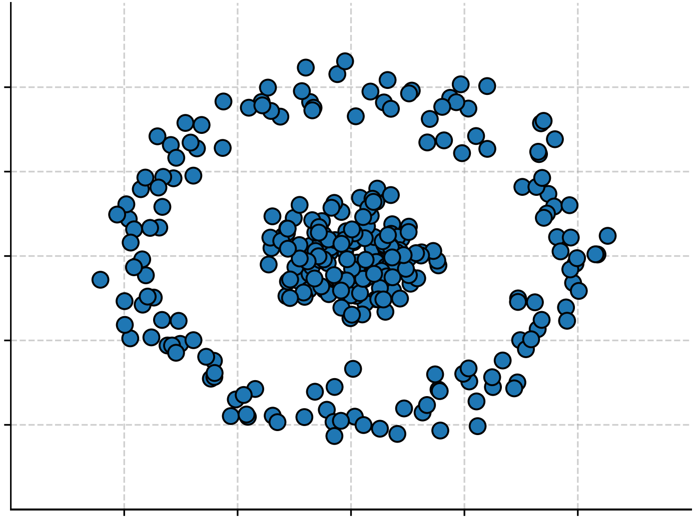

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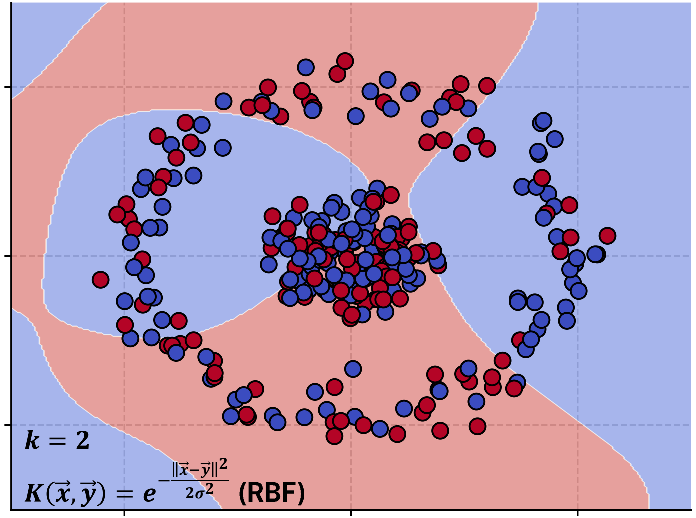

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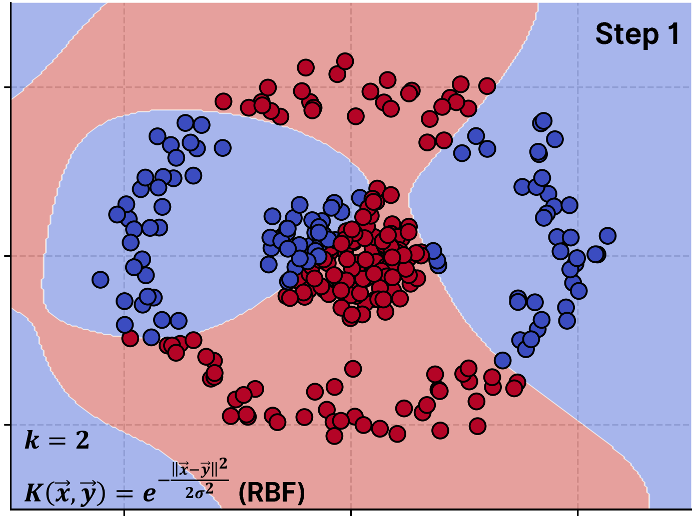

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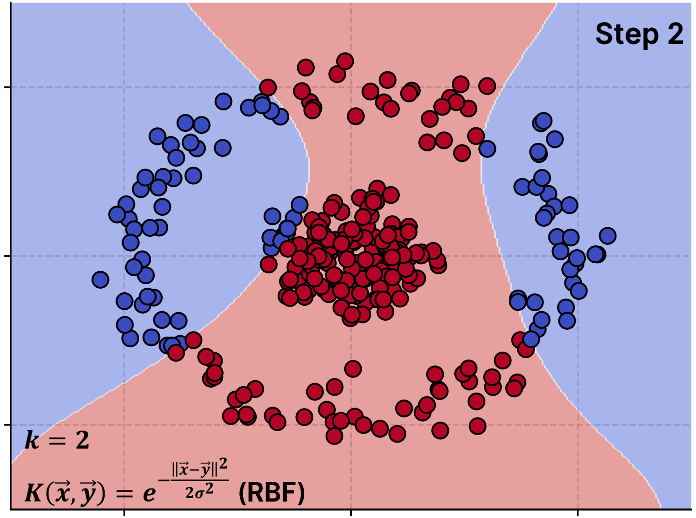

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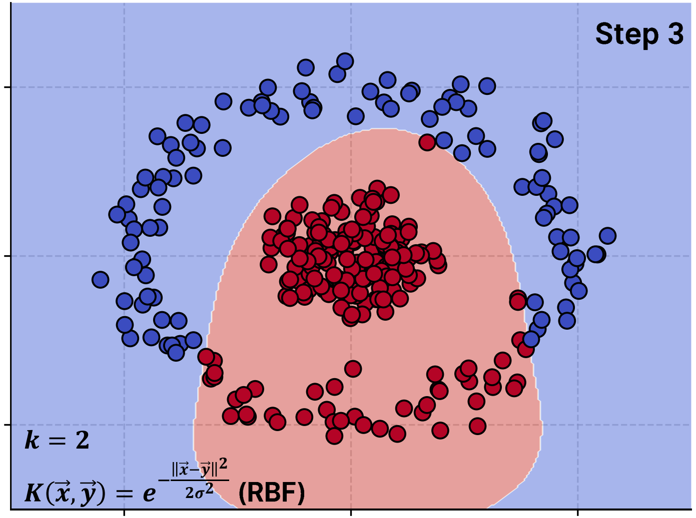

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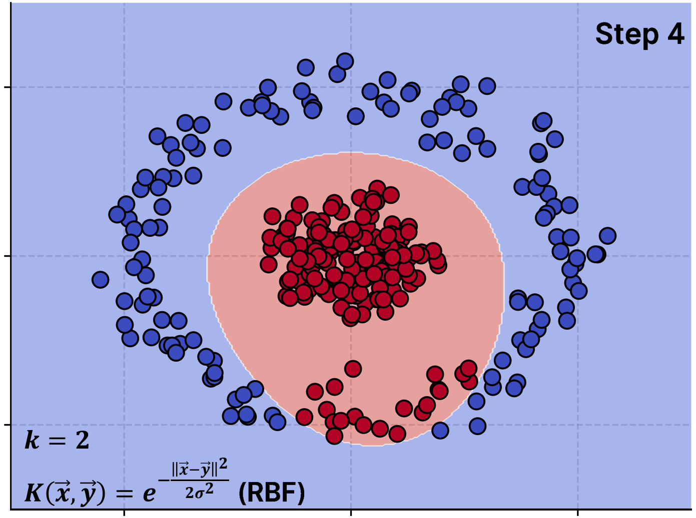


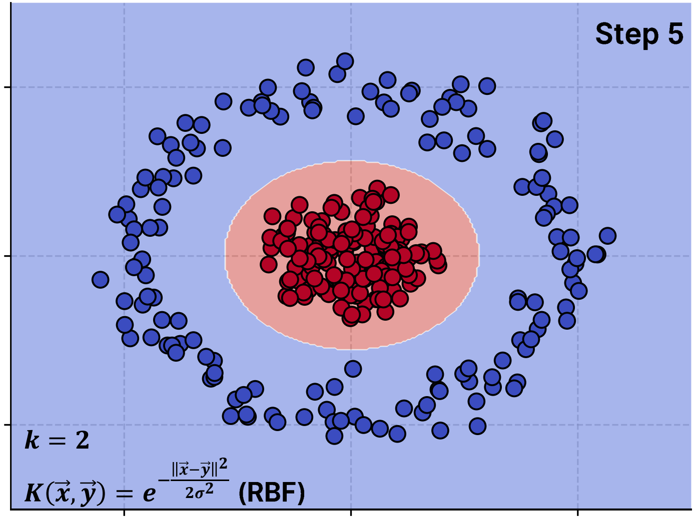
Kernel K-means

- Assign each point to a random cluster.
- **Repeat until no change occurs:**

$$\mathbf{z_{ij^*}} \coloneqq \begin{cases} \mathbf{1} & \textbf{if } \boldsymbol{j^*} = \mathbf{argmin}_{\boldsymbol{j}} \left(-2 \dfrac{1}{|C_j|} \sum_{\vec{x}' \in C_j} K\left(\vec{x}^{(i)}, \vec{x}'\right) + \dfrac{1}{|C_j|^2} \sum_{\vec{x}' \in C_j} \sum_{\vec{x}'' \in C_j} K(\vec{x}', \vec{x}'') \right) \\ \mathbf{0} & \textbf{otherwise} \end{cases}$$

Where:

- $z_{ij} = \begin{cases} 1 & \text{if } \vec{x}^{(i)} \in C_j \\ 0 & \text{otherwise} \end{cases}$
- $K: \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ is a kernel function.



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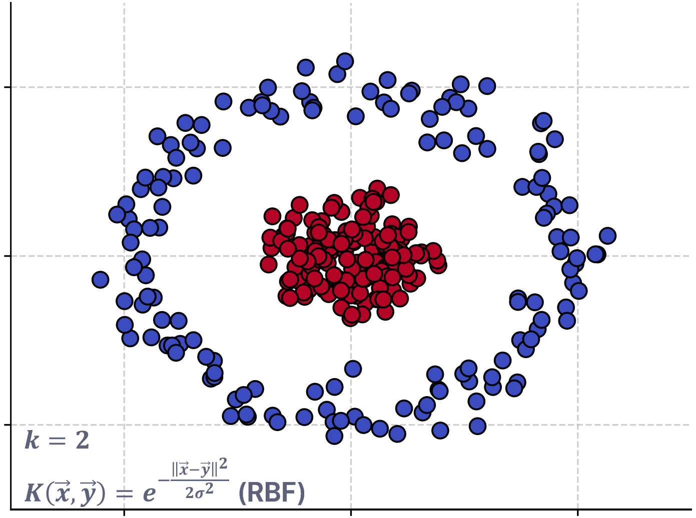

K-means in Python

```python
from sklearn.cluster import KMeans
from sklearn.metrics import silhouette_score, silhouette_samples, adjusted_rand_score
from sklearn.mixture import GaussianMixture

km = KMeans(n_clusters = 4) # k = 4, by default it uses k-means++ initialization and does 10 runs
km.fit(X) # run the algorithm, compute the cluster centers
y = km.predict(X) # cluster assignment for the points it was fitted on
km.cluster_centers_
km.inertia_ # final distortion value

silhouette_score(X, y) # mean silhouette score over all samples
```

Summary

- **K-means** is a clustering algorithm which *partitions* the data points into a *fixed* number of clusters *k*.
- Each cluster is represented by a **centroid** and points are assigned to the cluster with the closest centroid.
- It uses an iterative **expectation-maximization** method to optimize the objective function and might get stuck in local optima.
- Number of clusters *k* is a *hyperparameter* which can be tuned by using the **elbow** method and the **silhouette** coefficient.
- K-means can only obtain *non-convex spherical* clusters and tends to produce clusters of *equal sizes*.
- **Soft K-means**, **Gaussian Mixture Models** and **Kernel K-means** are extensions which can deal with some of the limitations of k-means.

History of K-means

- ***"Sur la division des corps matériels en parties"***
  - First introduced the idea — Hugo Steinhaus, 1957
- ***"Least square quantization in PCM"***
  - First proposed the algorithm, but published it outside Bell Labs only in 1982 — S. P. Lloyd, 1957
  - Sometimes called Lloyd's algorithm
- ***"Cluster analysis of multivariate data: efficiency versus interpretability of classification"***
  - Basically published the same method as Lloyd — E.W. Forgy,1965
    - which is why it is sometimes referred to as Lloyd-Forgy
- ***"Some methods for classification and analysis of multivariate observations"***
  - First use of the term *"k-means"*. — J. MacQueen, 1967

Keywords

Clustering

K-Means

Expectation-Maximization

Cluster Centers (Centroids)

Partition

Elbow Method

Silhouette Coefficient

K-means++

Rand Index

Soft K-means

Gaussian Mixture Models

Kernel K-means