Aprendizado de Máquina e Reconhecimento de Padrões

Kmeans

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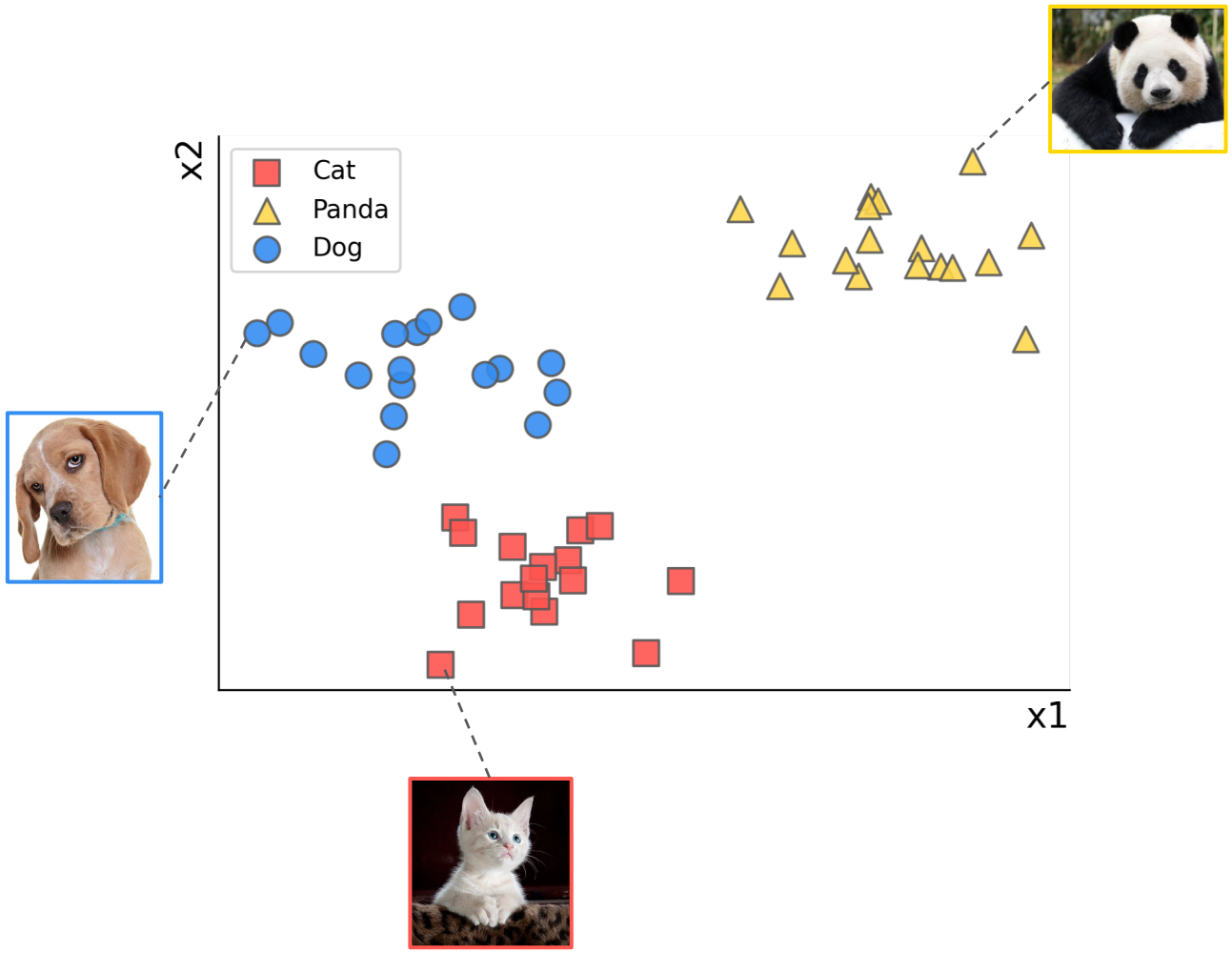
São Paulo
Campus Campinas

Supervised Learning (e.g., classification)

Previously **annotated/labeled** **training data**.



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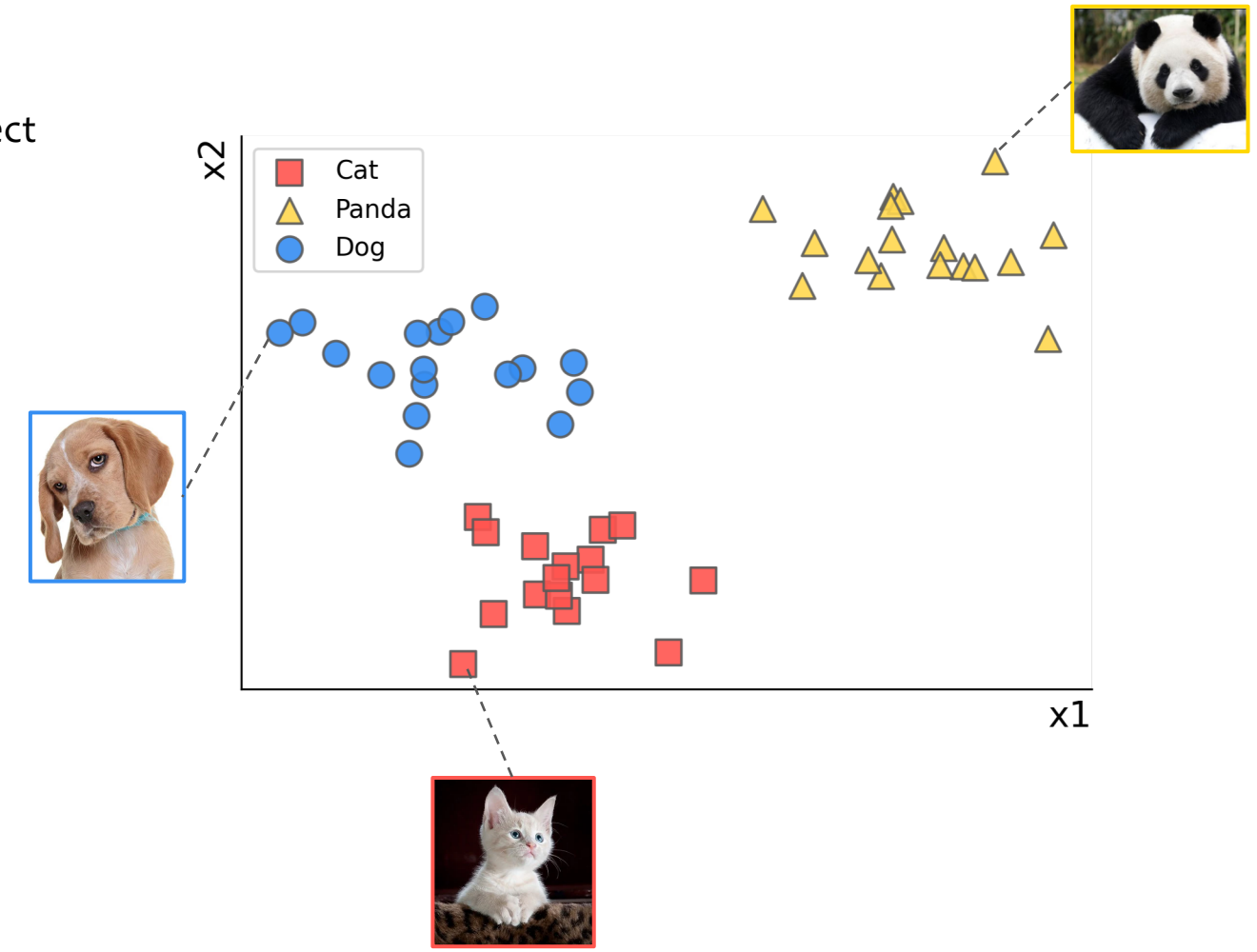

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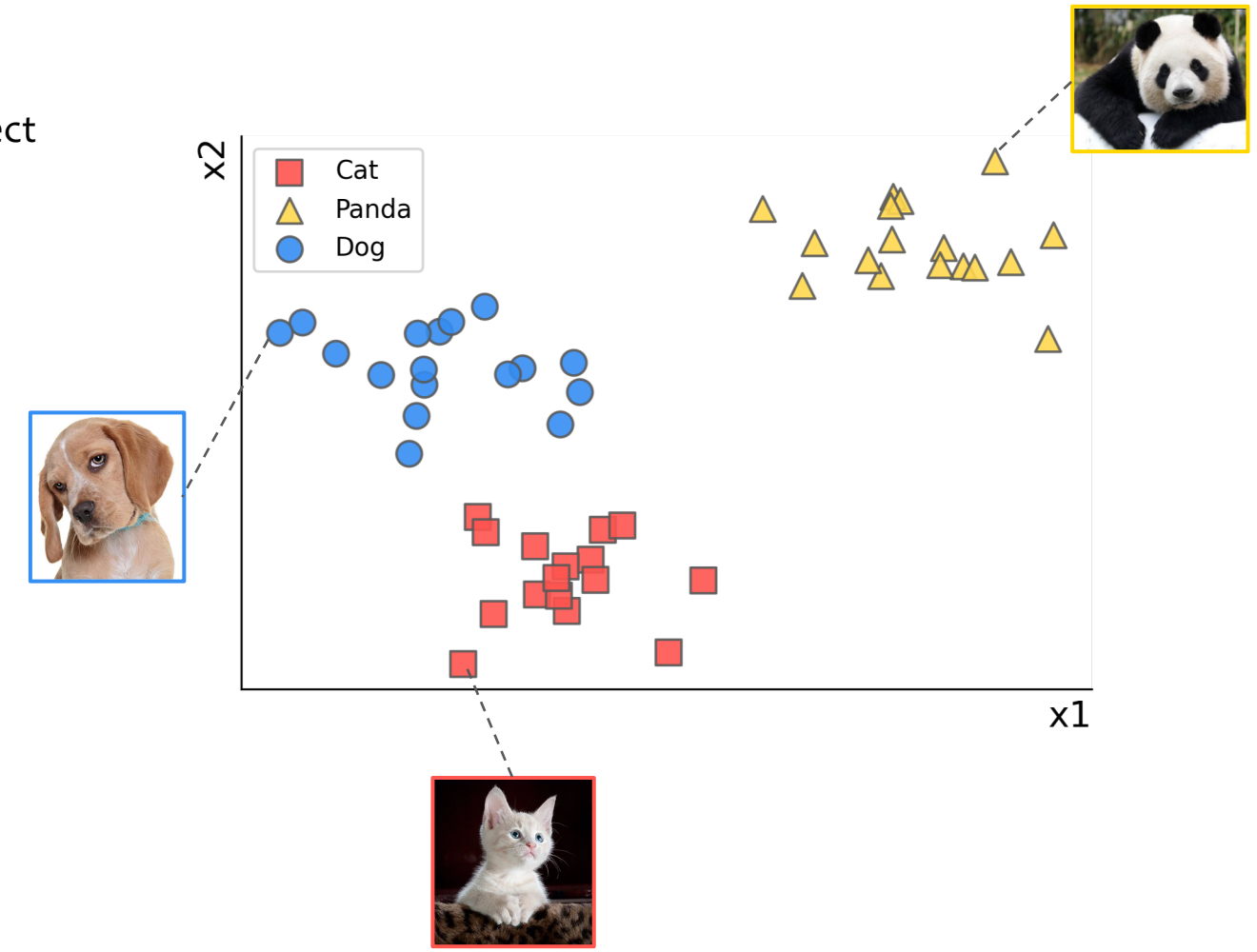

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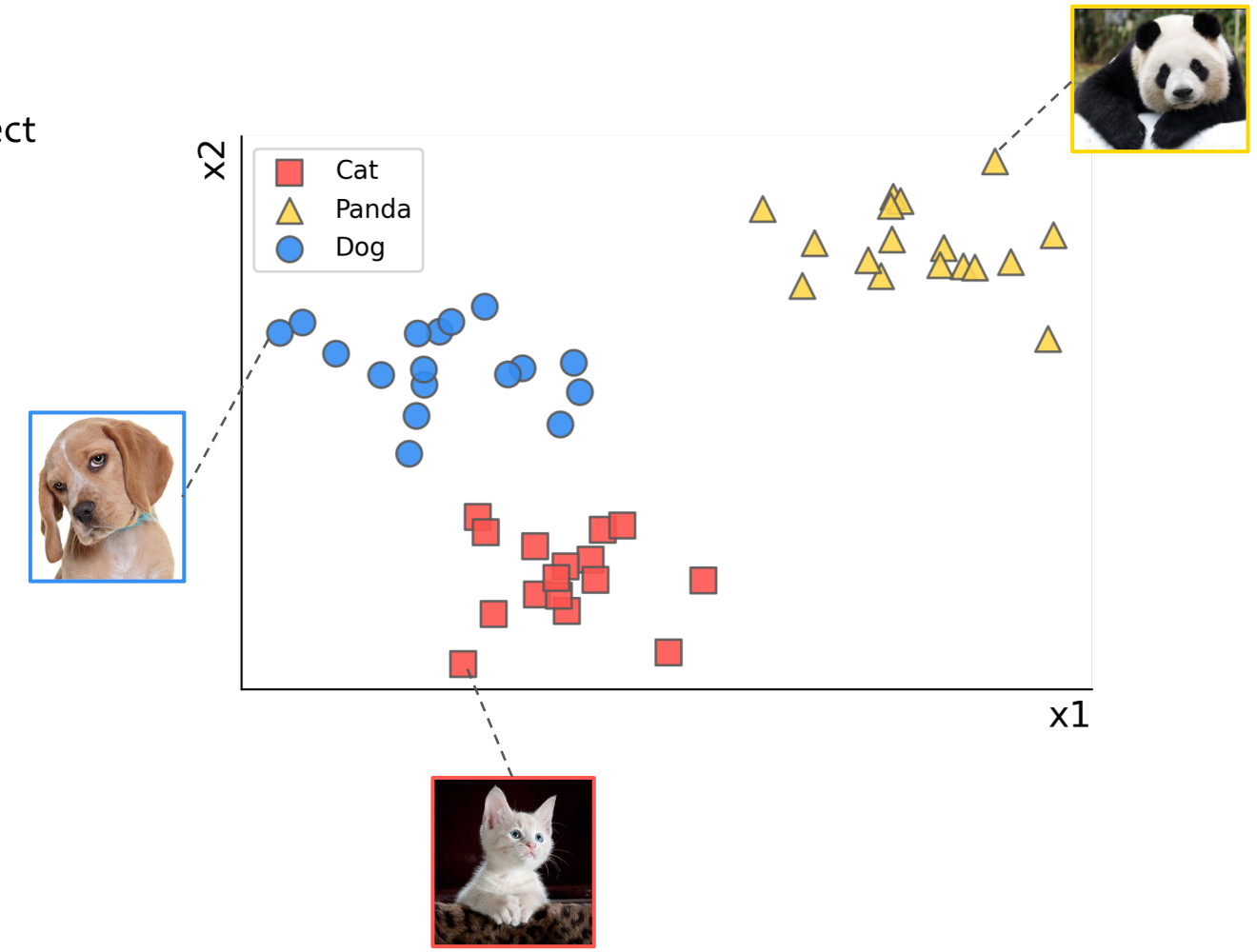

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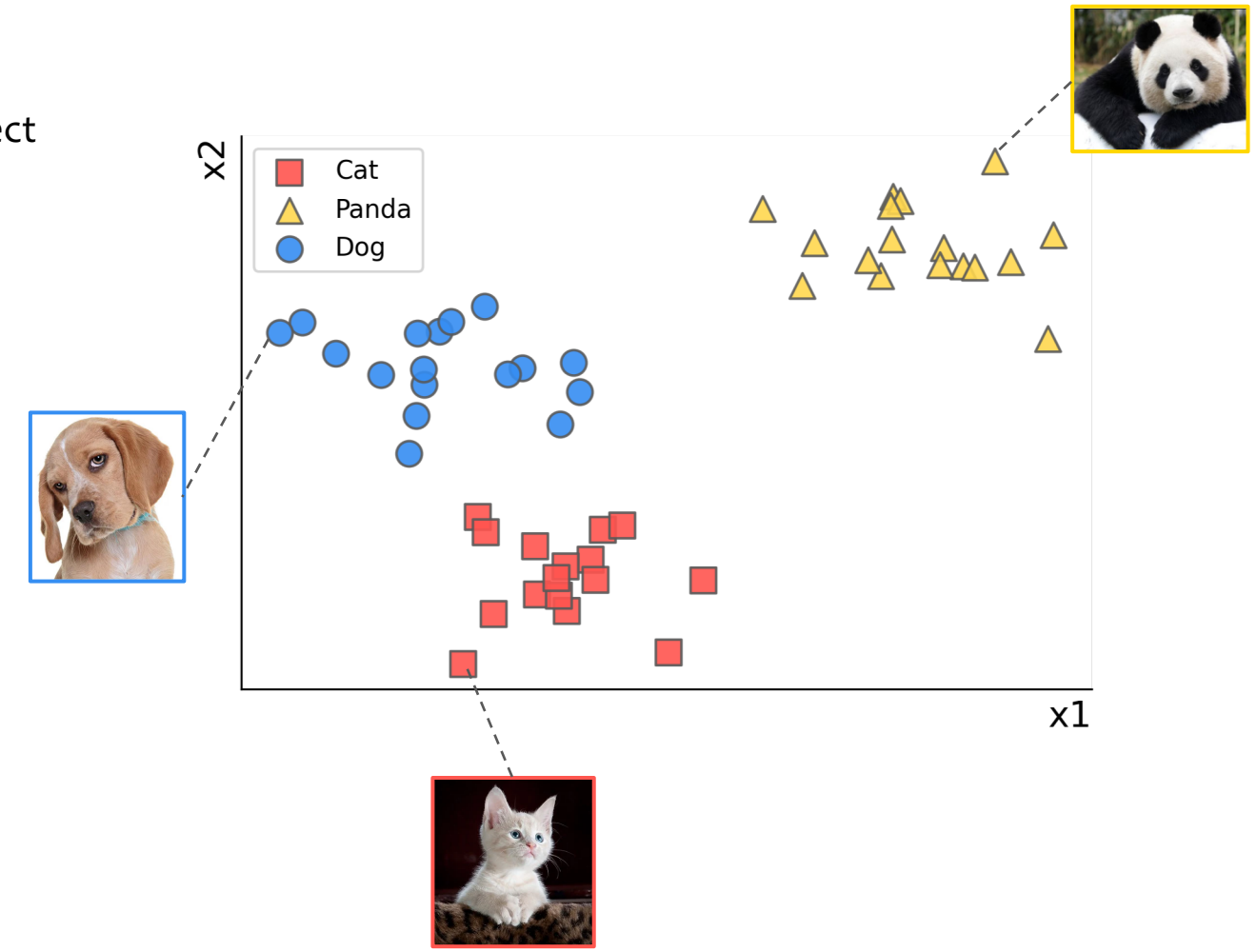

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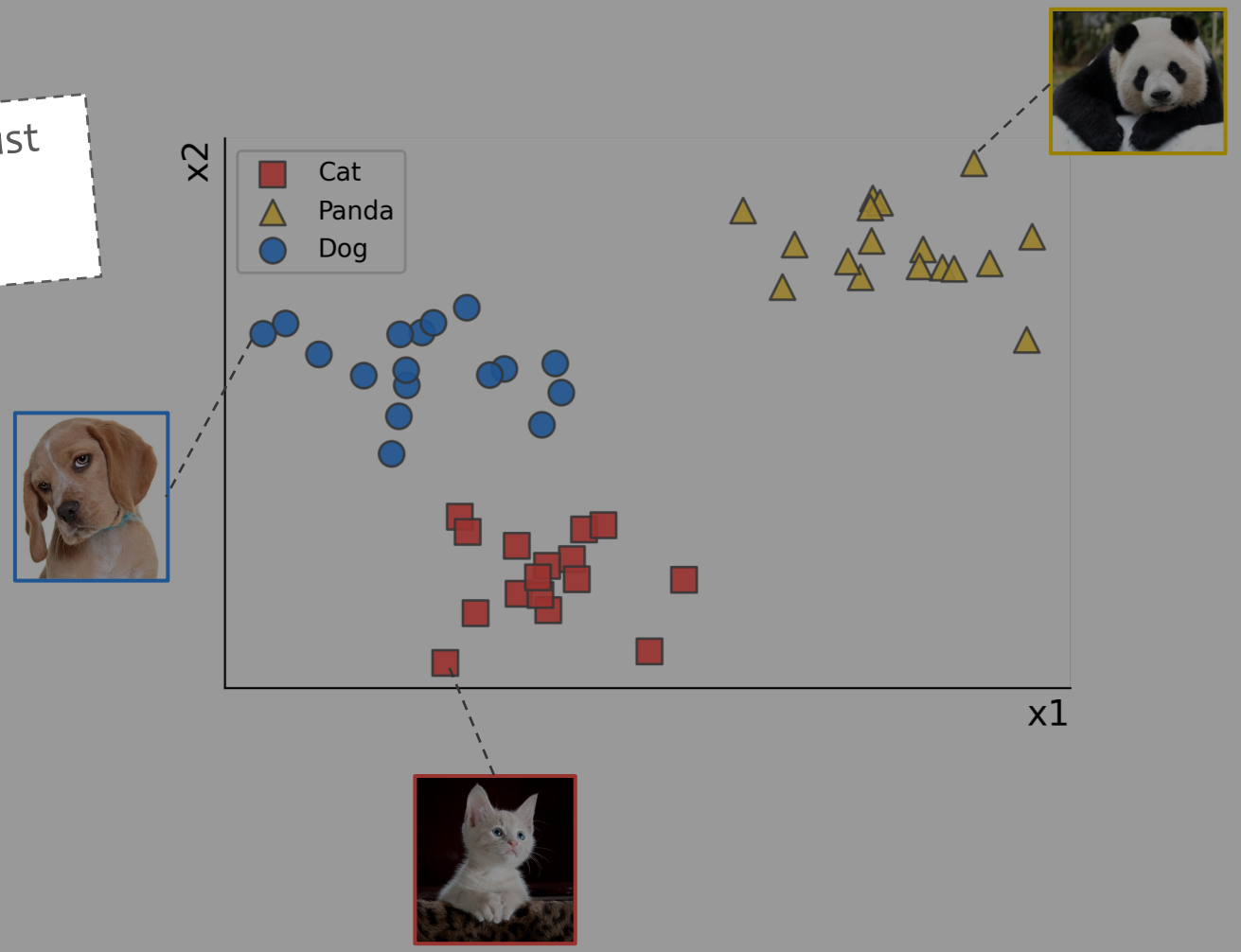

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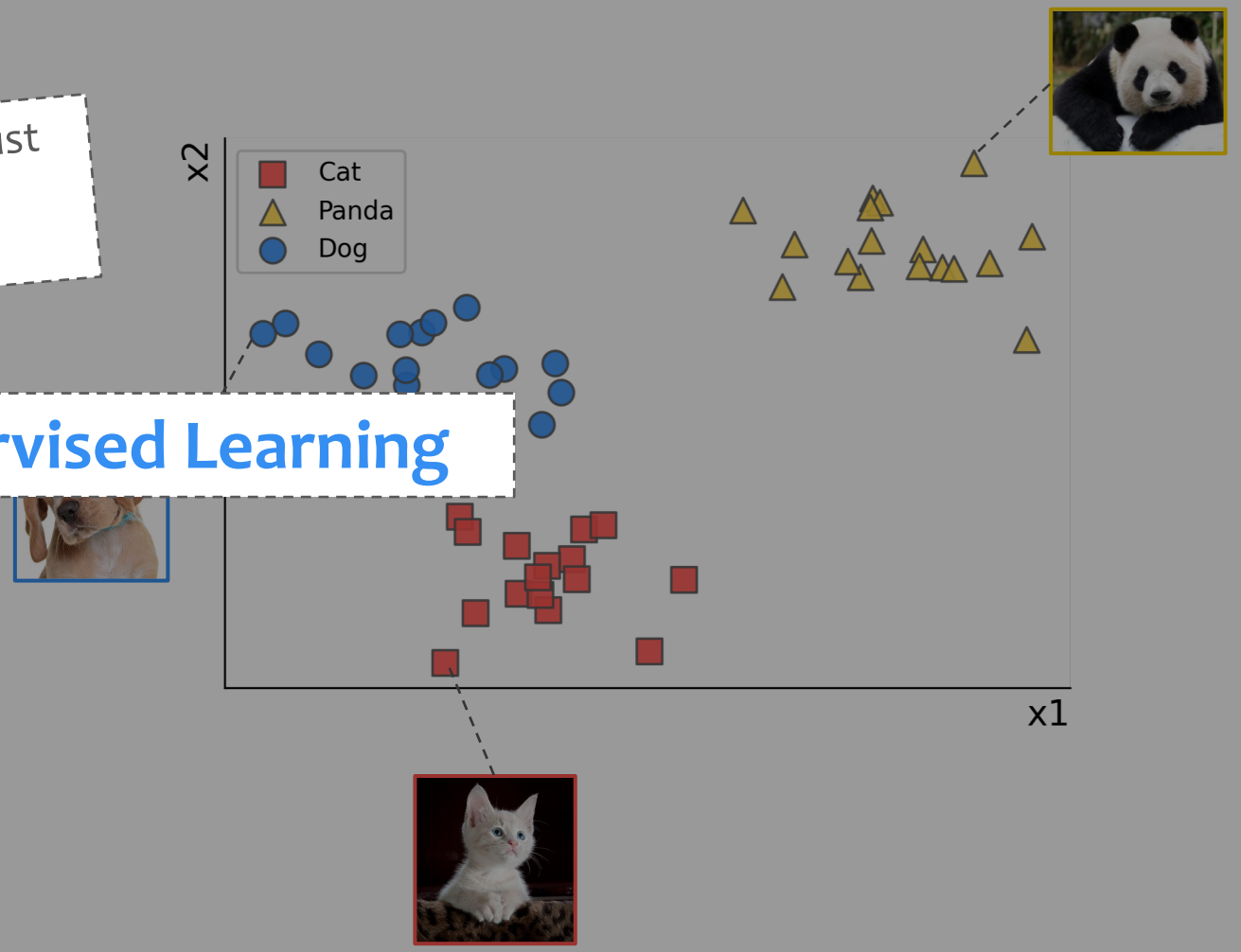

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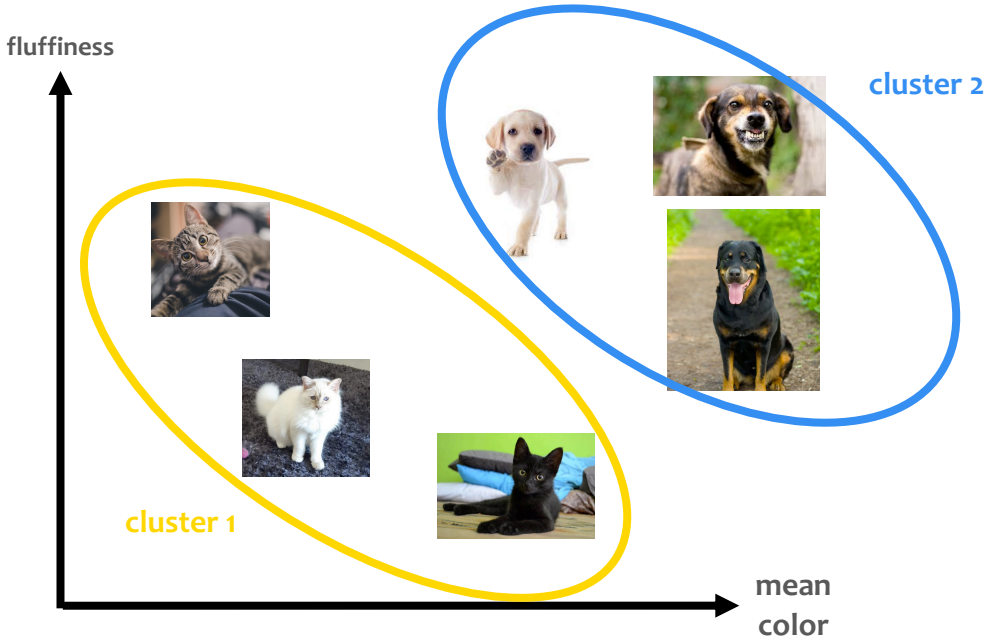
Unsupervised Learning

no supervision → **no** labels / annotations

Clustering



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- DBSCAN
- Mean-shift
- OPF Clustering
- Hierarchical Clustering
- ...

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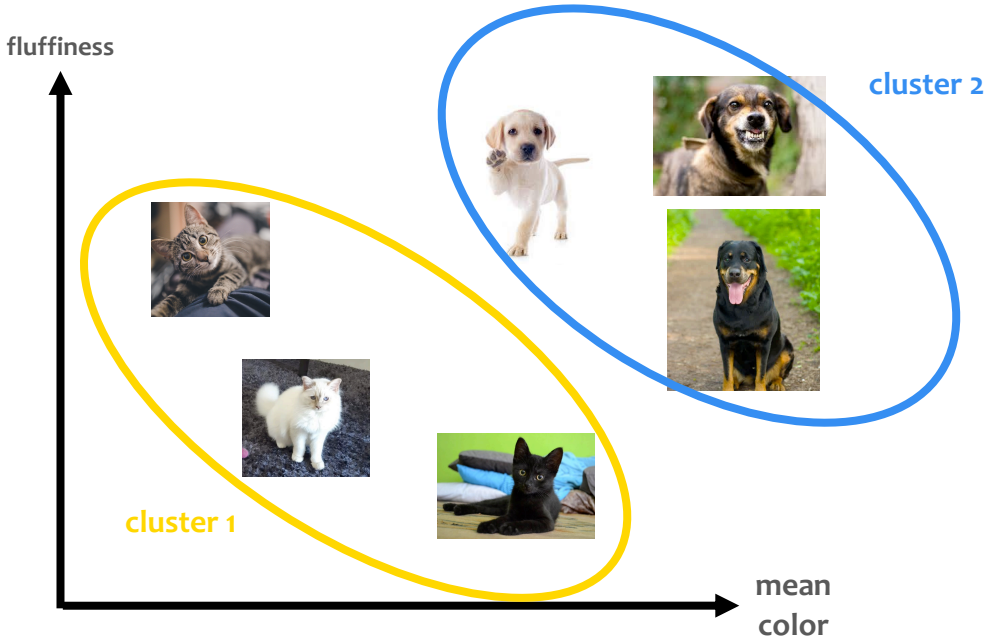

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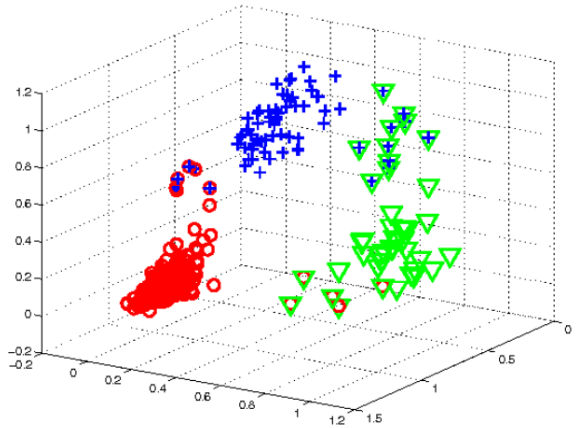
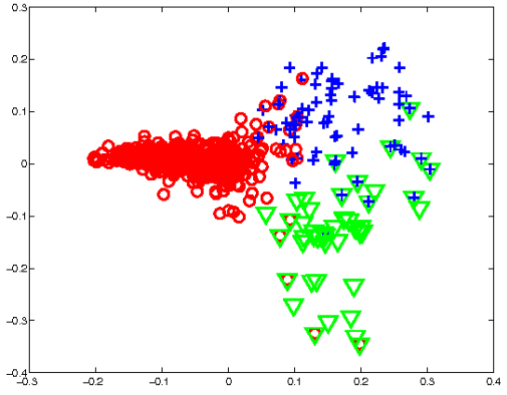
Dimensionality Reduction / Projection

Project a **high-dimensional data** on to a **lower-dimensional feature space** without losing much information.

Projection on to a **2D** or **3D** space is used to **visualize and understand** the data.



high-dimensional data



projection

- Principal Component Analysis (PCA)
- Locally Linear Embedding (LLE)
- t-SNE
- UMAP
- ...

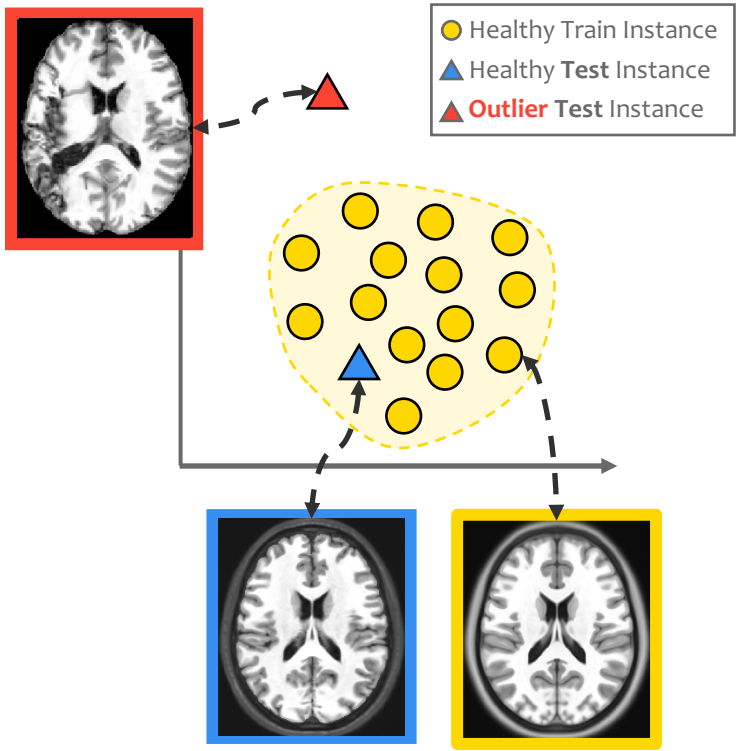
Unsupervised Learning

Anomaly/Novelty/Outlier Detection

The algorithm is fed with **training data** containing **only** a **single class** (normal, control, healthy).

New unseen instances (test) that **DOES NOT** look a **normal one** is an **outlier**, being considered as an **anomaly**.

The **training set** must be very **clean** and **representative**.



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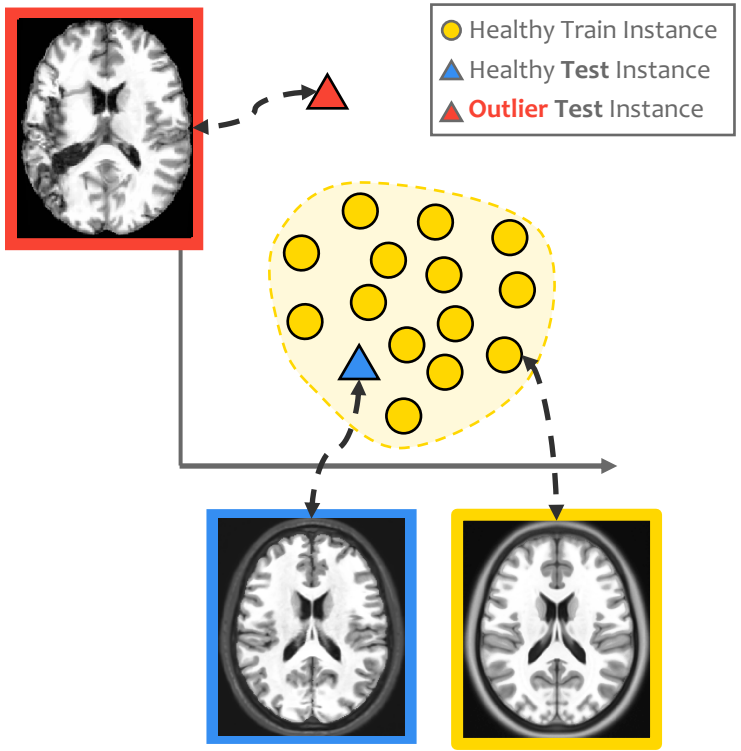
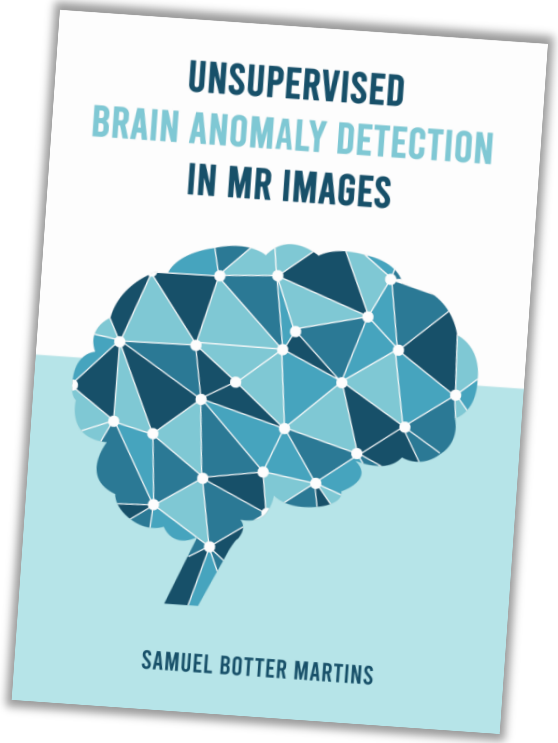
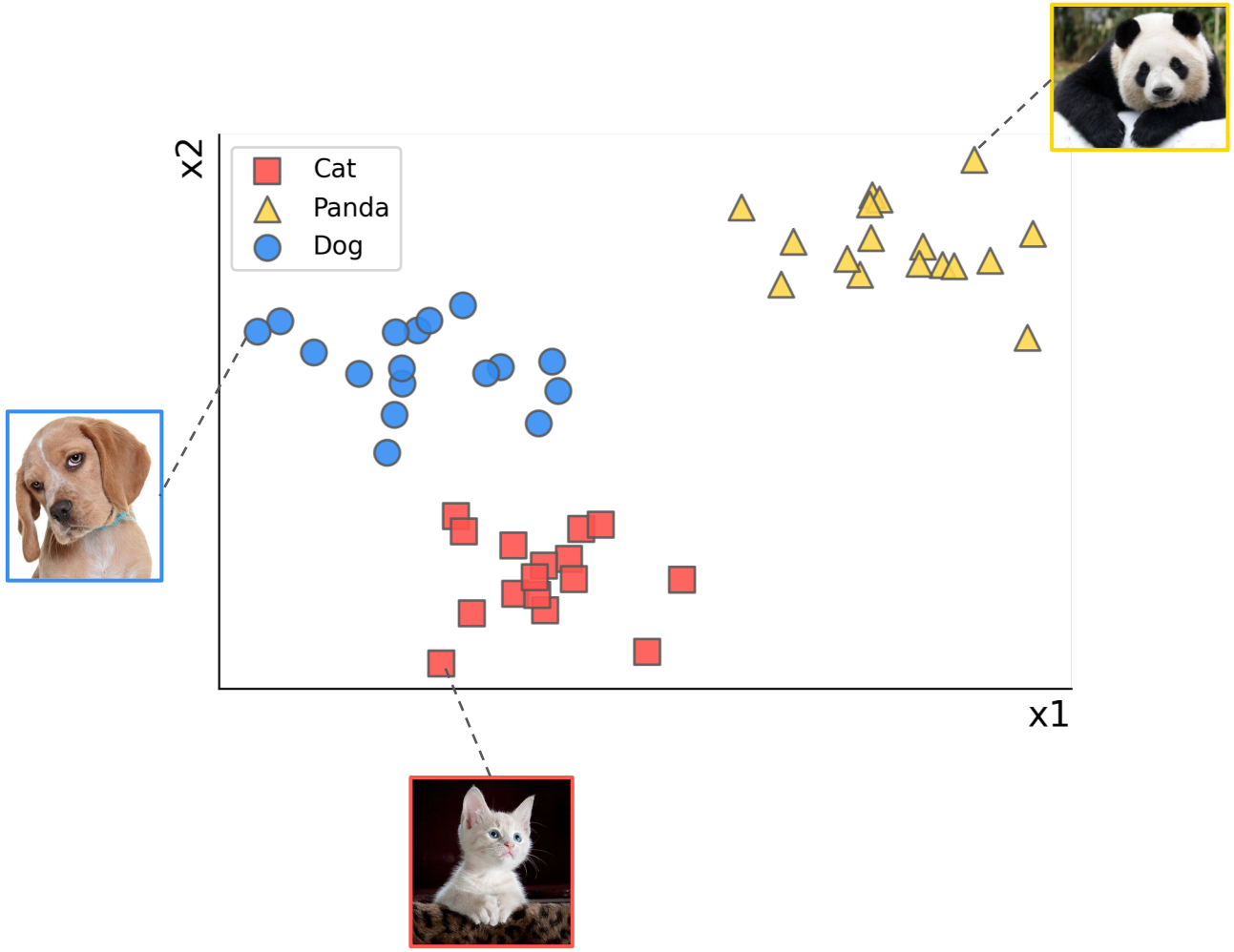




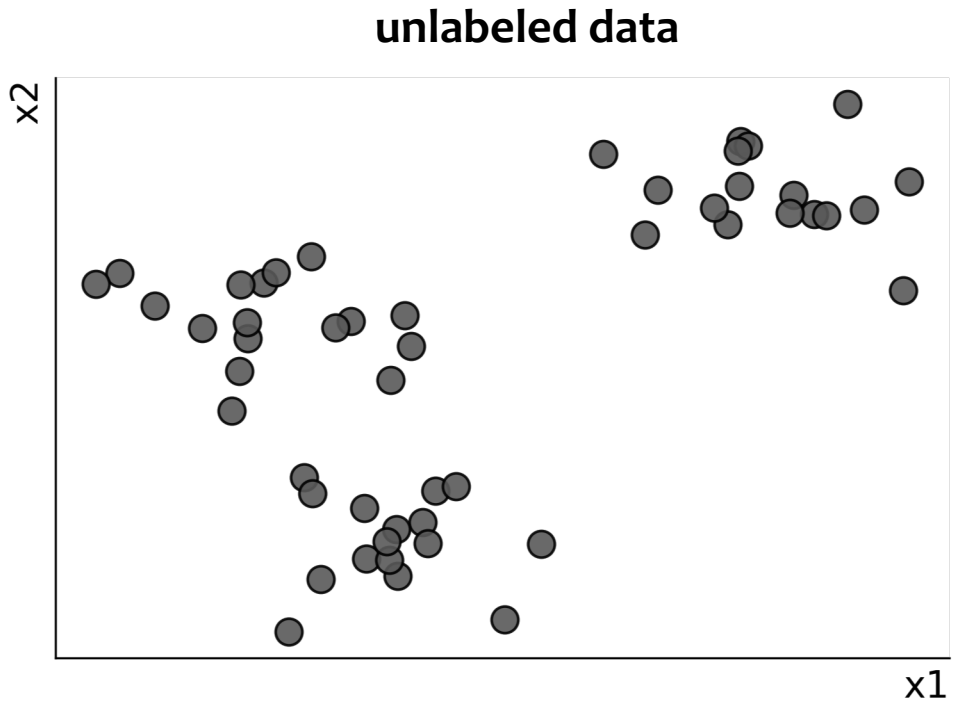
https://research.rug.nl/en/publications/unsupervised-brain-anomaly-detection-in-mr-images

Let’s start with **Clustering!**

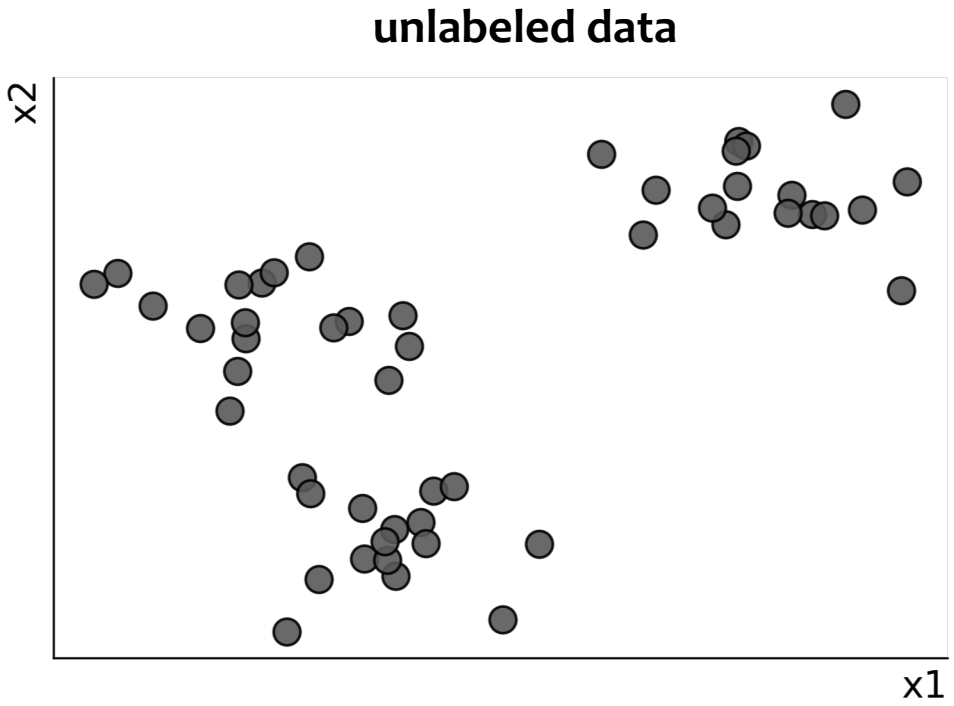
What if instead of having a set of previously labeled data...



What if instead of having a set of previously labeled data, the **data were unlabeled**?



One could use some **clustering algorithm** **to group similar instances** together into *clusters/groups.*



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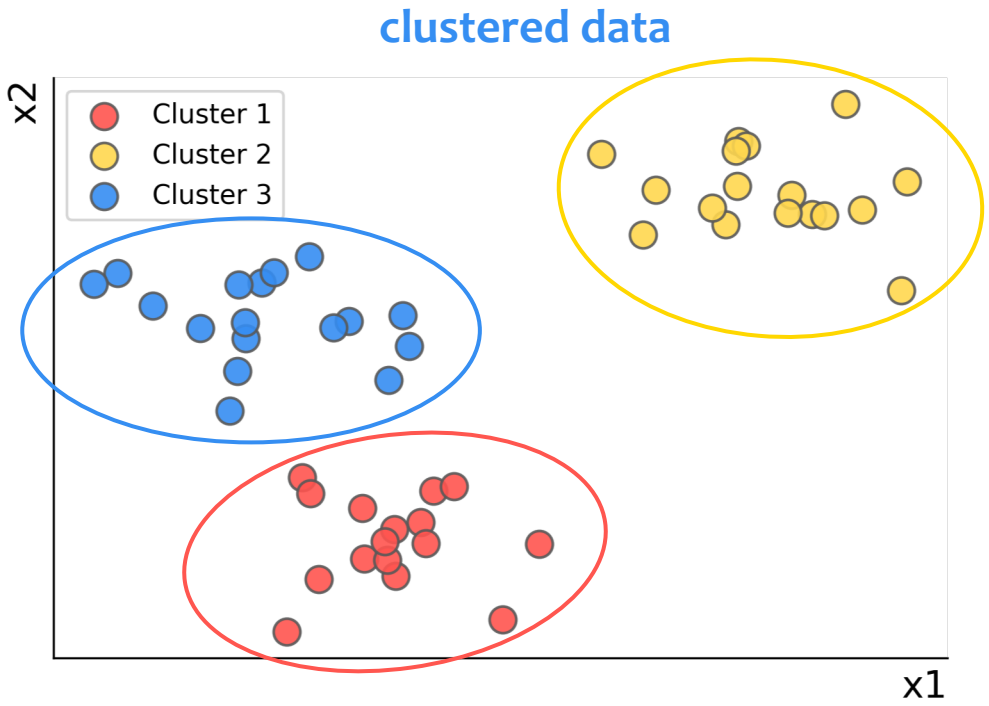

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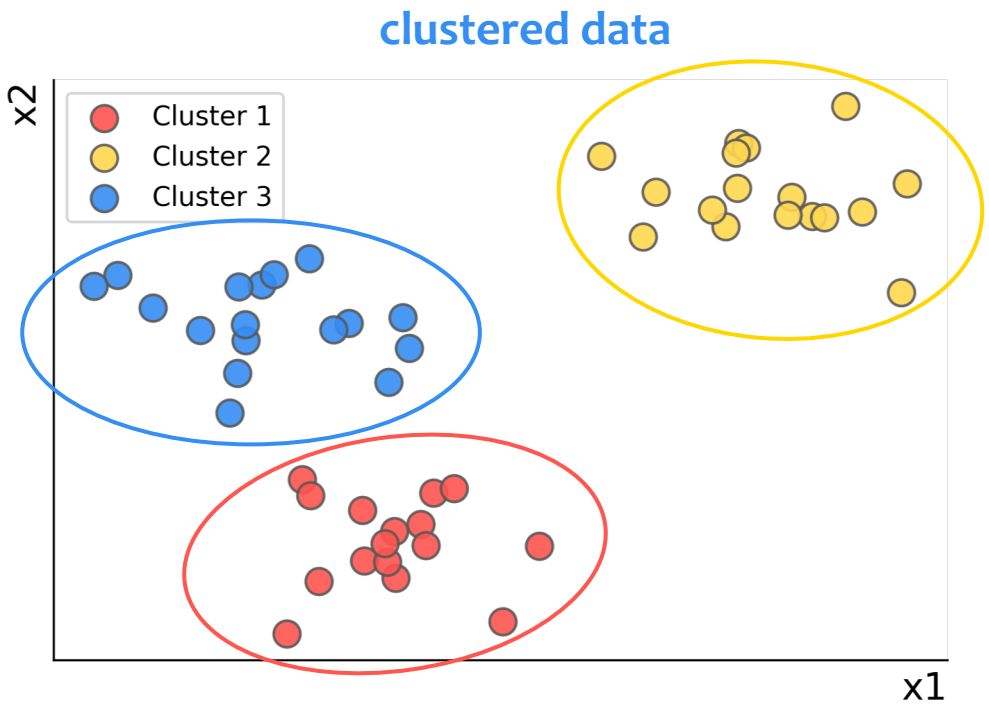

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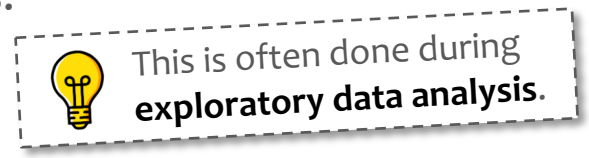
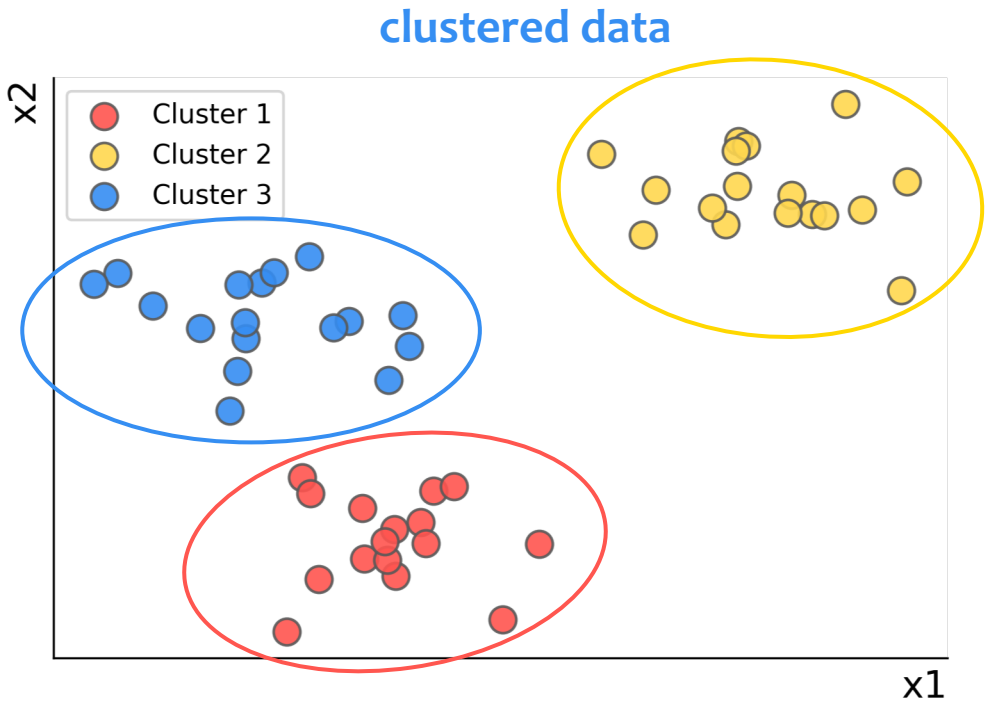


This is often done during **exploratory data analysis**.



Clustering Approaches

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Partition methods

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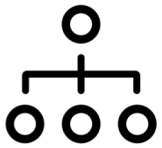

Hierarchical methods

- Creates a **hierarchical decomposition** of the given dataset (agglomerative or divisive).
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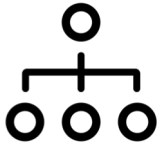

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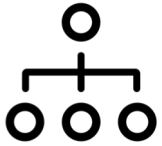

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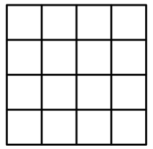

- First divide the space into regular grids, then perform **clustering** on the grids;

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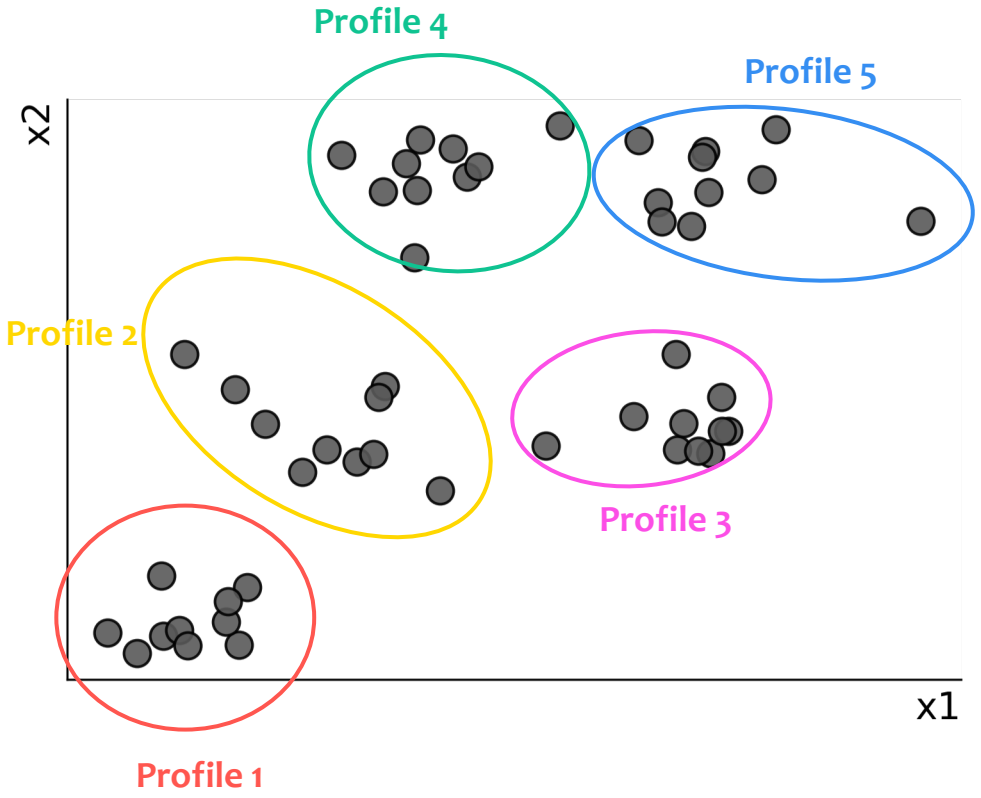

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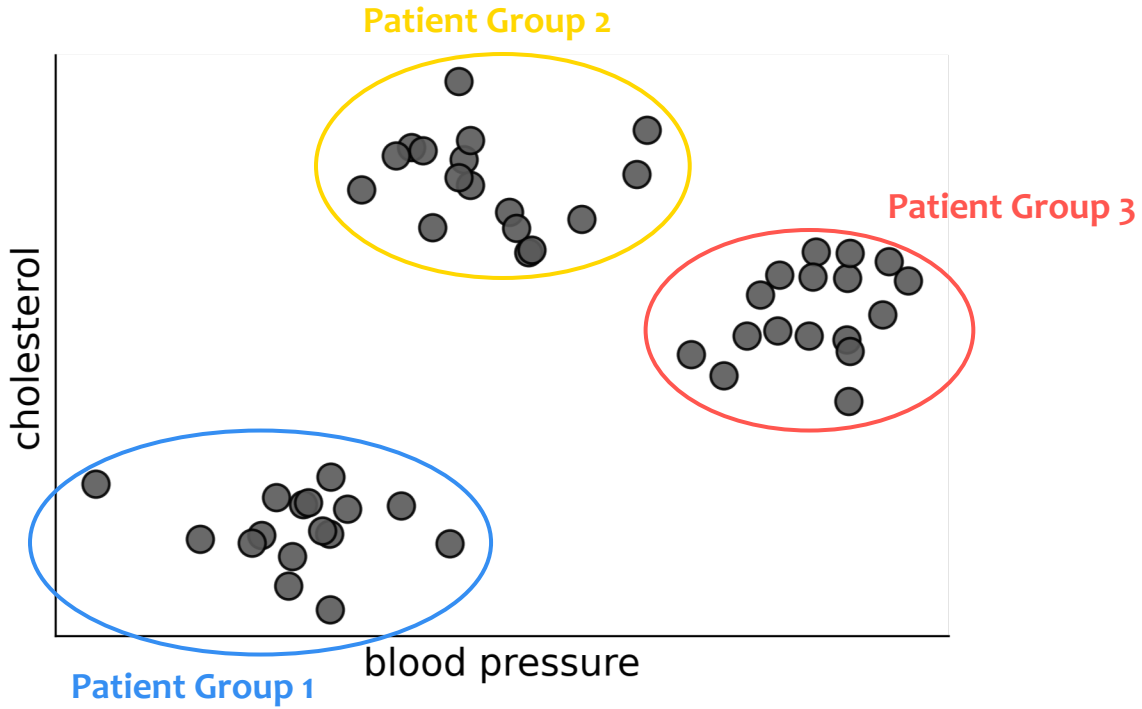

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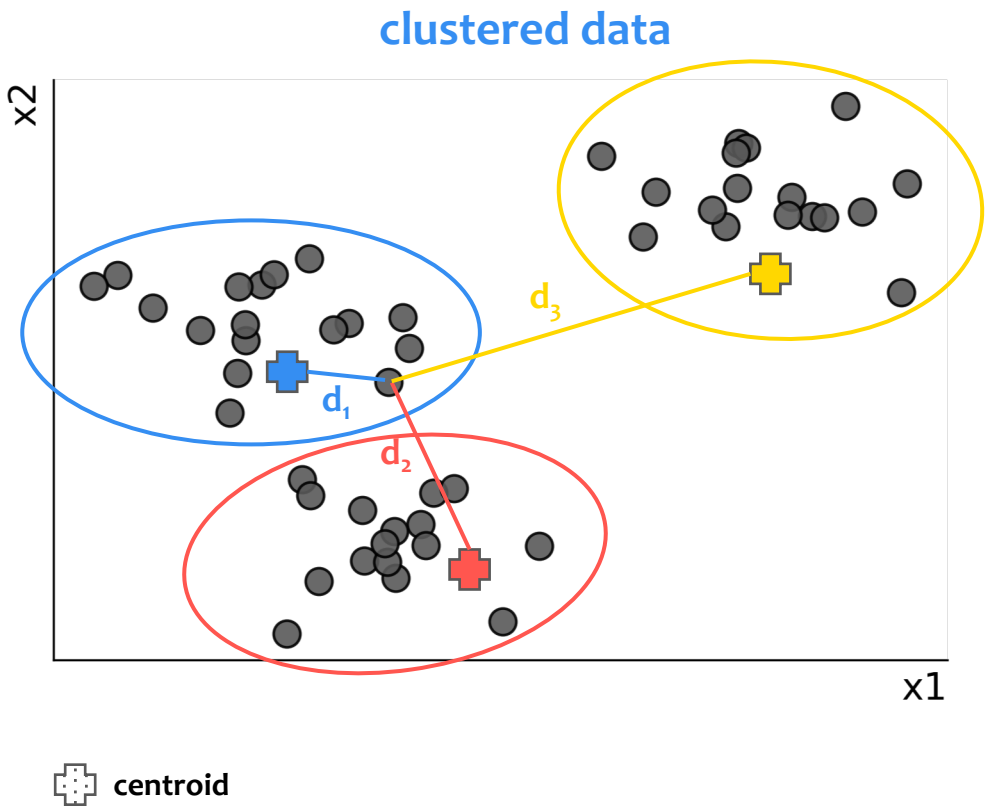

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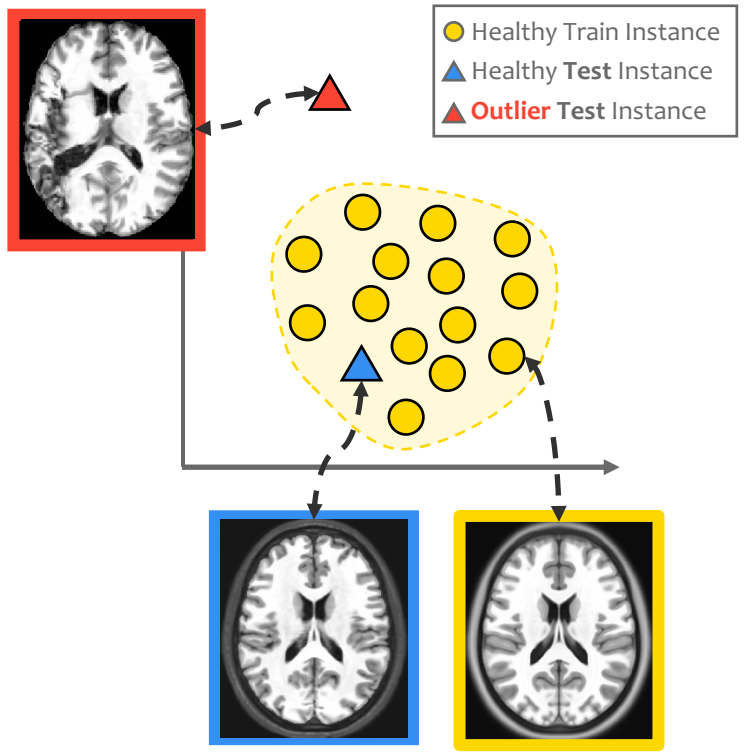

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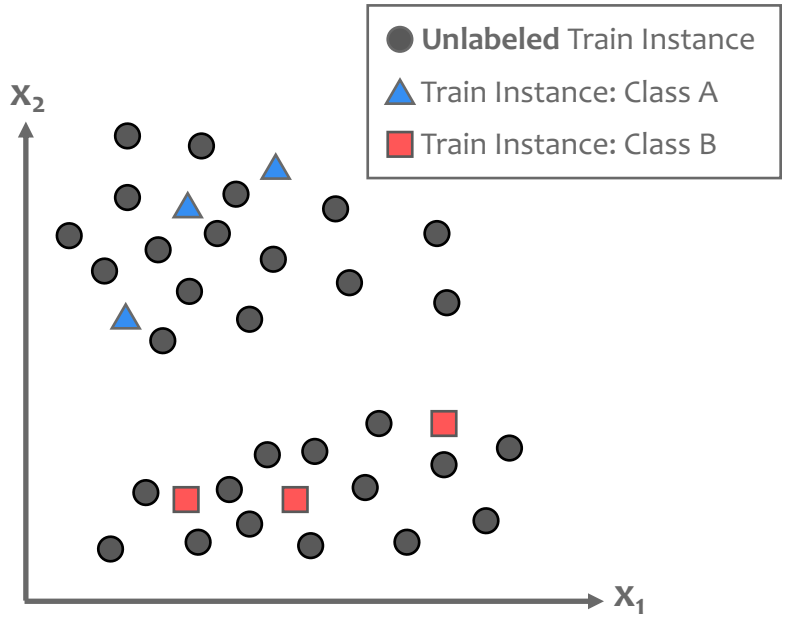

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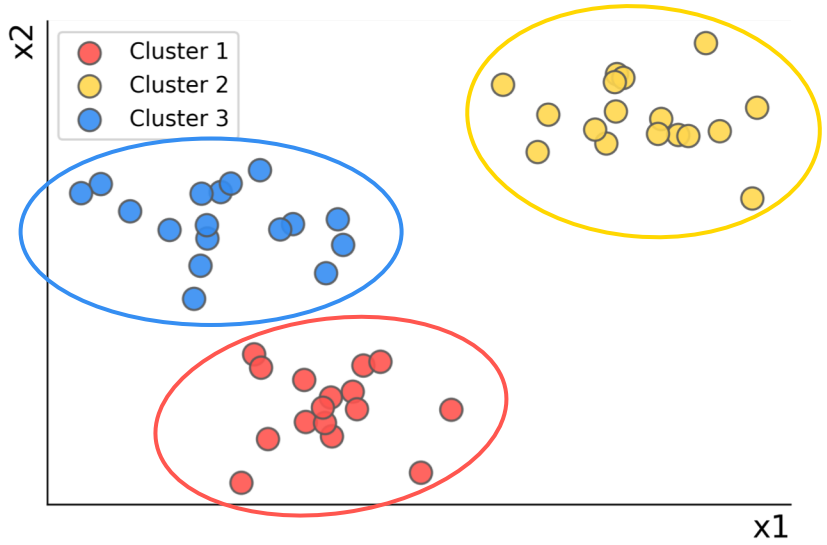
Let's see **KMeans:** the most classical clustering algorithm!

KMeans



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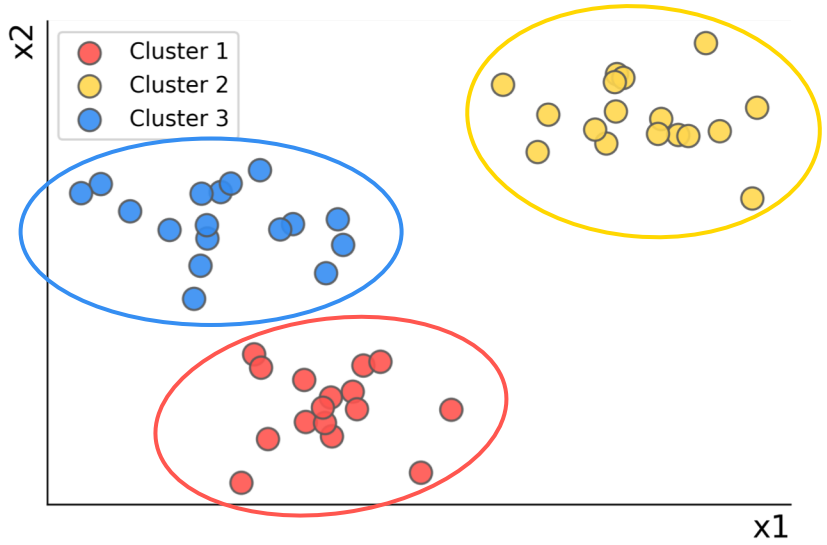

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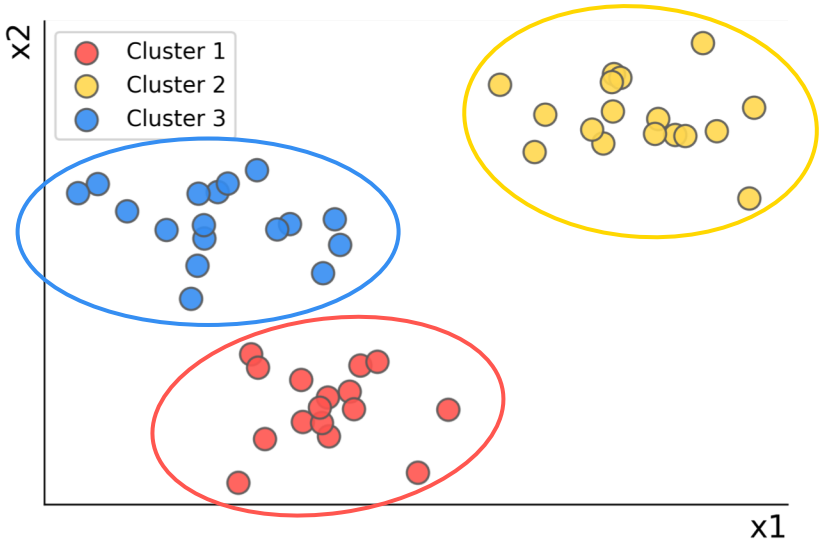
Goal

- **To partition** the dataset into k **clusters**:
  - Each cluster must contain **at least one** sample;
  - Each sample must belong to **exactly one** cluster;
  - The **mass center (mean)** of a cluster corresponds to its **centroid**;



KMeans

Initialization:

1) Choose the **number k** of clusters;

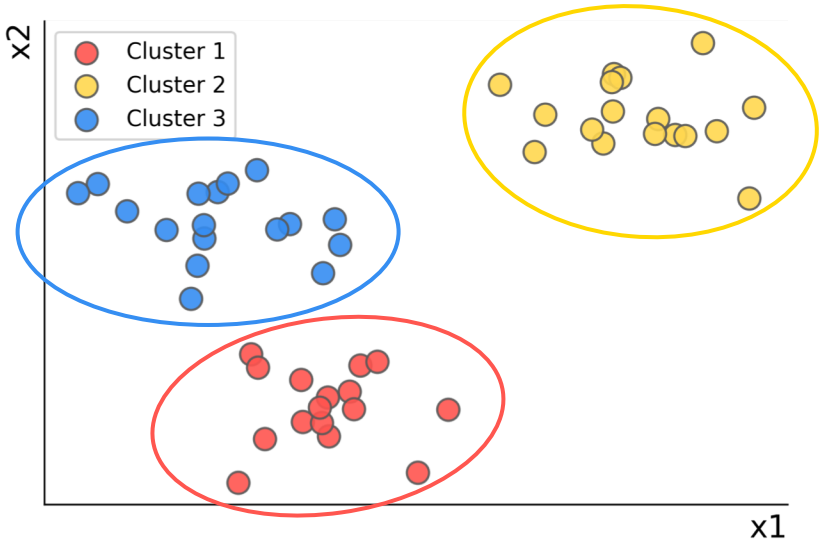
2) Choose the **initial k centroids** (cluster centers);

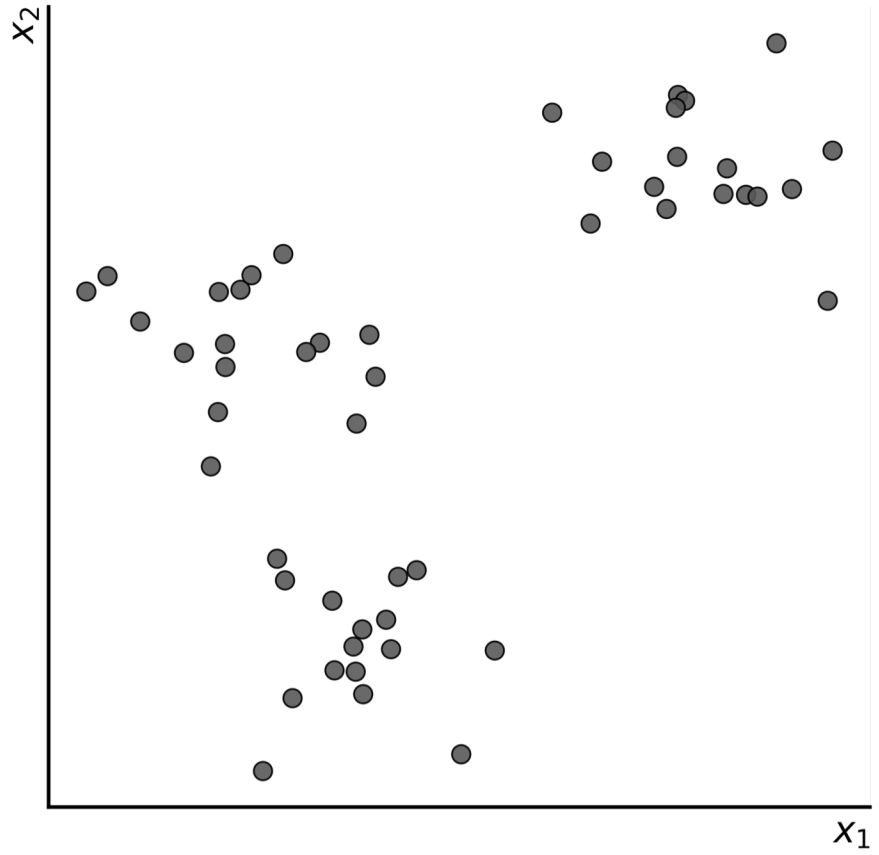
Learning:

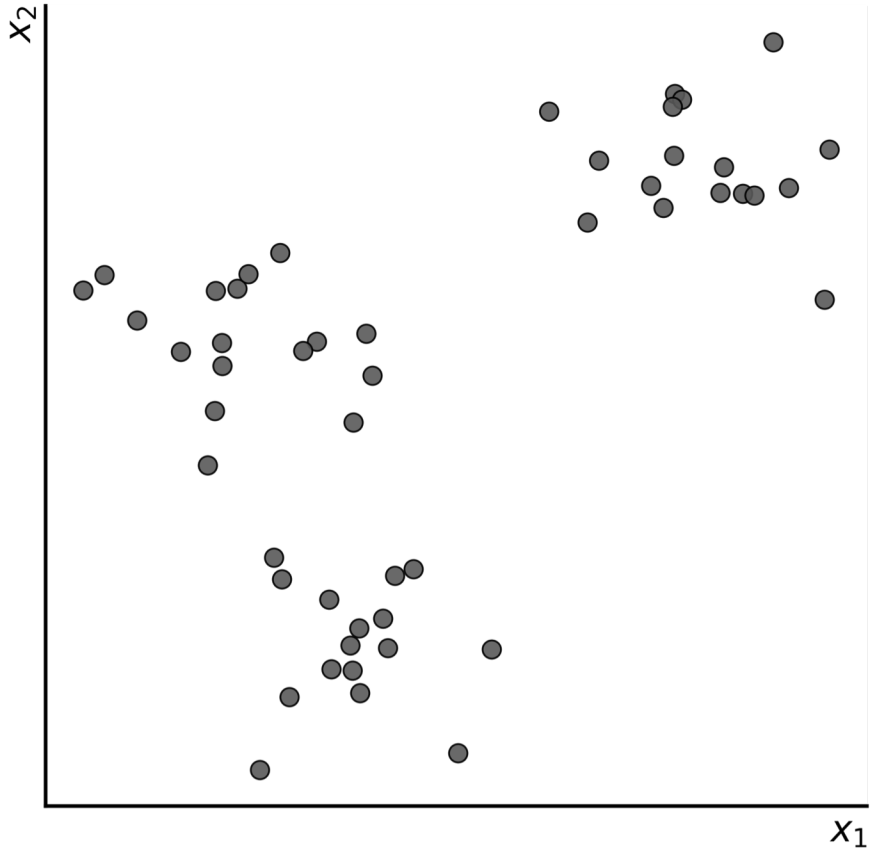
3) Repeat until **convergence**:

- **4)** Assign each instance to **the nearest** centroid;
- **5)** Move the centroids to the centers of their clusters;

6) Assign each instance to **the final nearest** centroid;

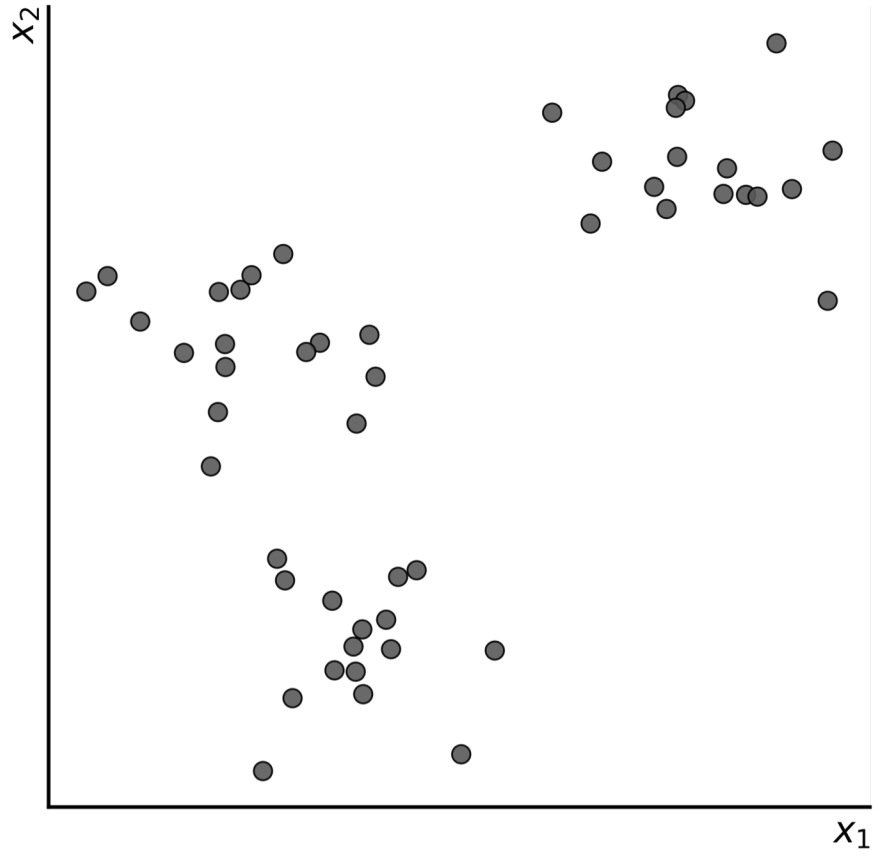



x_2
x_1



Consider that $\mathbf{x_1}$ and $\mathbf{x_2}$ have the **same scale**.

1) Choose the **number k** of clusters;



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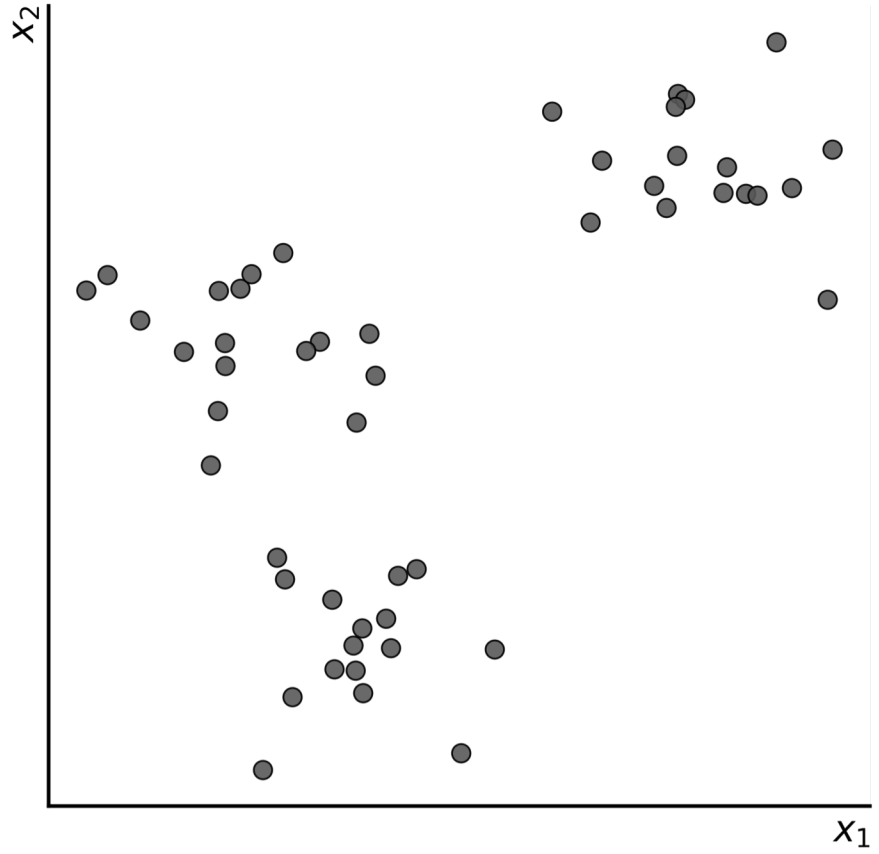
Let's consider: **k=3**



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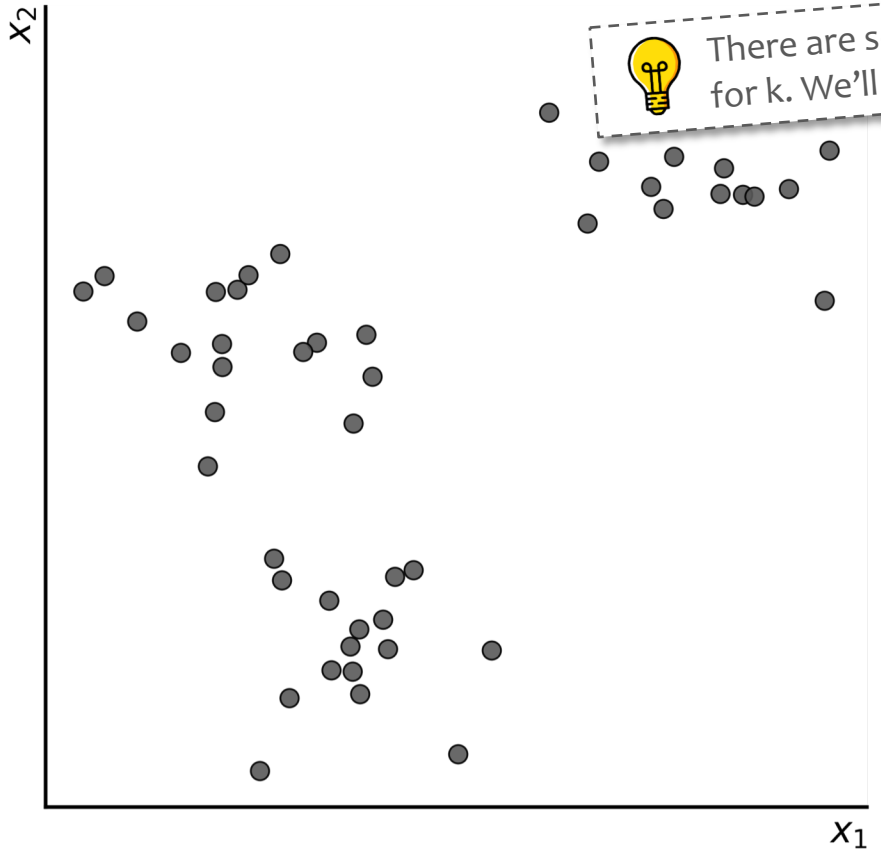
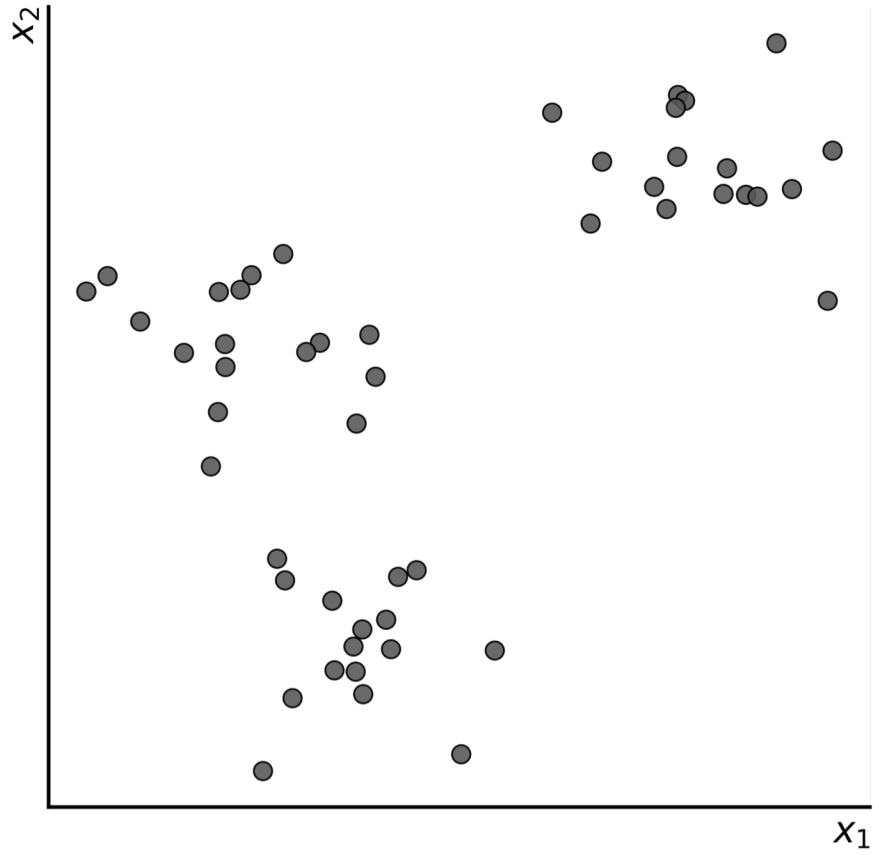


This **hyperparameter is crucial** to obtain high-quality models.

There are some ways to find a proper value for k. We'll see them soon!

2) Choose the **initial k centroids** (cluster centers)



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- random instances from the dataset (Forgy initialization); or
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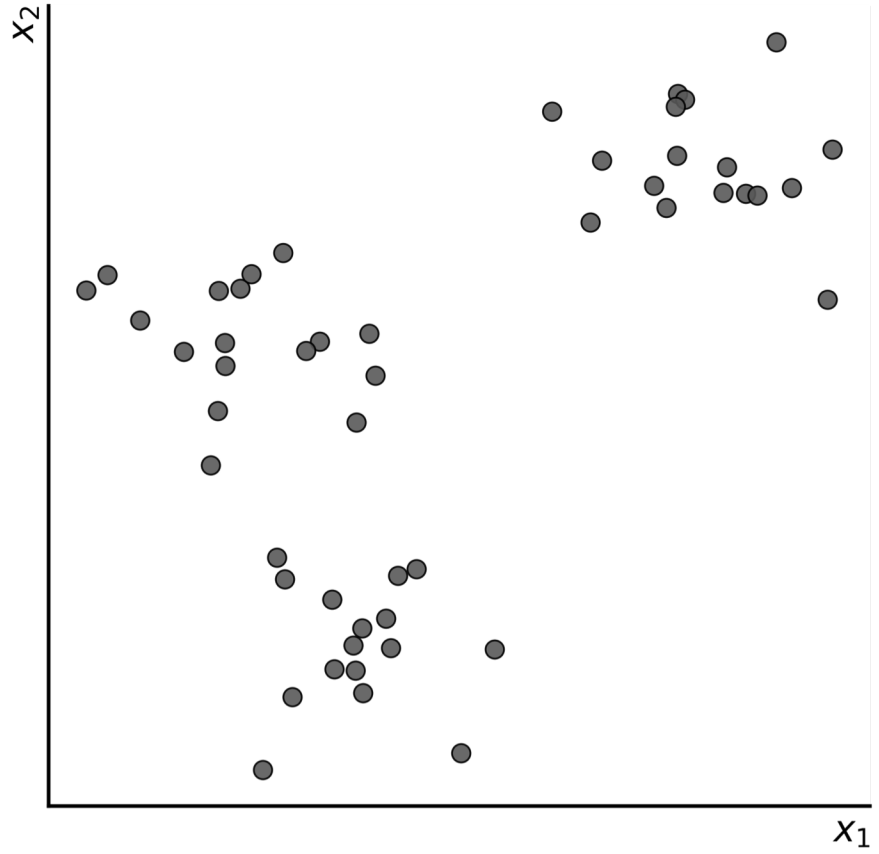

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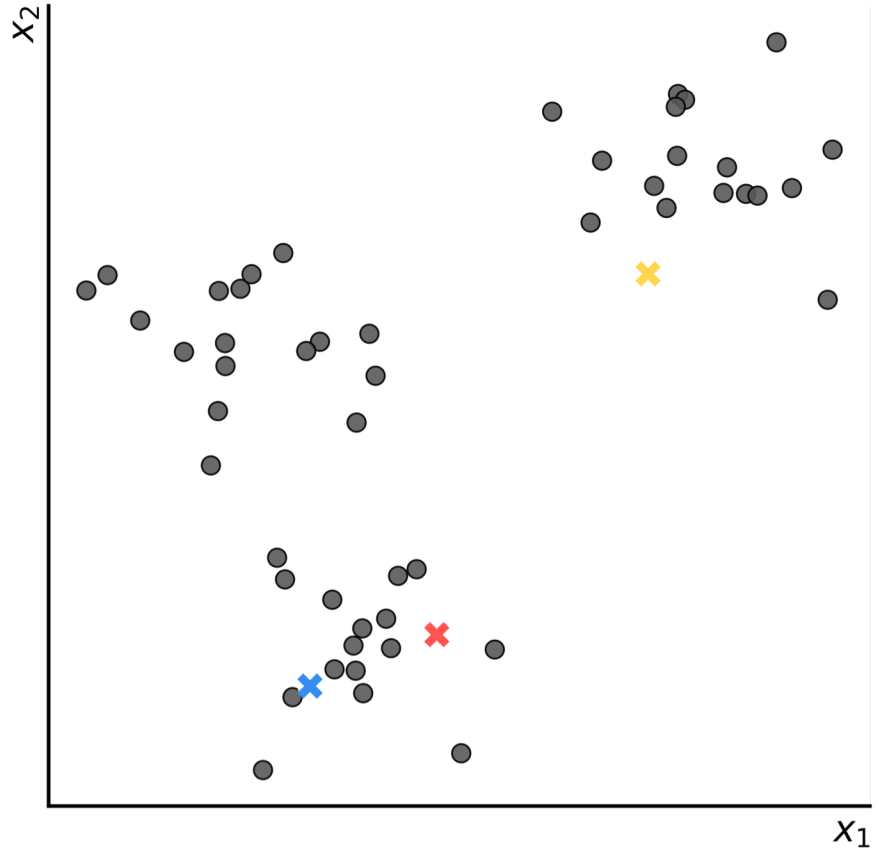

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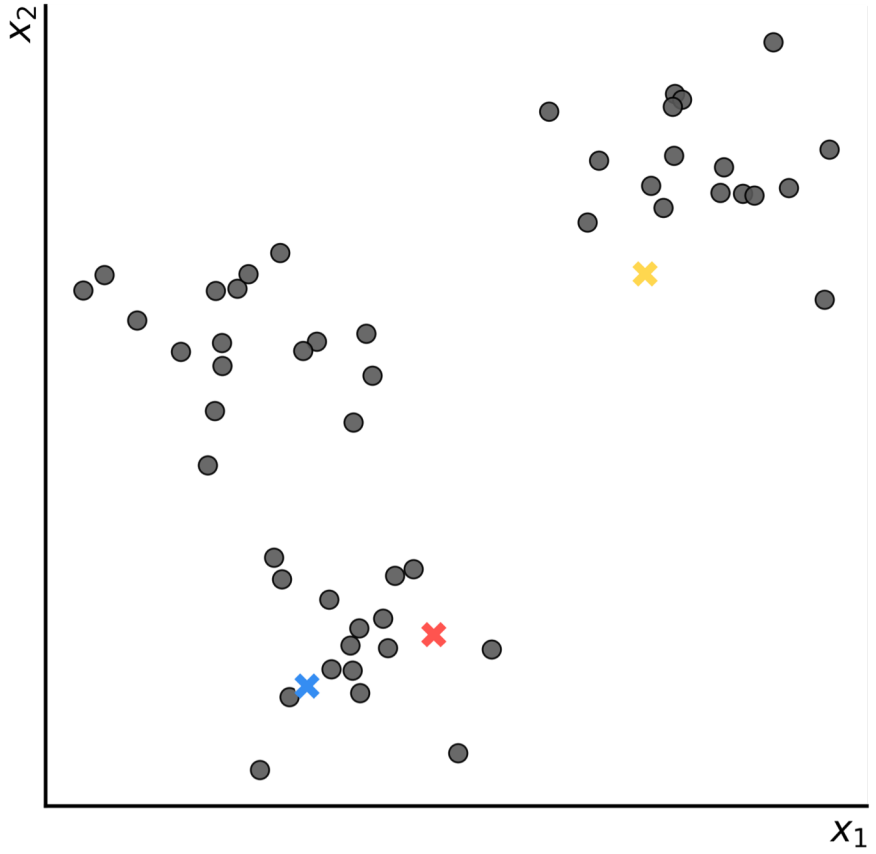
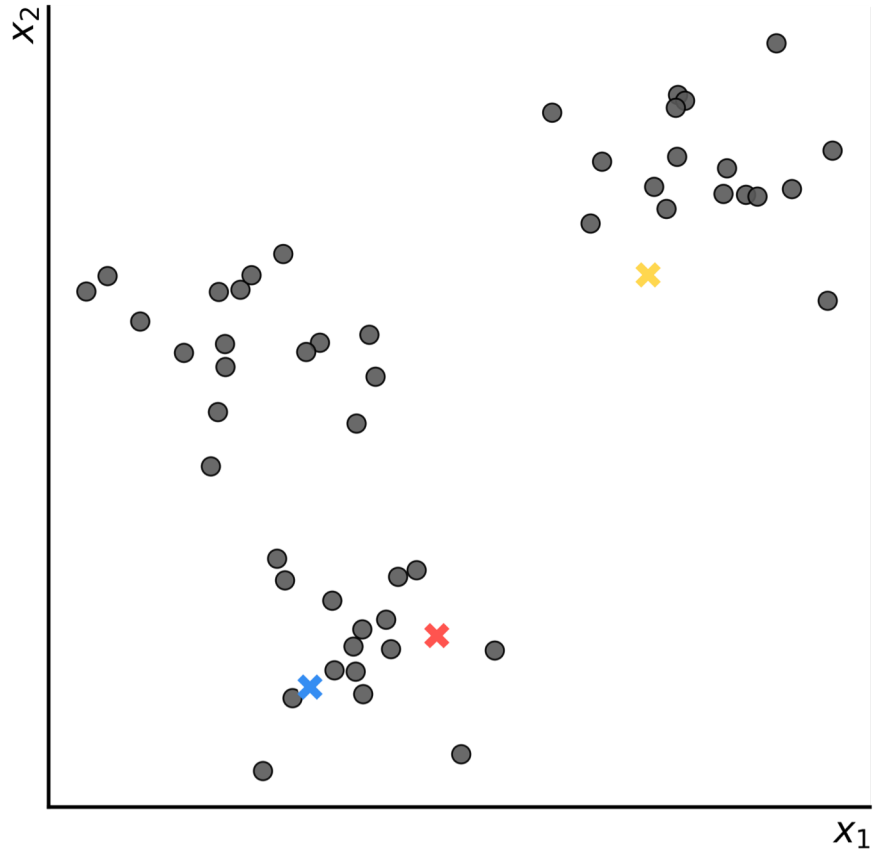


3) Repeat until **convergence**:



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- No reassigment occurrs; and/or
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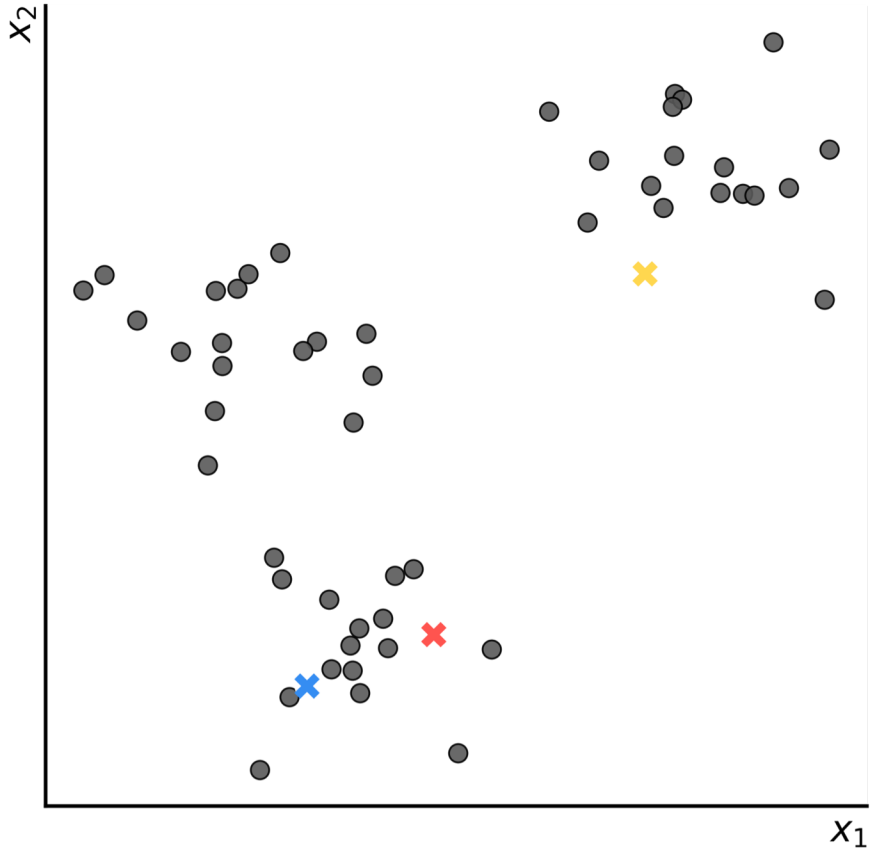

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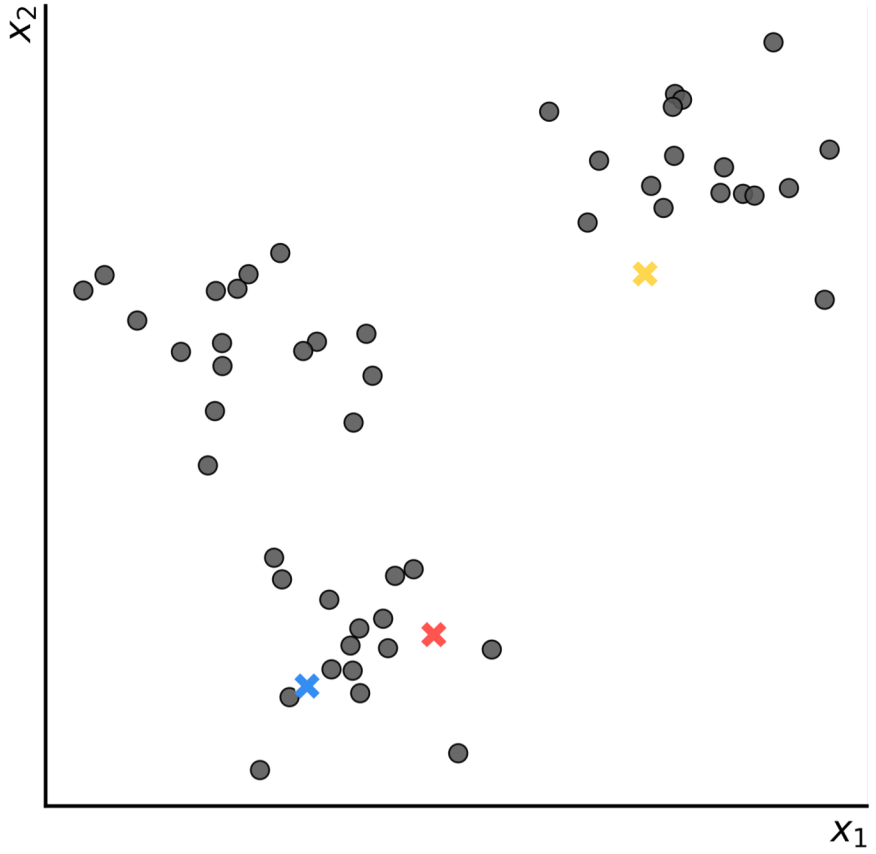

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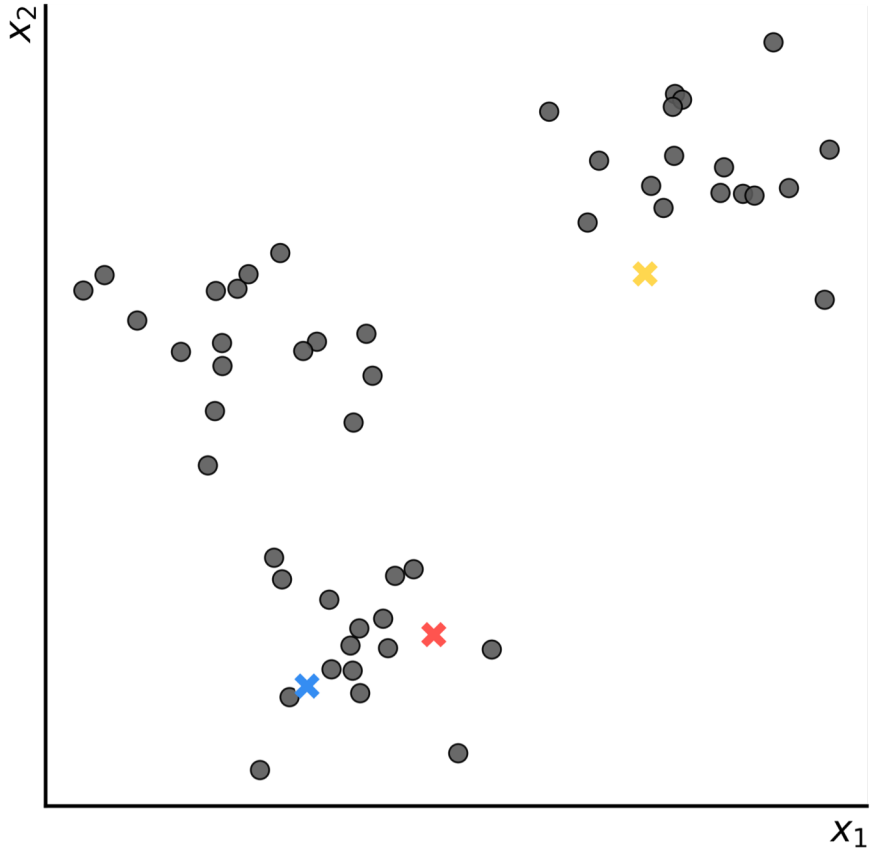

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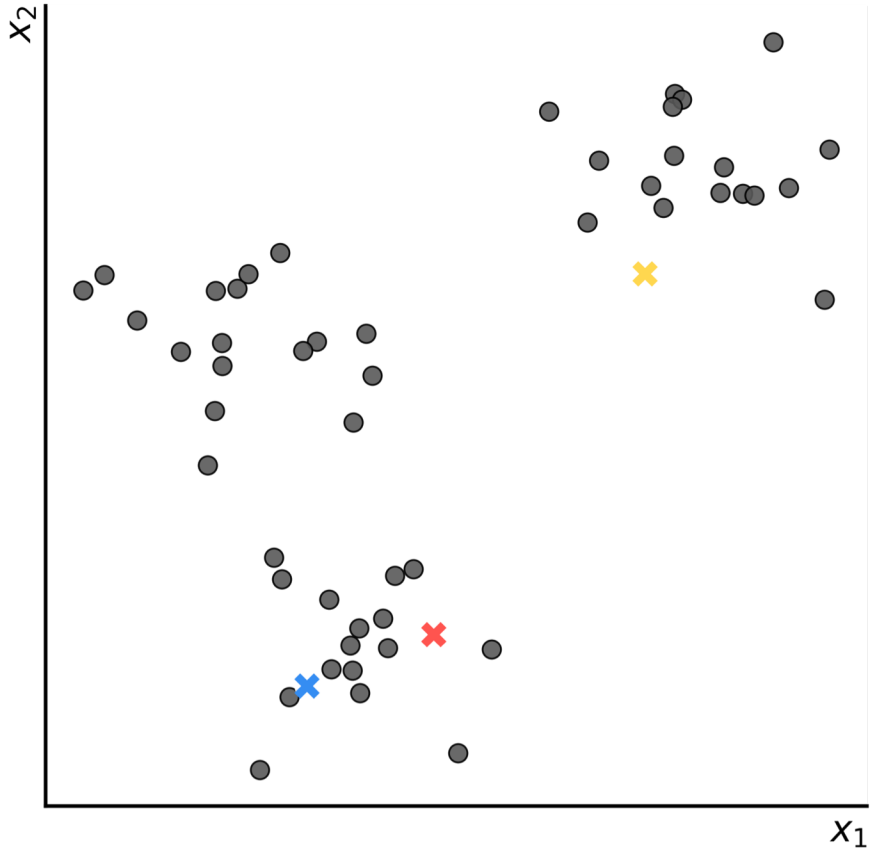

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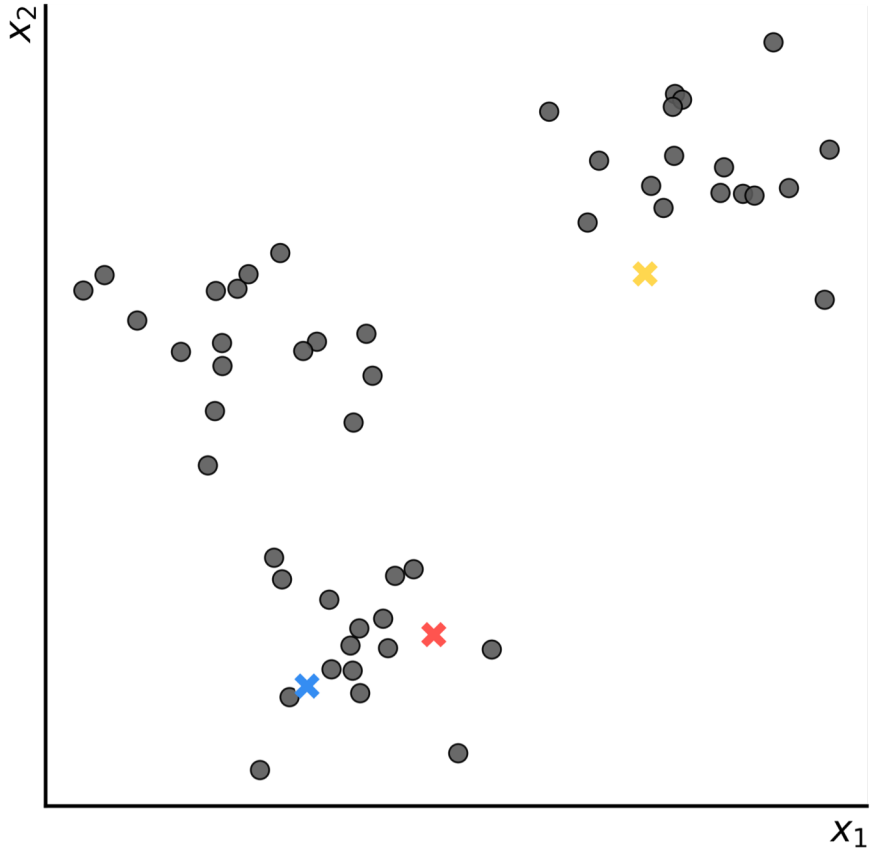
iteration 1



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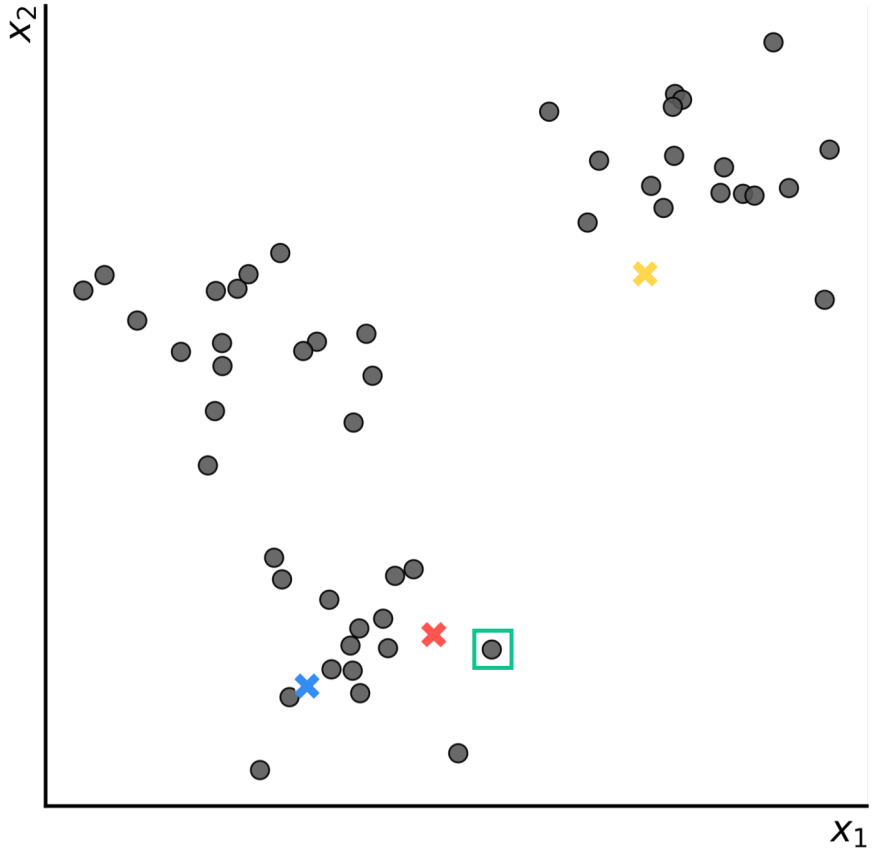

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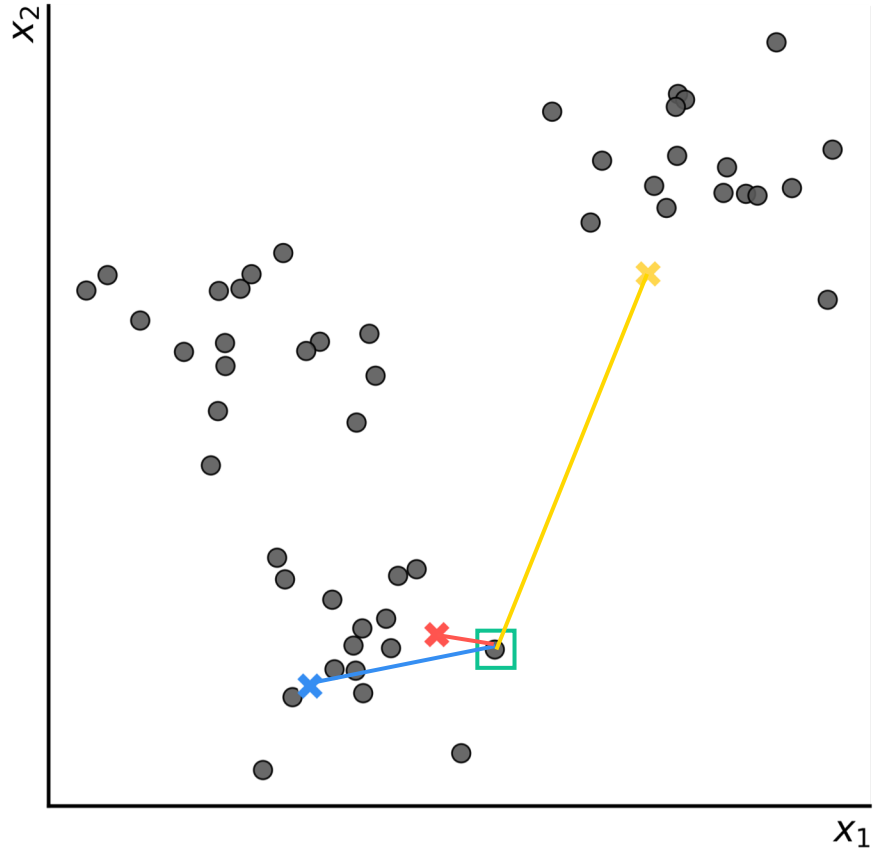

Euclidean distance is the common metric (default) used in KMeans.

iteration 1

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- For each sample $\boldsymbol{x}^{(i)}$:
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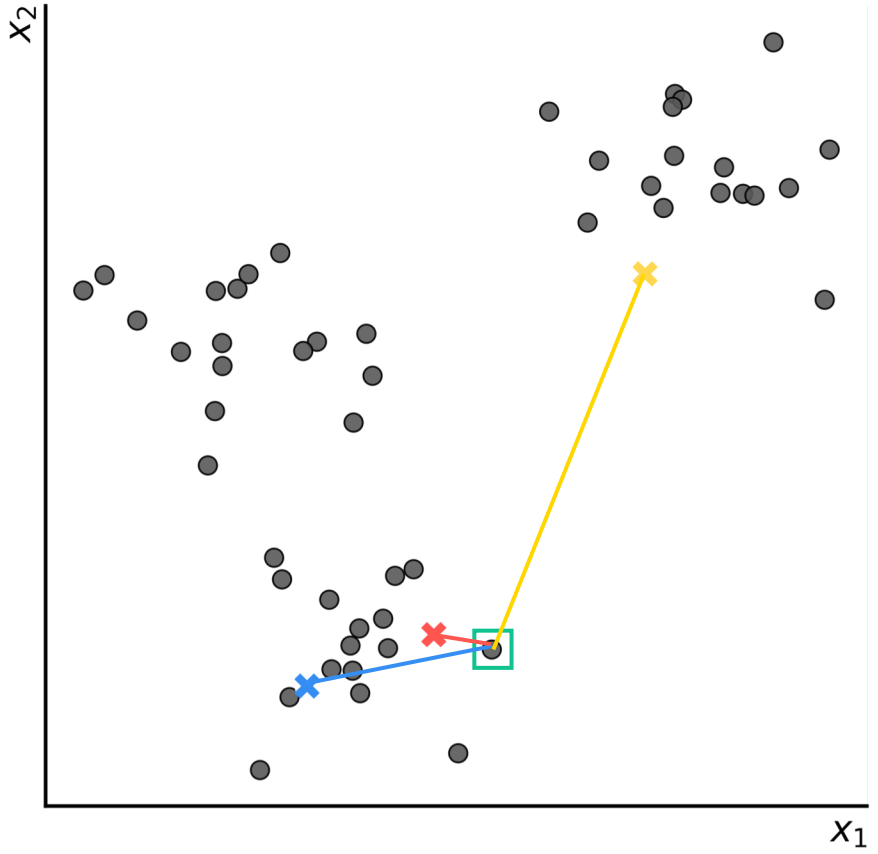

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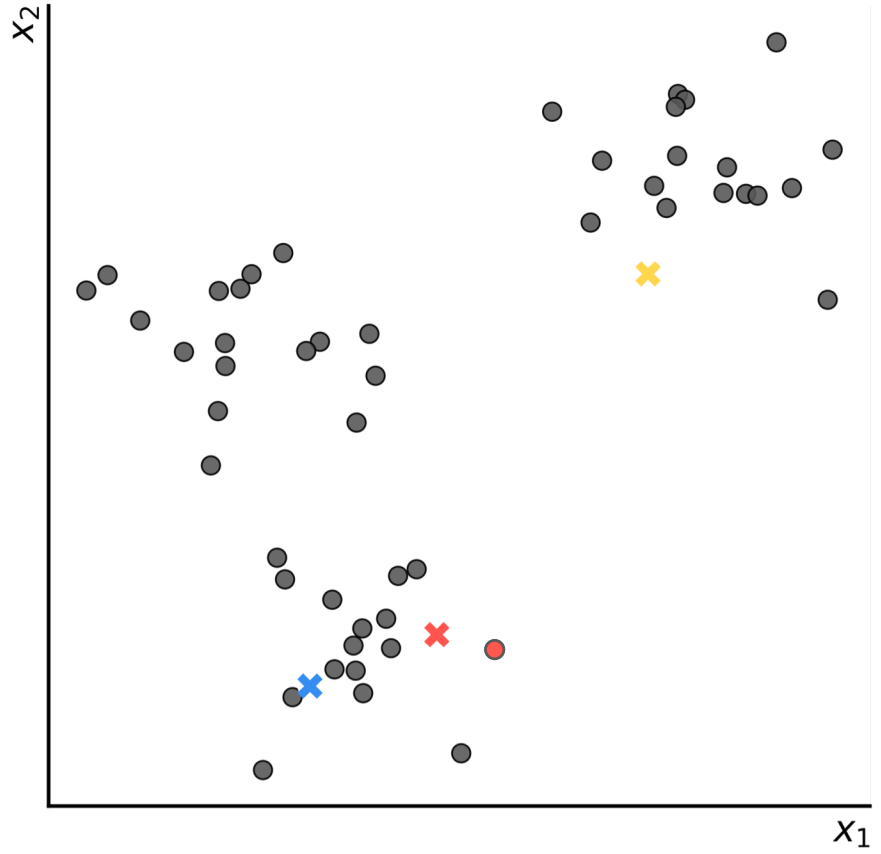

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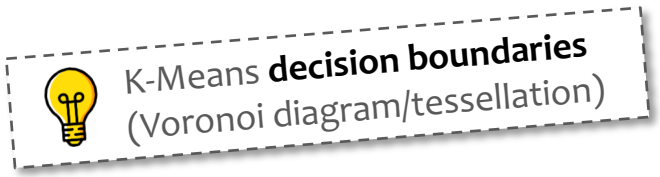
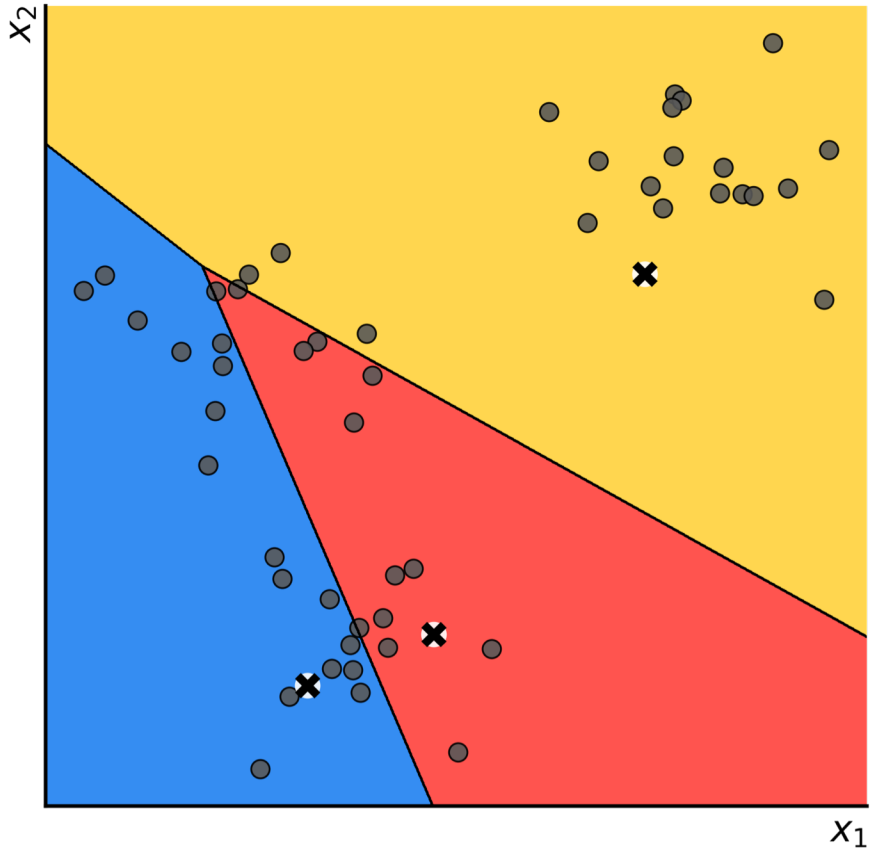
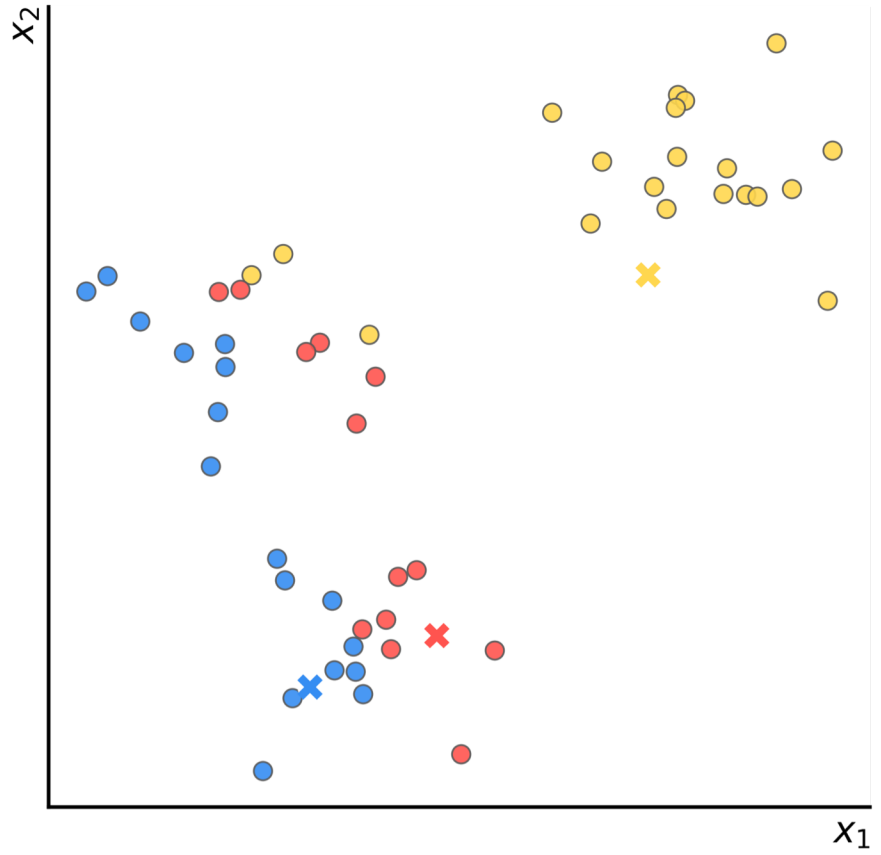




5) Move the centroids to the centers of their clusters

iteration 1



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- For each cluster $c^{(j)} = [c_1^{(j)}, c_2^{(j)}, \cdots]$:
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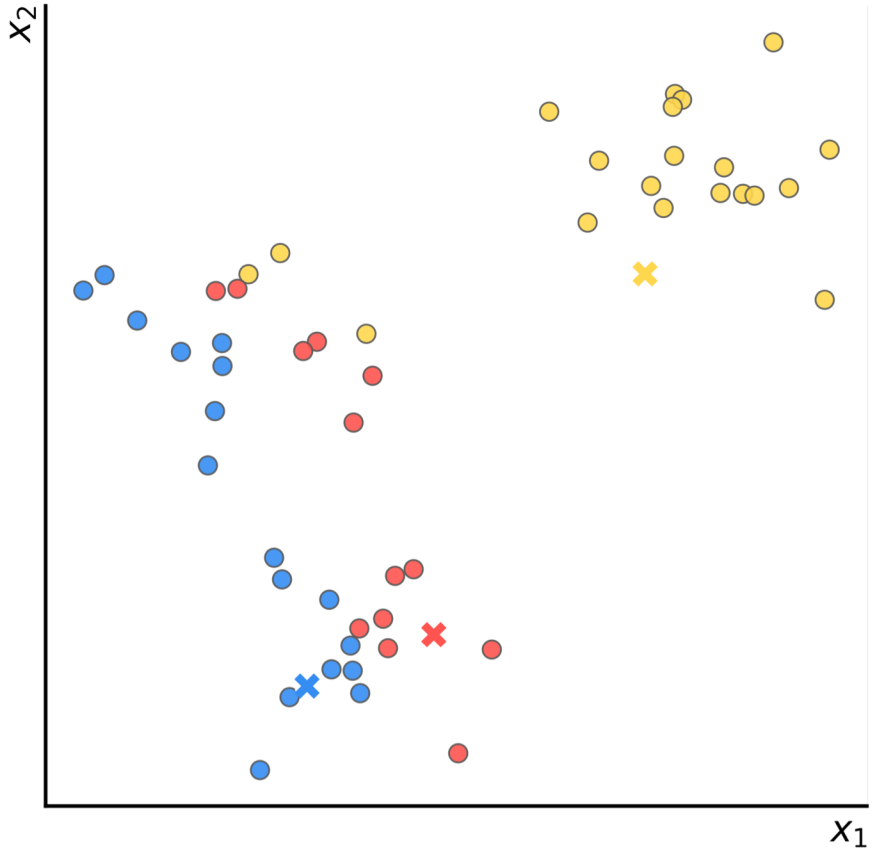
number of samples in **cluster j**



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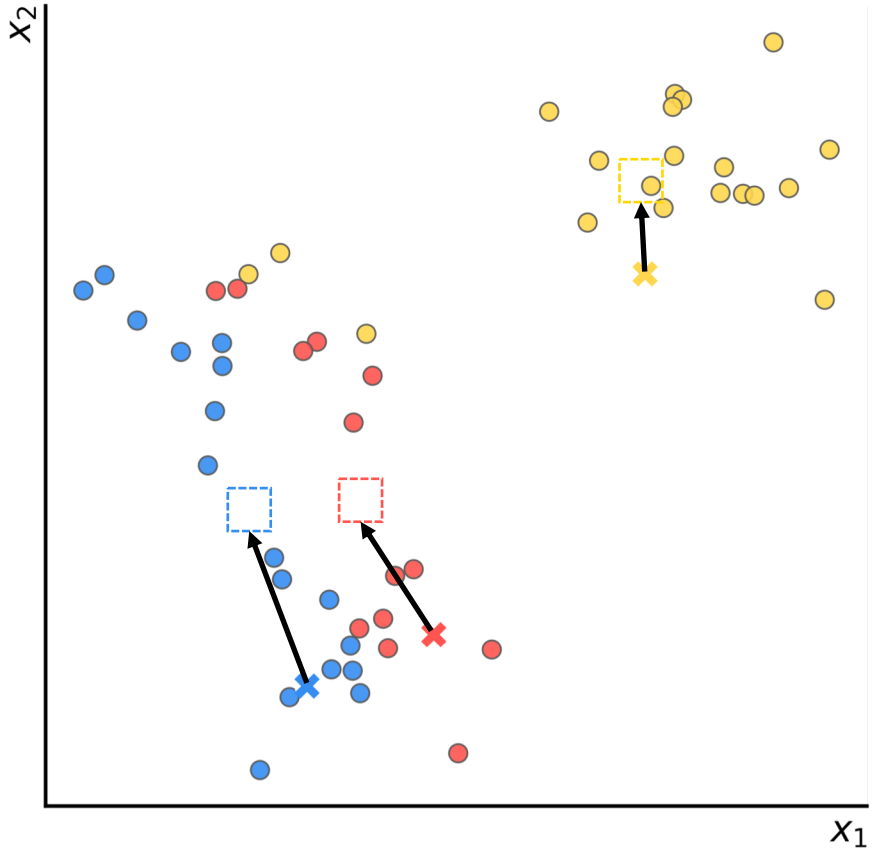

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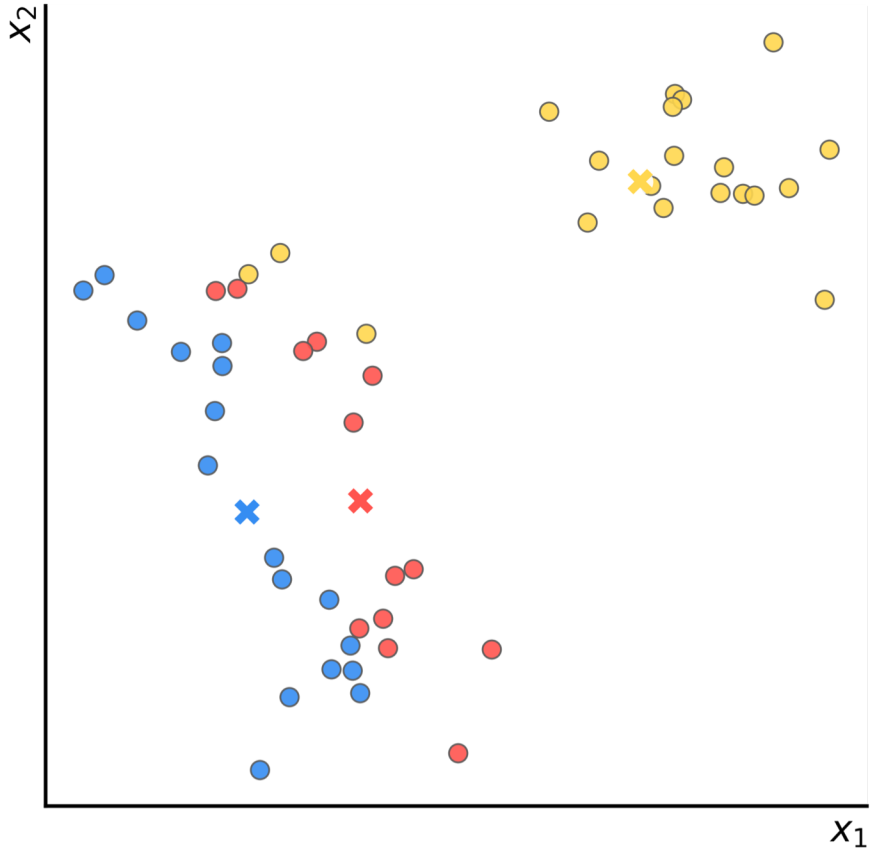

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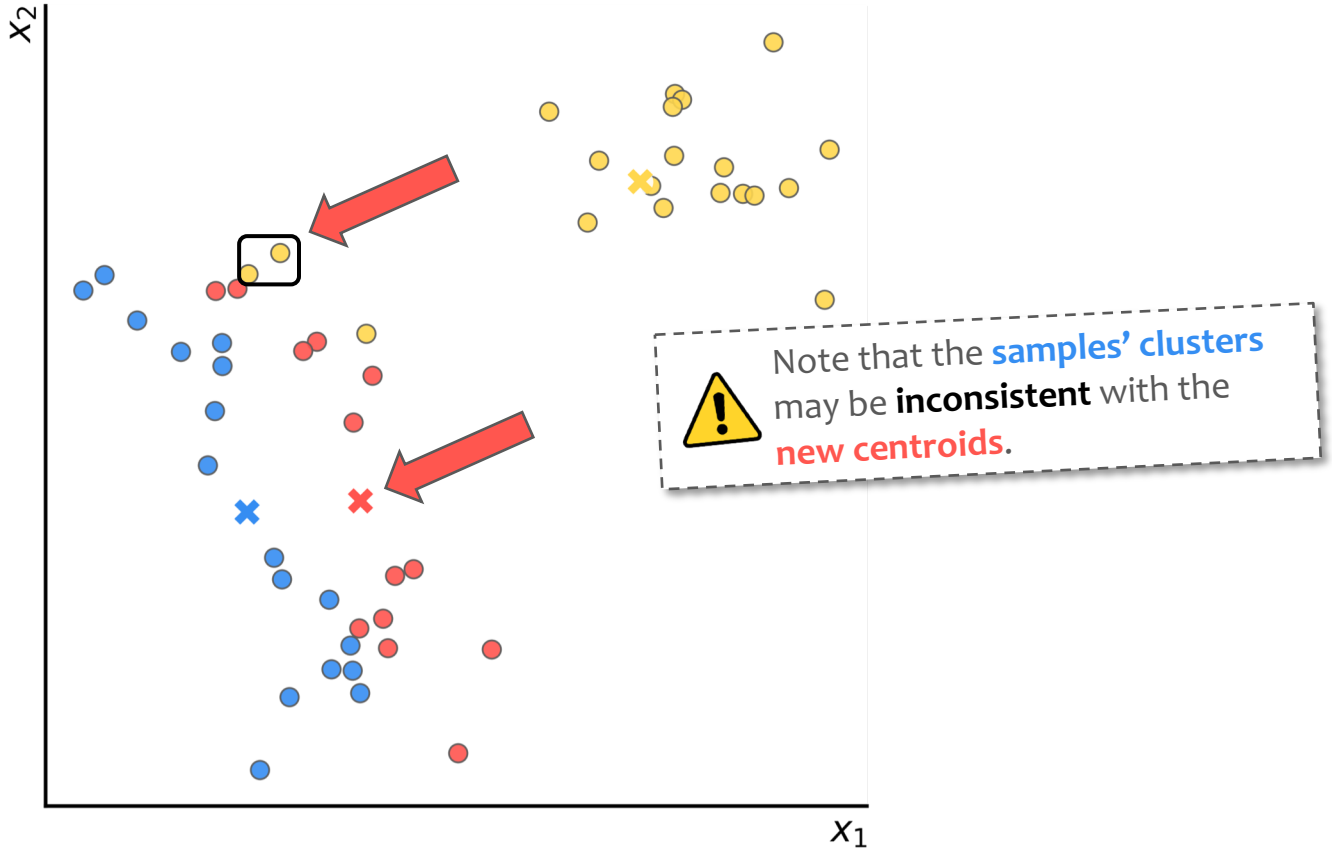

3) Repeat until **centroids do not move significantly**:

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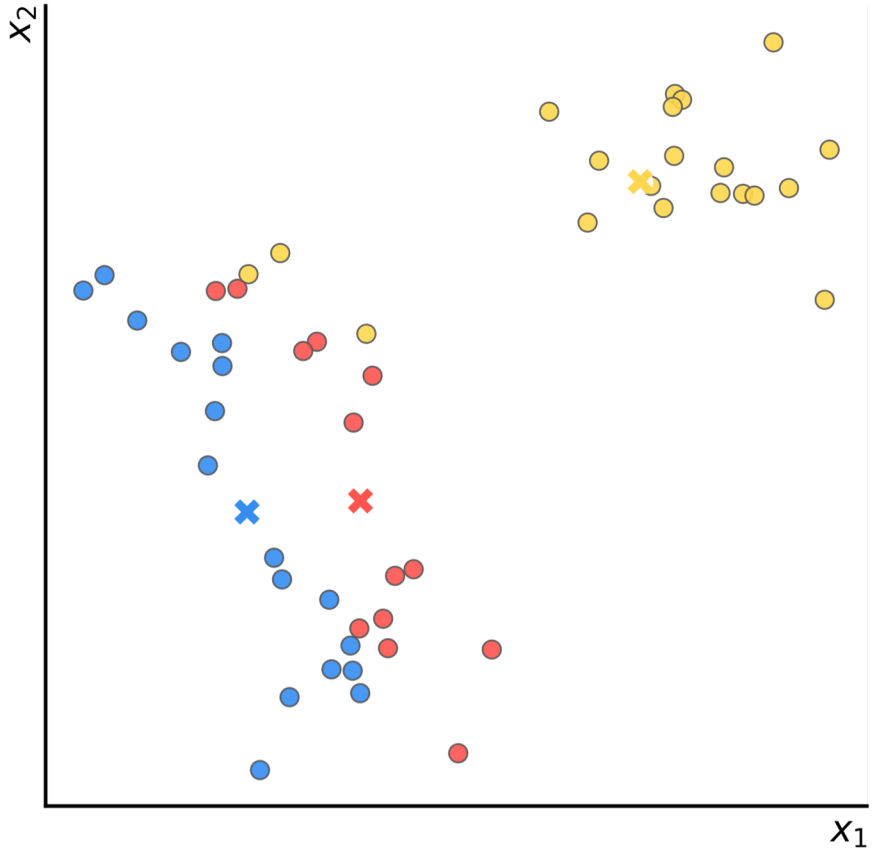

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iteration 2

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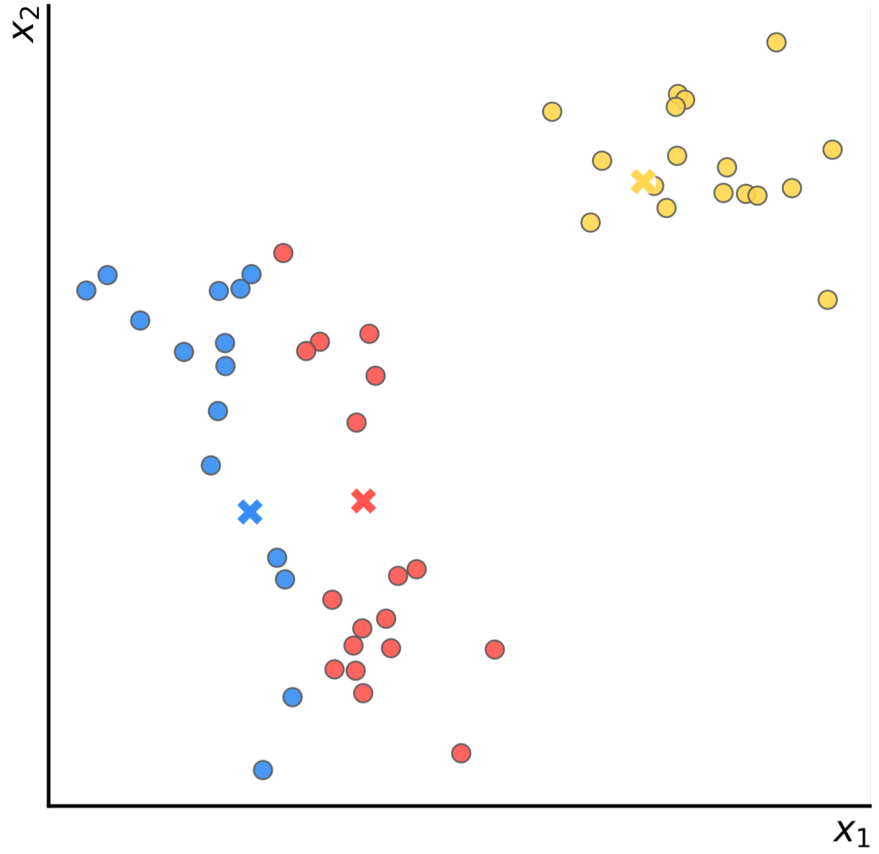

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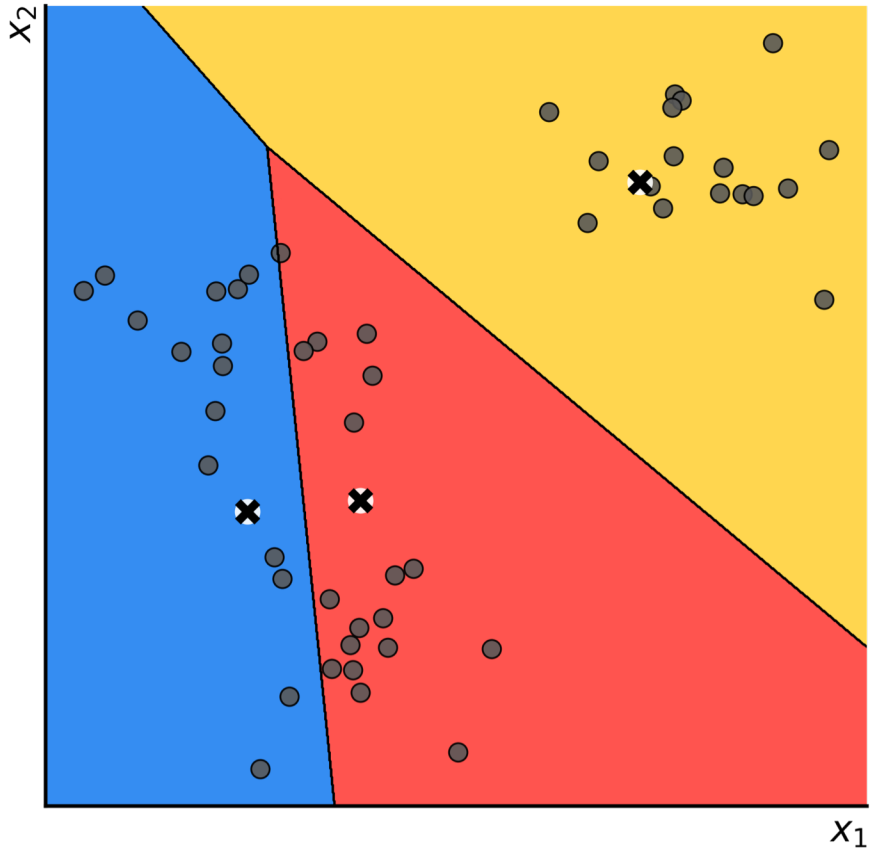

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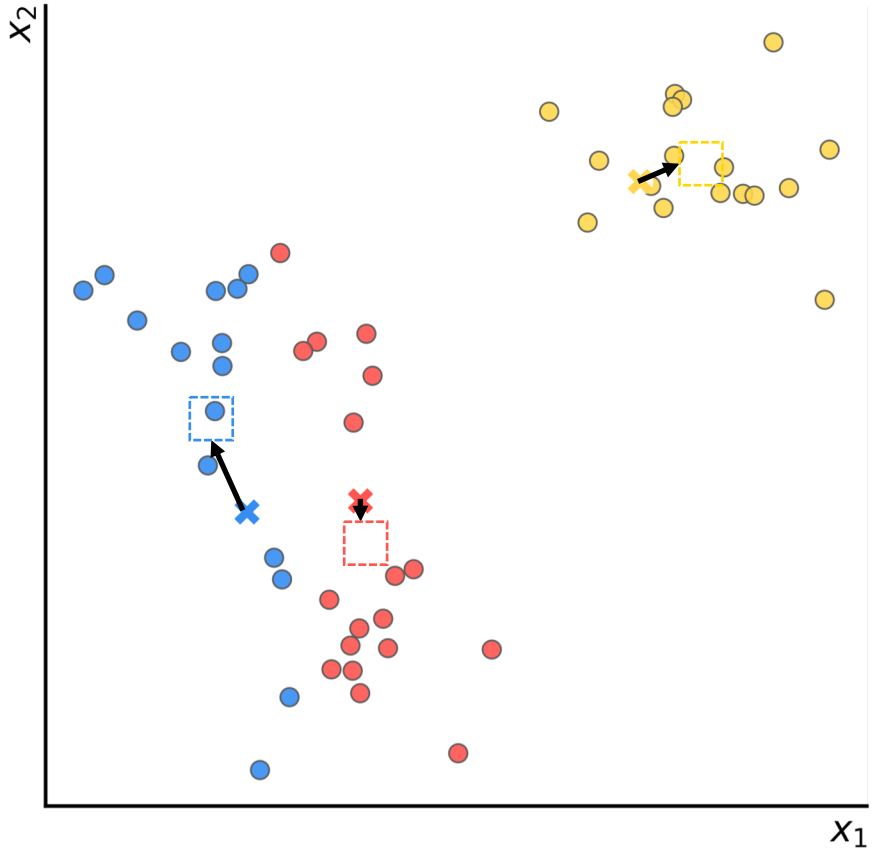

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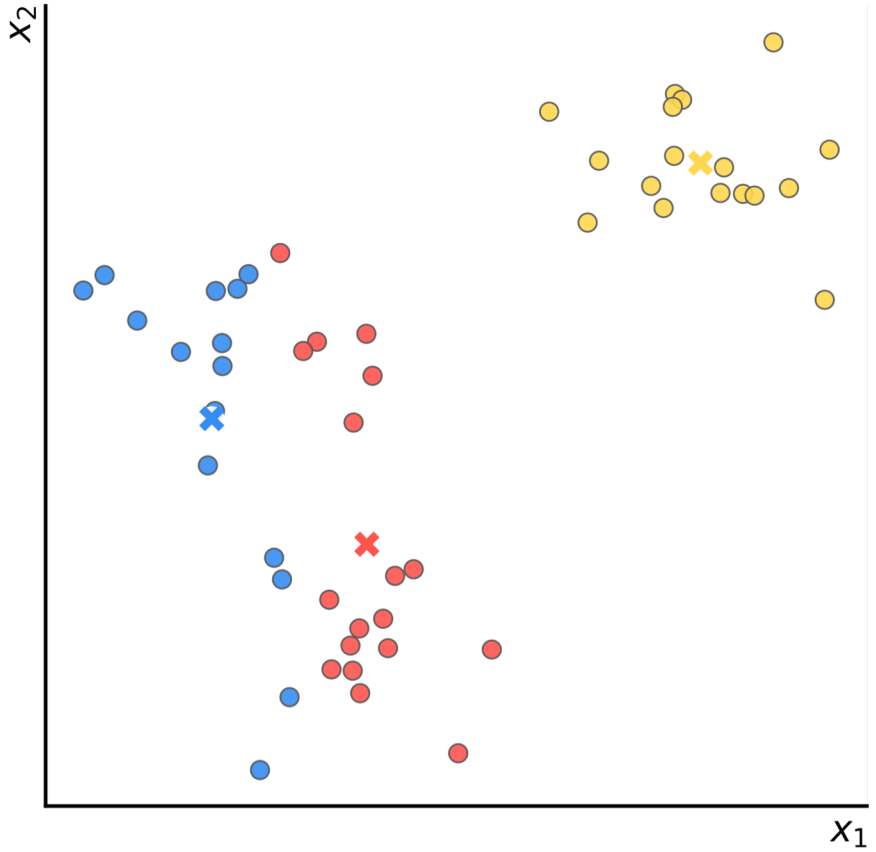

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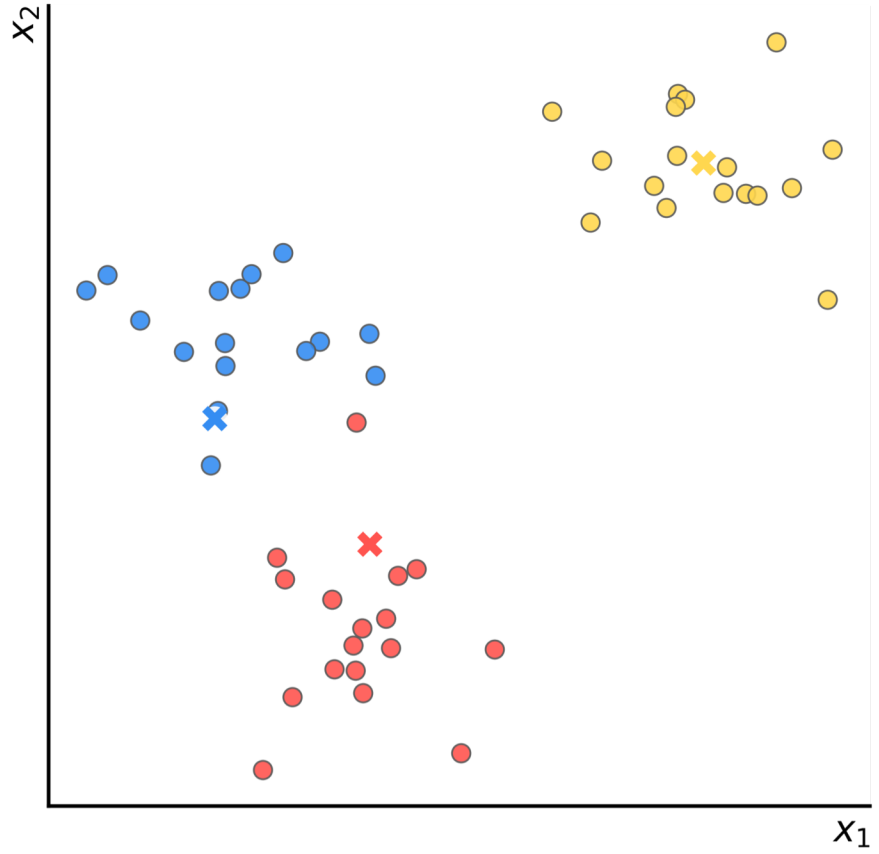

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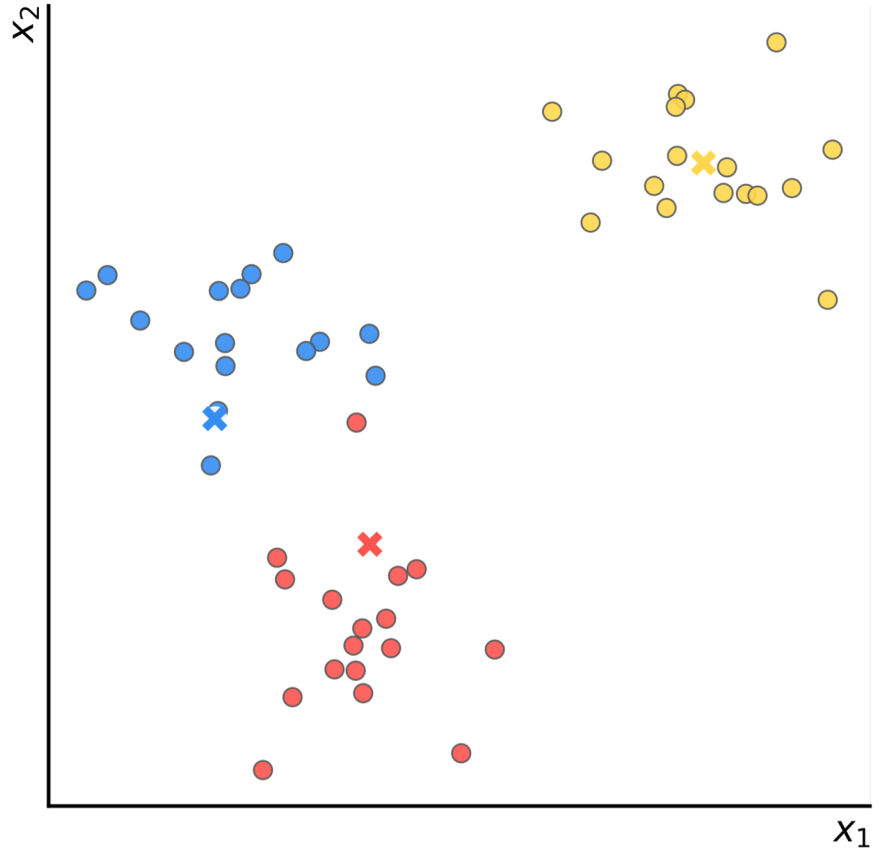

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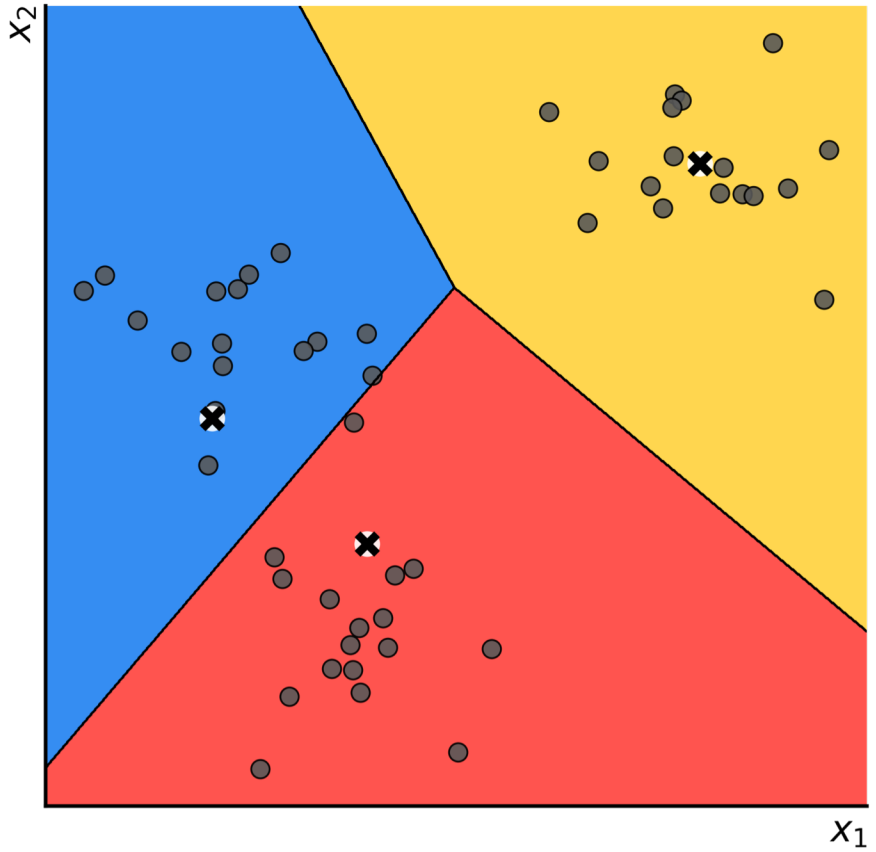

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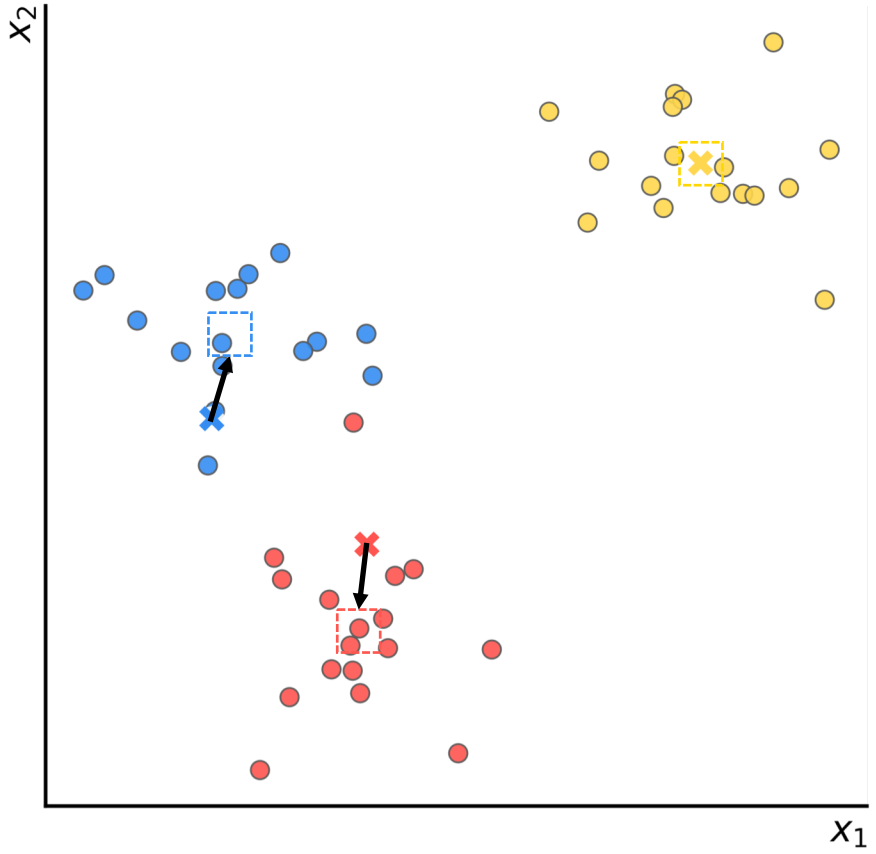

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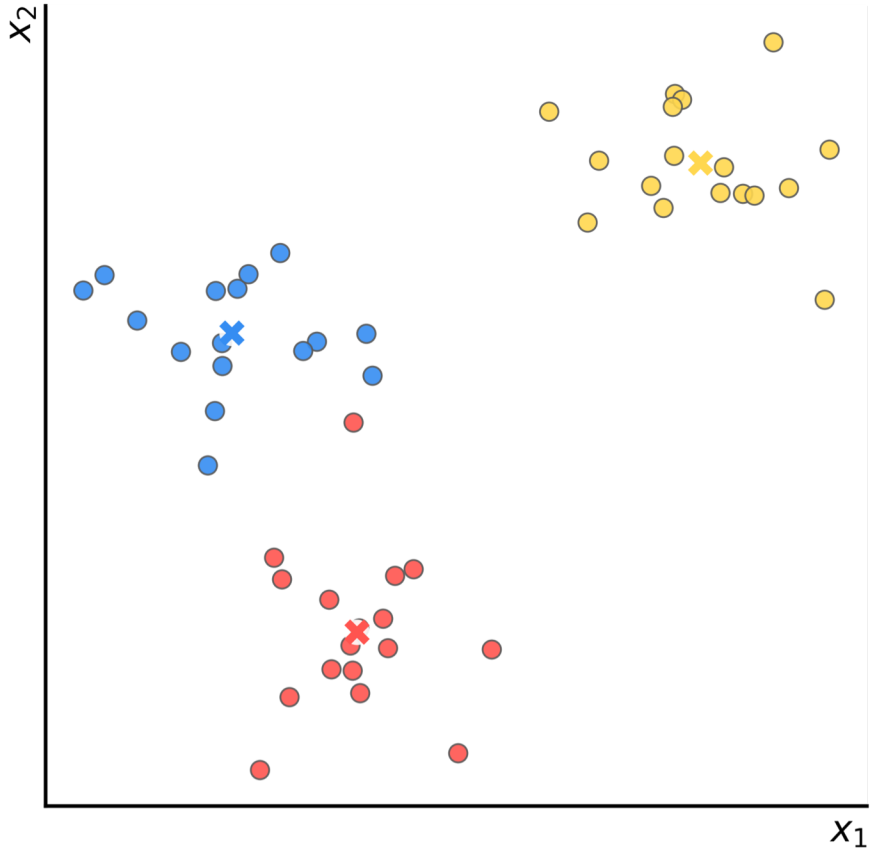

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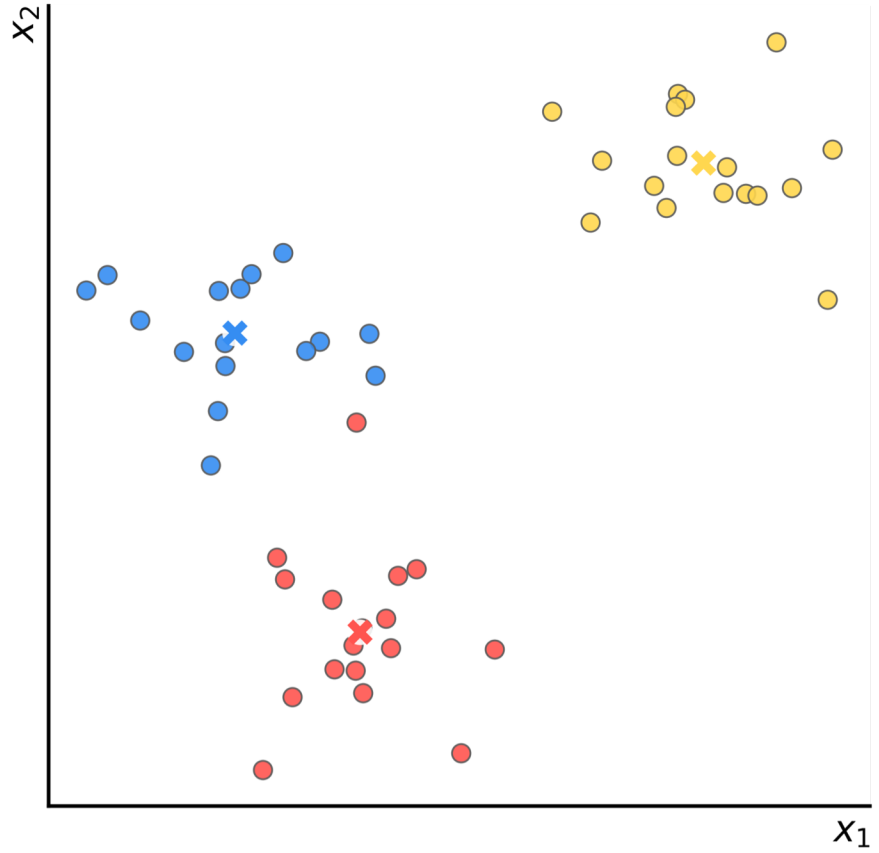

3) Repeat until **centroids do not move significantly**:

iteration 4

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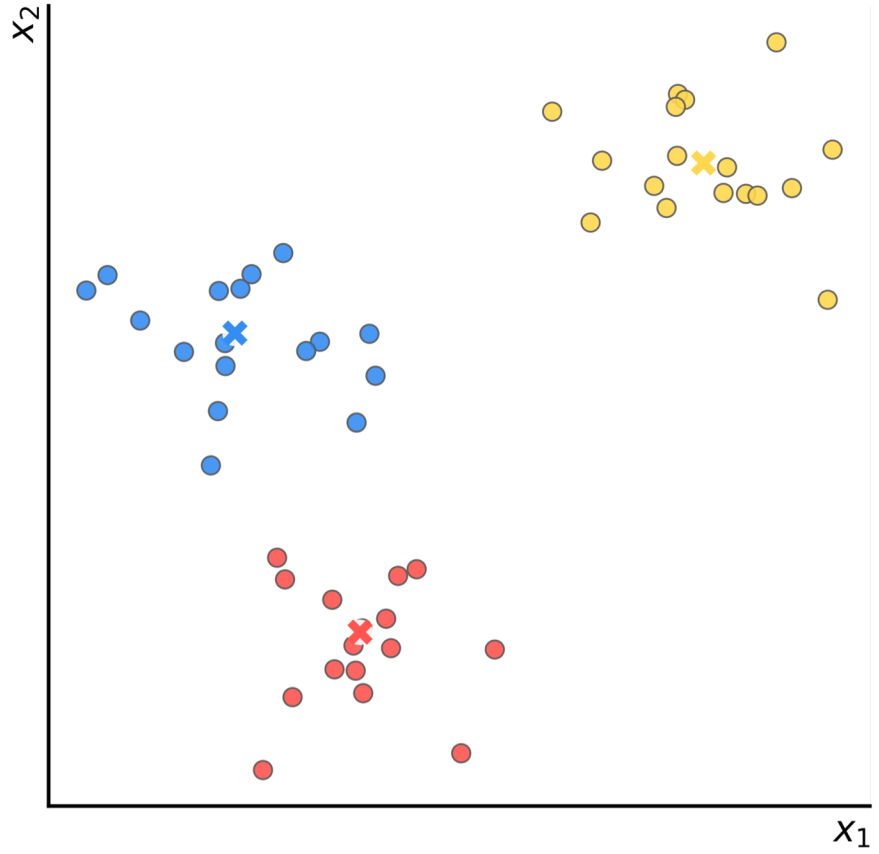

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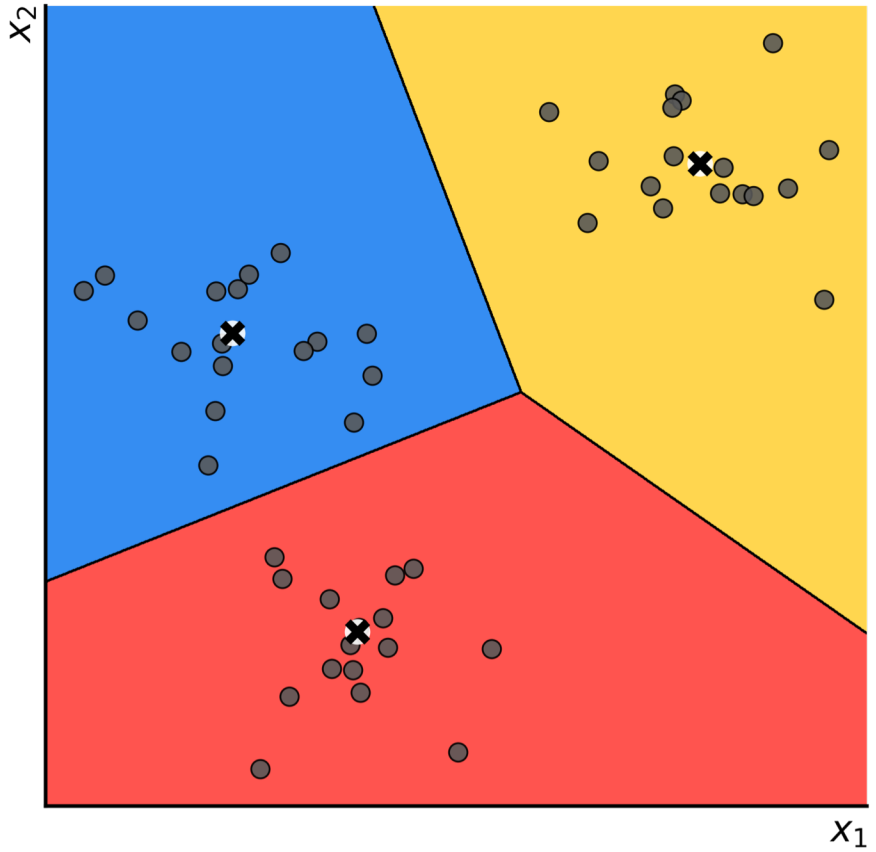

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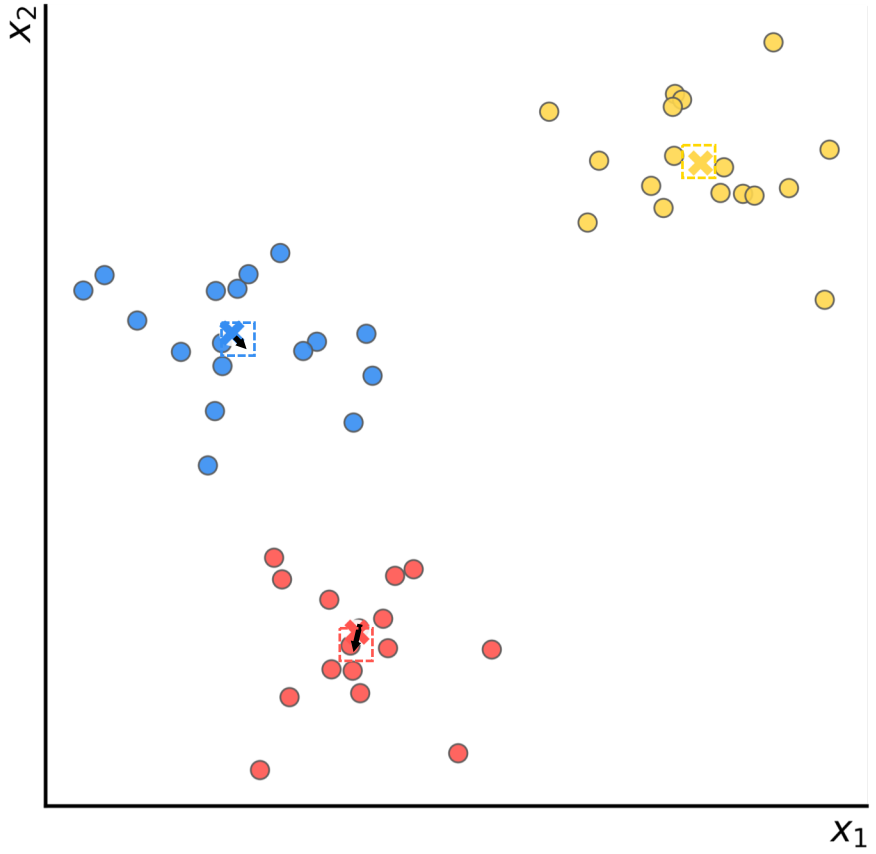

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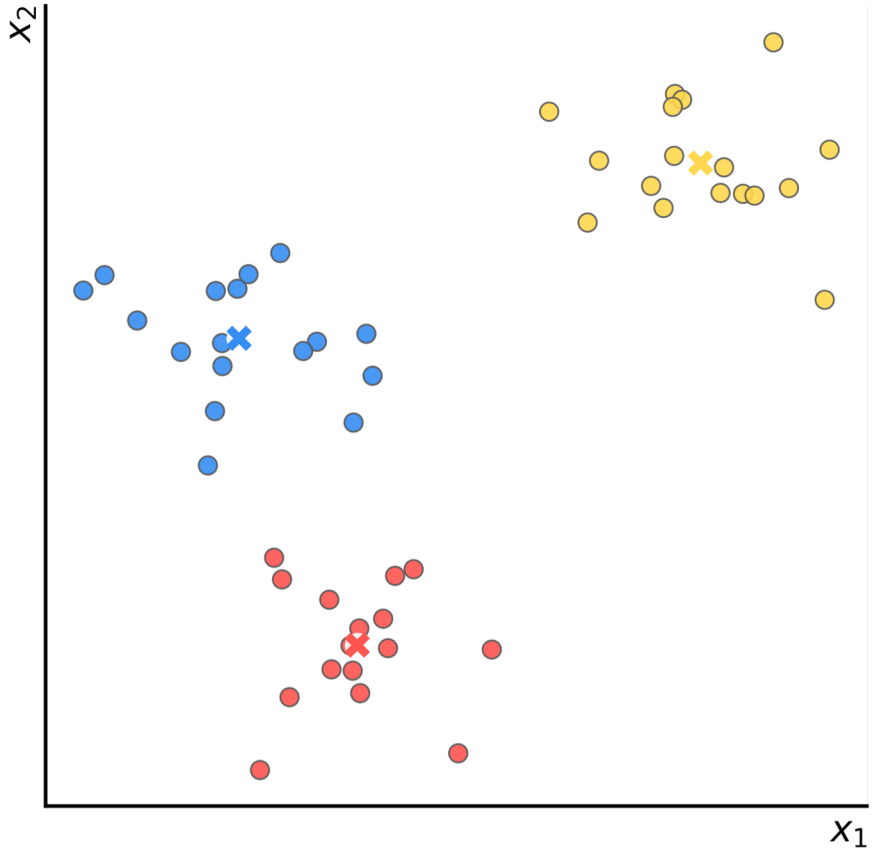

Note that the **samples' clusters** may be **inconsistent** with the **new centroids**.

3) Repeat until **centroids do not move significantly**:

- **4)** Assign each instance to **the nearest** centroid;
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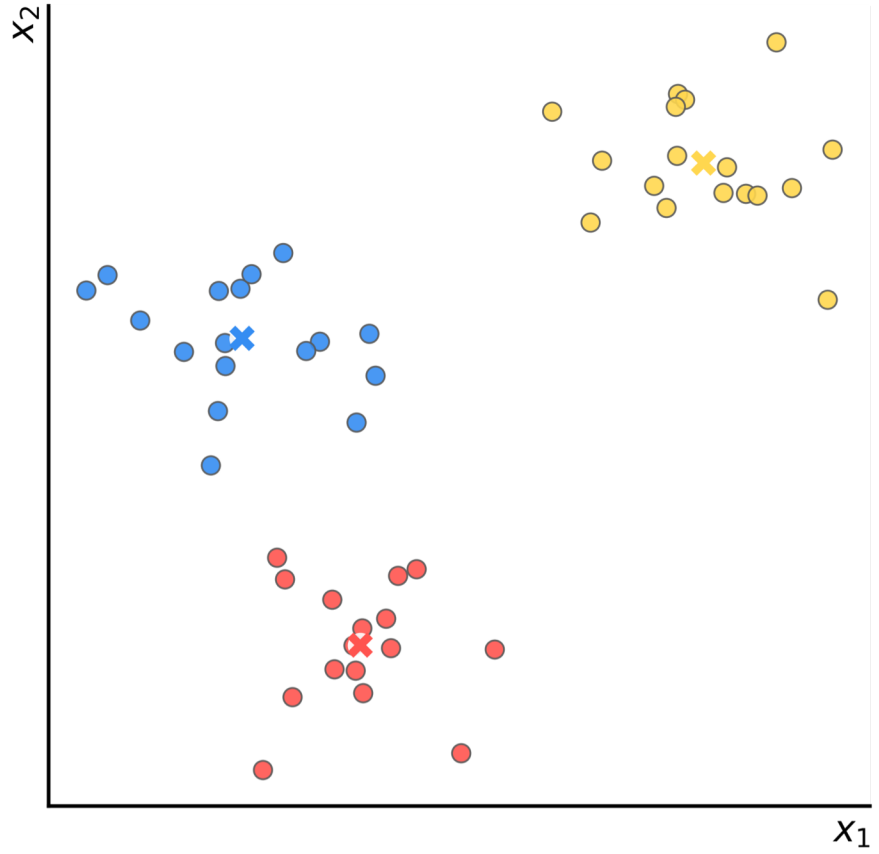

3) Repeat until **centroids do not move significantly**:

iteration 5

- **4)** Assign each instance to **the nearest** centroid;
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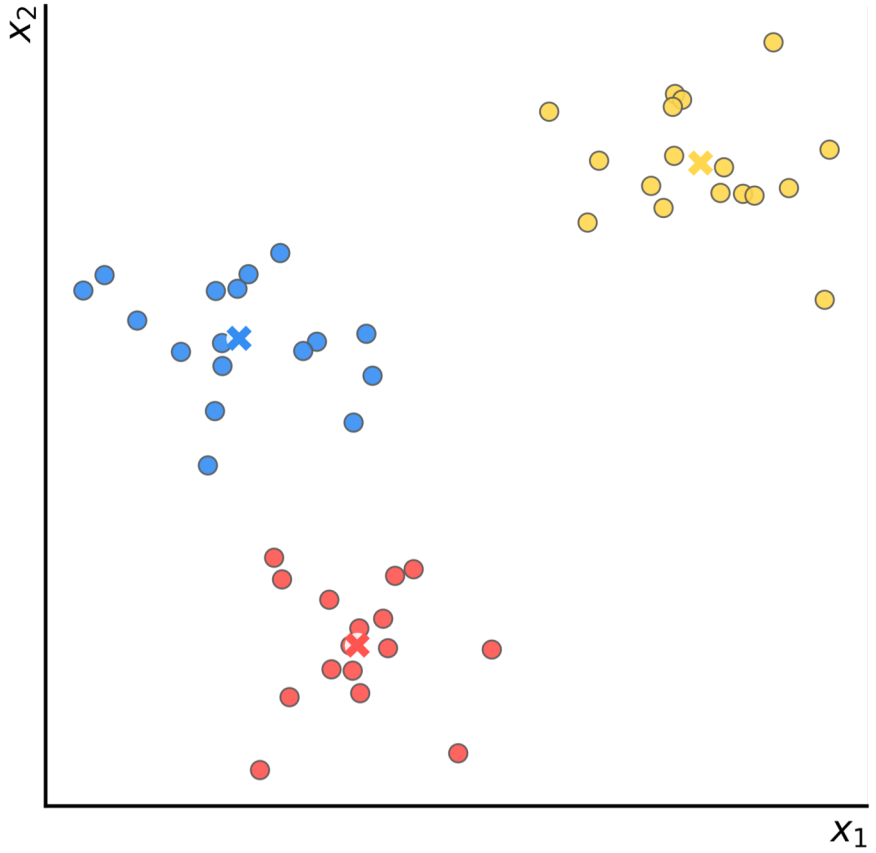

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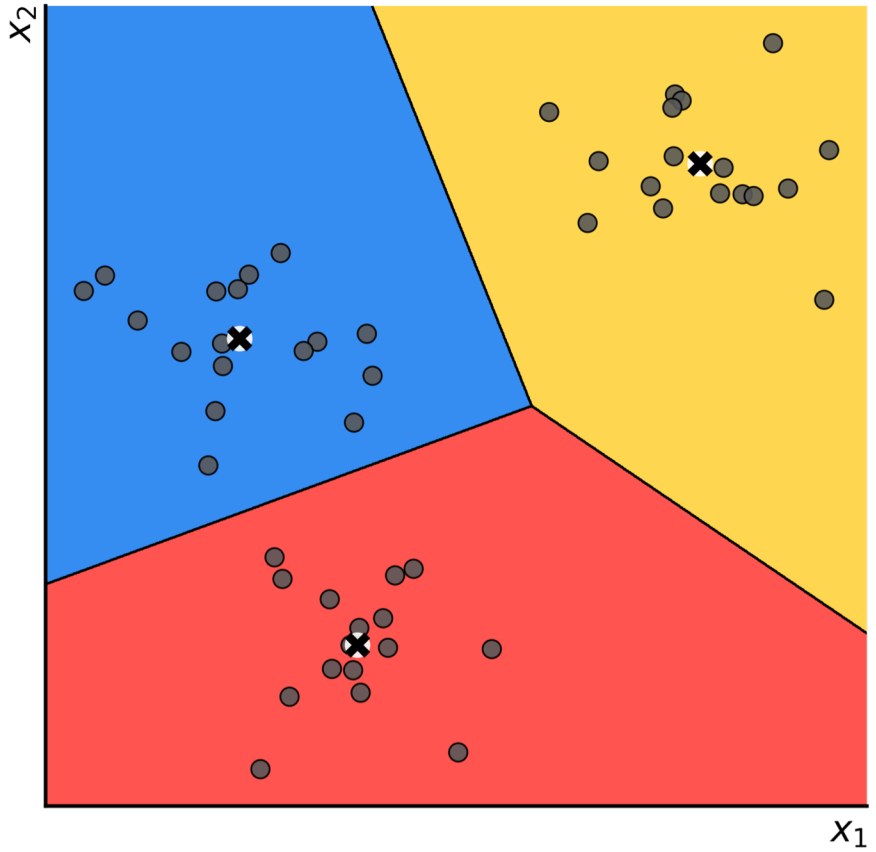

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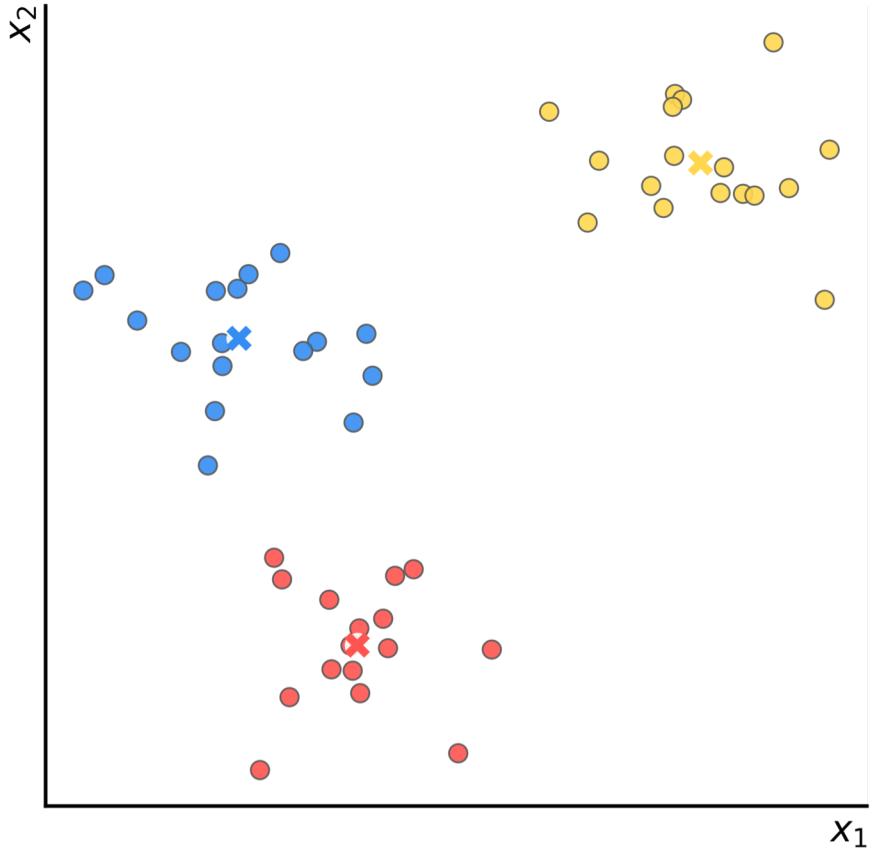

no centroid reposition

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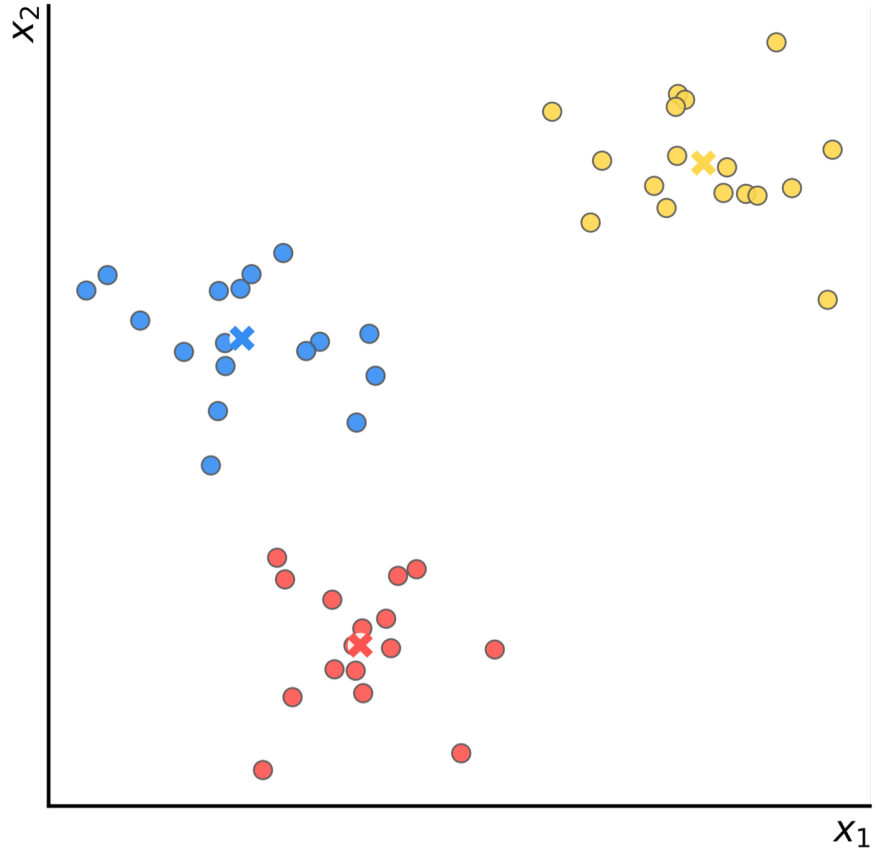

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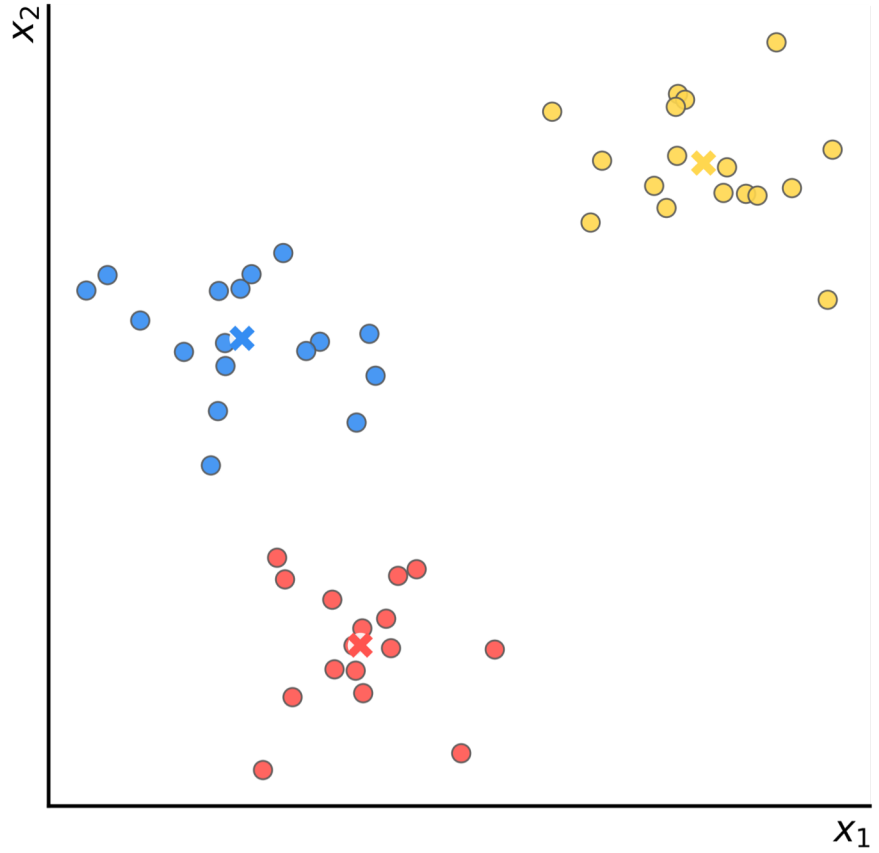
Stop!



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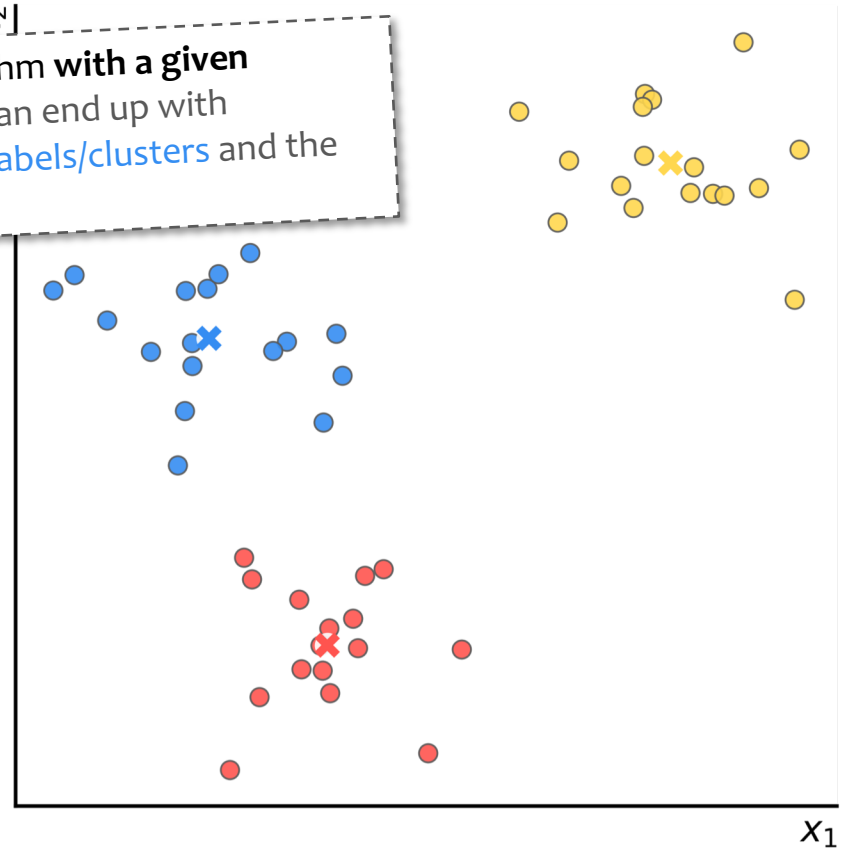
If you consider allow to stop the algorithm **with a given tolerance for centroid reposition**, we can end up with **inconsistencies** between the samples' labels/clusters and the final **centroids**!



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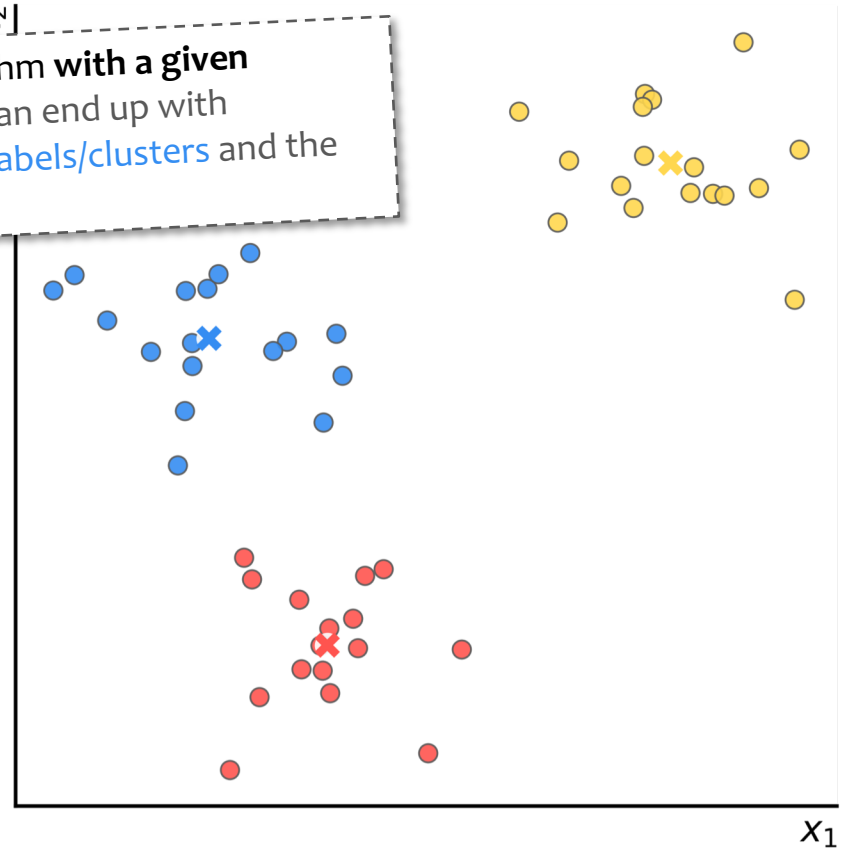

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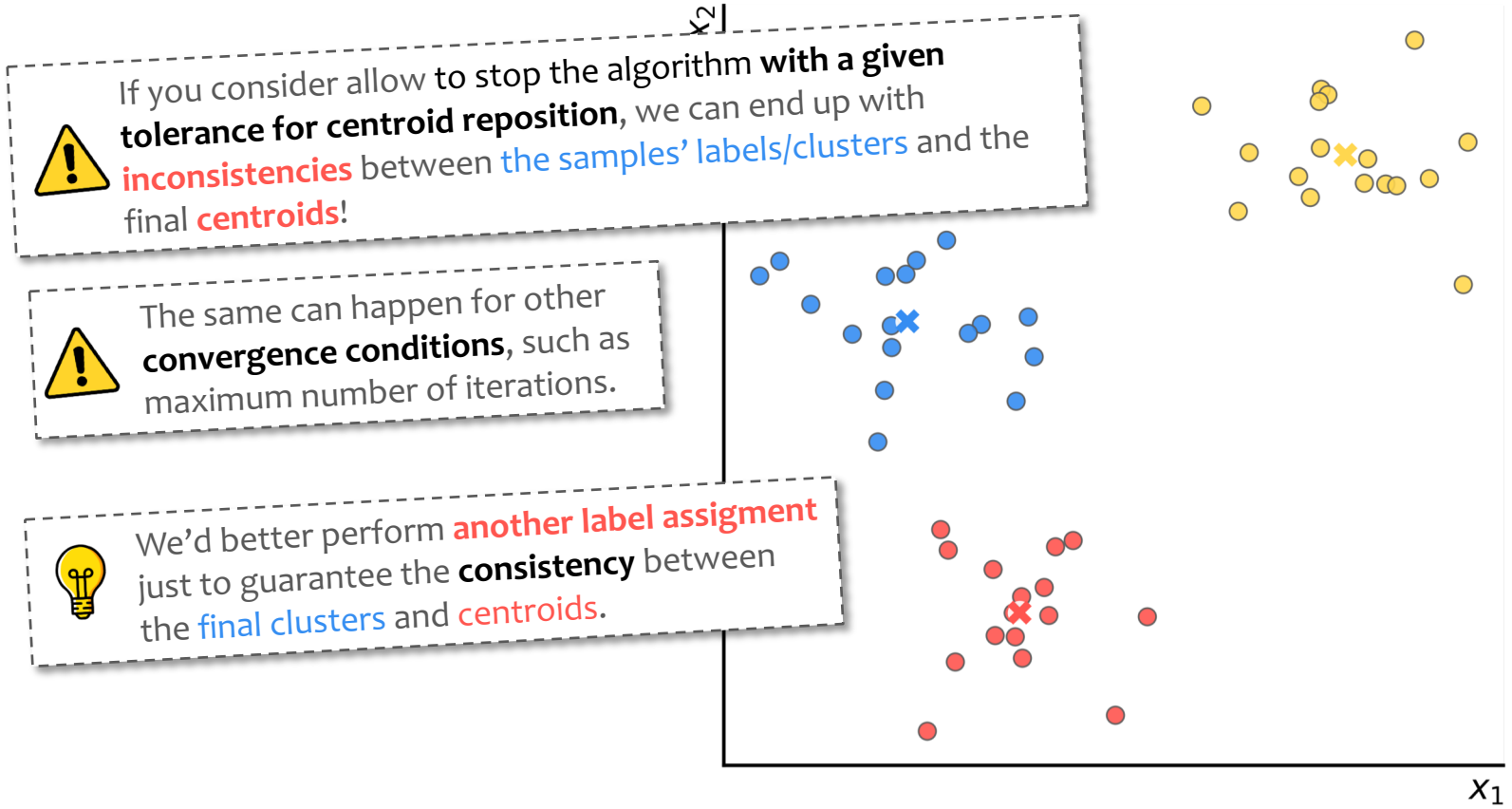


If you consider allow to stop the algorithm **with a given tolerance for centroid reposition**, we can end up with **inconsistencies** between the samples' labels/clusters and the final **centroids**!

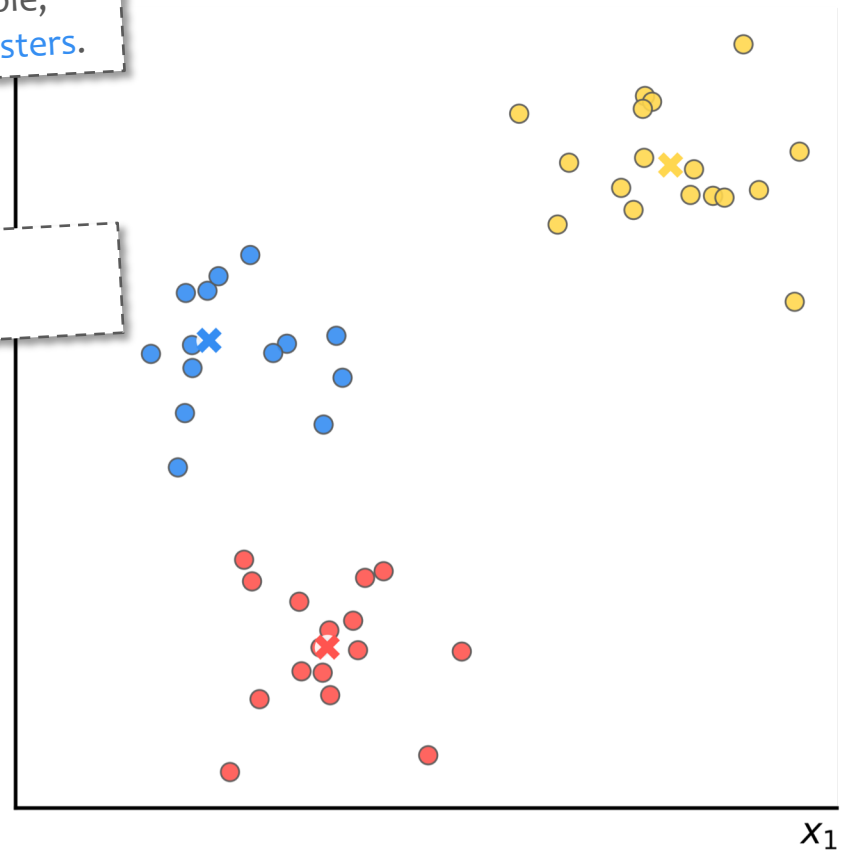
The same can happen for other **convergence conditions**, such as maximum number of iterations.

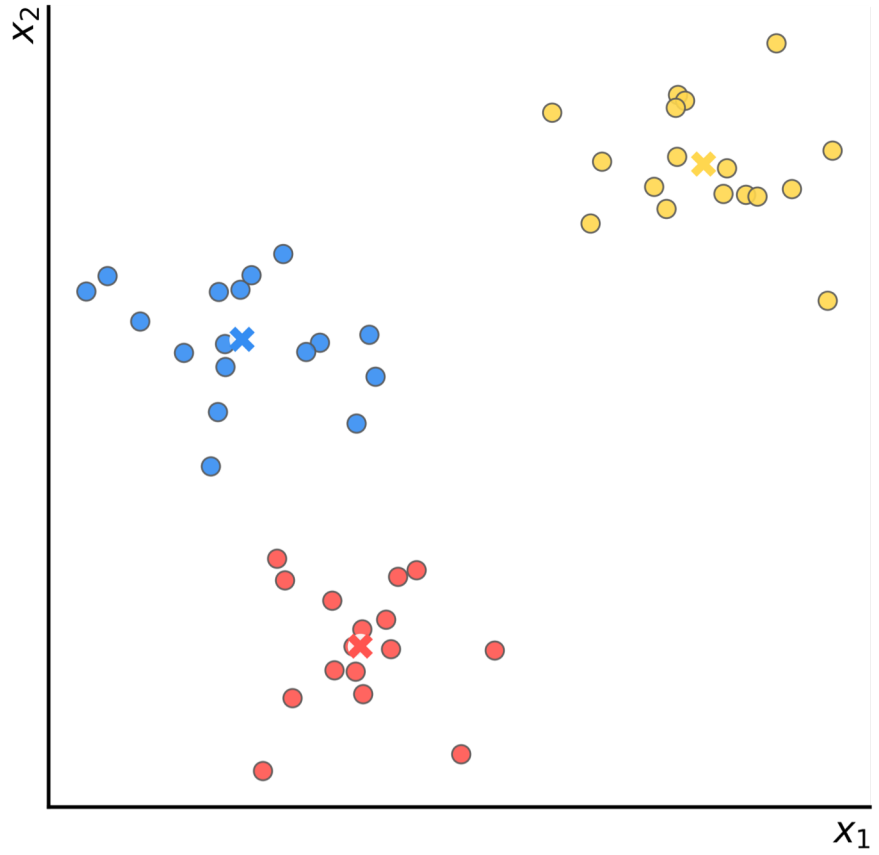
We'd better perform **another label assigment** just to guarantee the **consistency** between the final clusters and centroids.

6) Assign each instance to **the final nearest** centroid;

Since the final centroids are exactly the same from its previous iteration, for this example, this label assigment obtains the same clusters.

KMeans implementation in Scikit-Learn performs **this final label assignment.**

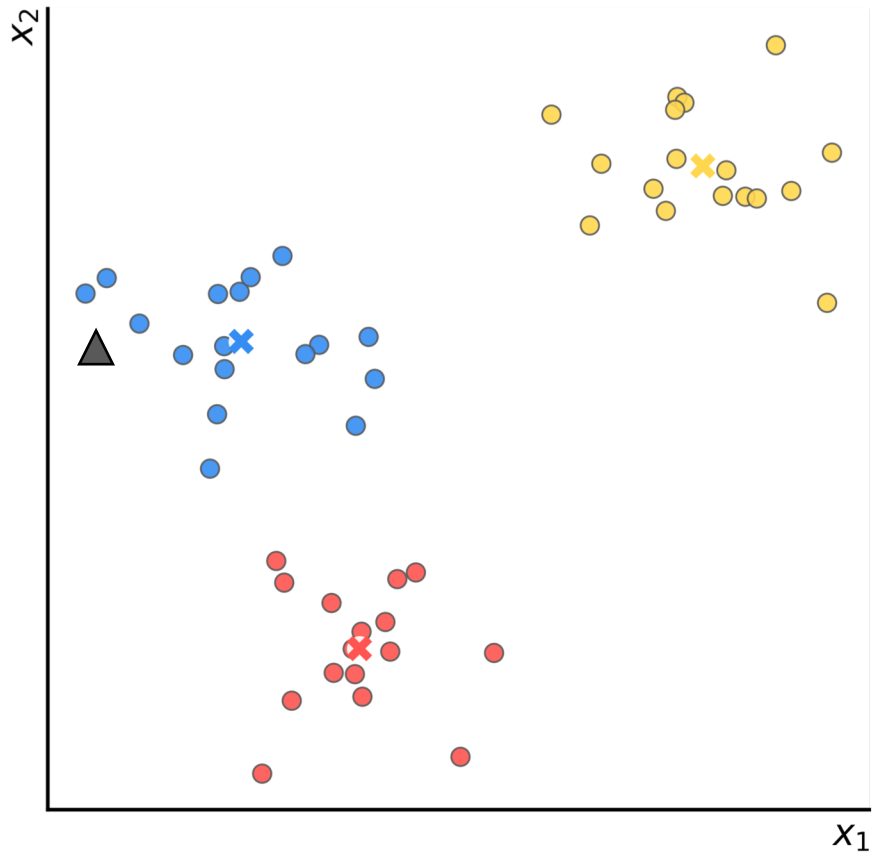



x_2
x_1

KMeans

Usage

- For each new **testing sample**:
  - Assign each instance to **the nearest** centroid;



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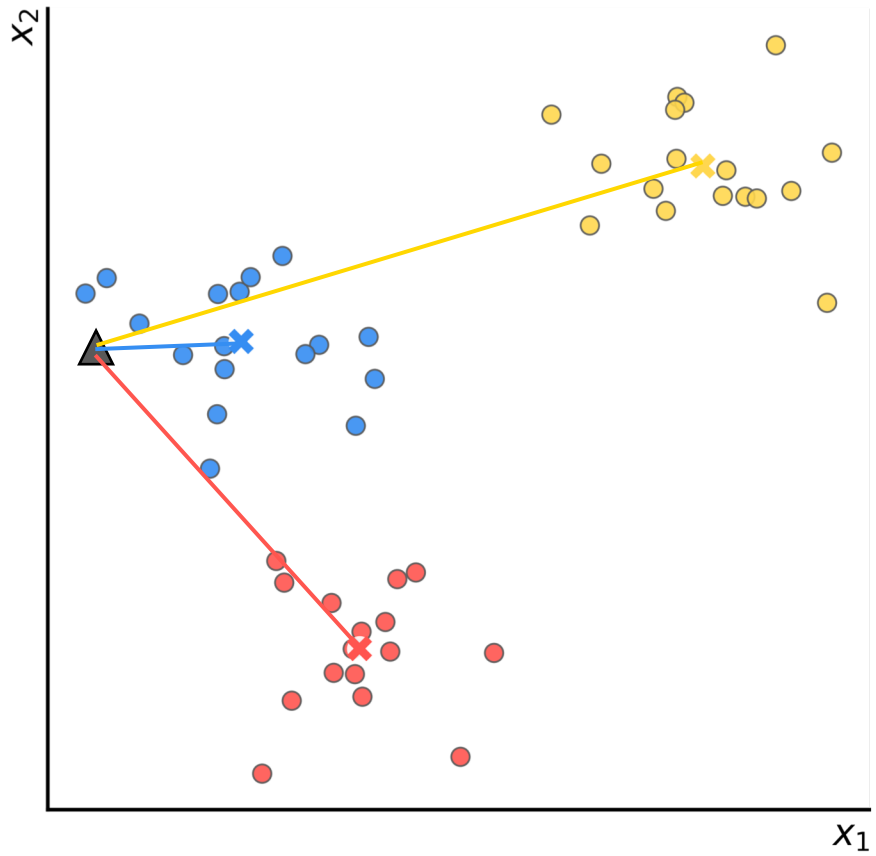

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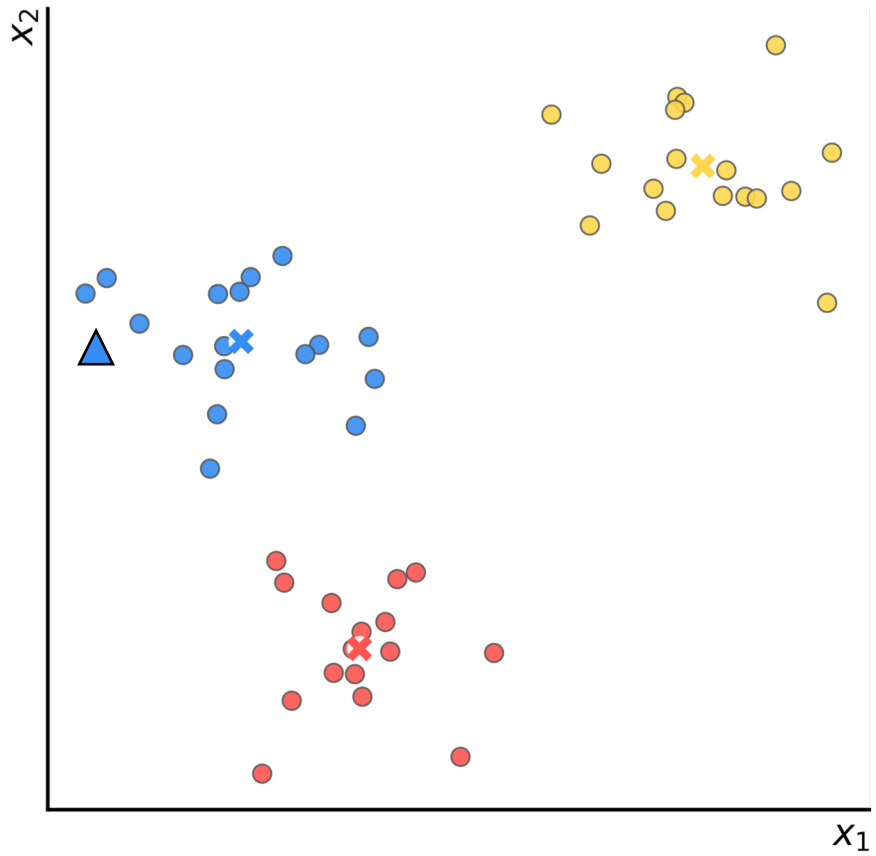
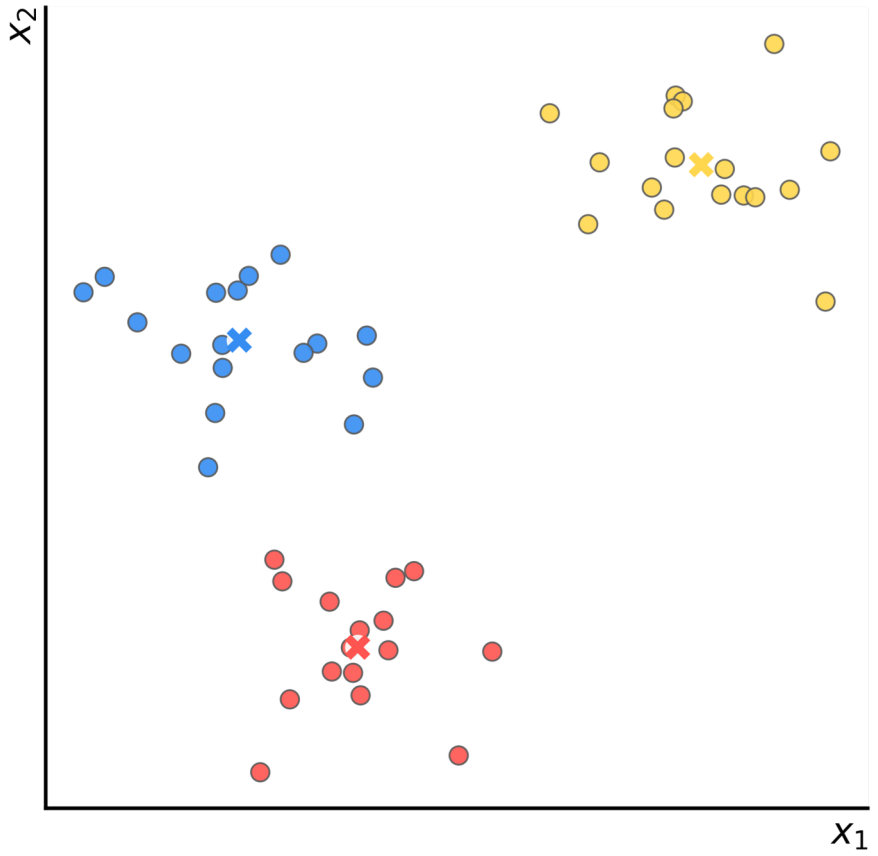


The algorithm is **guaranteed to converge**, but **it may not converge** to the **right solution** (*i.e.*, it may converge to **a local optimum**).



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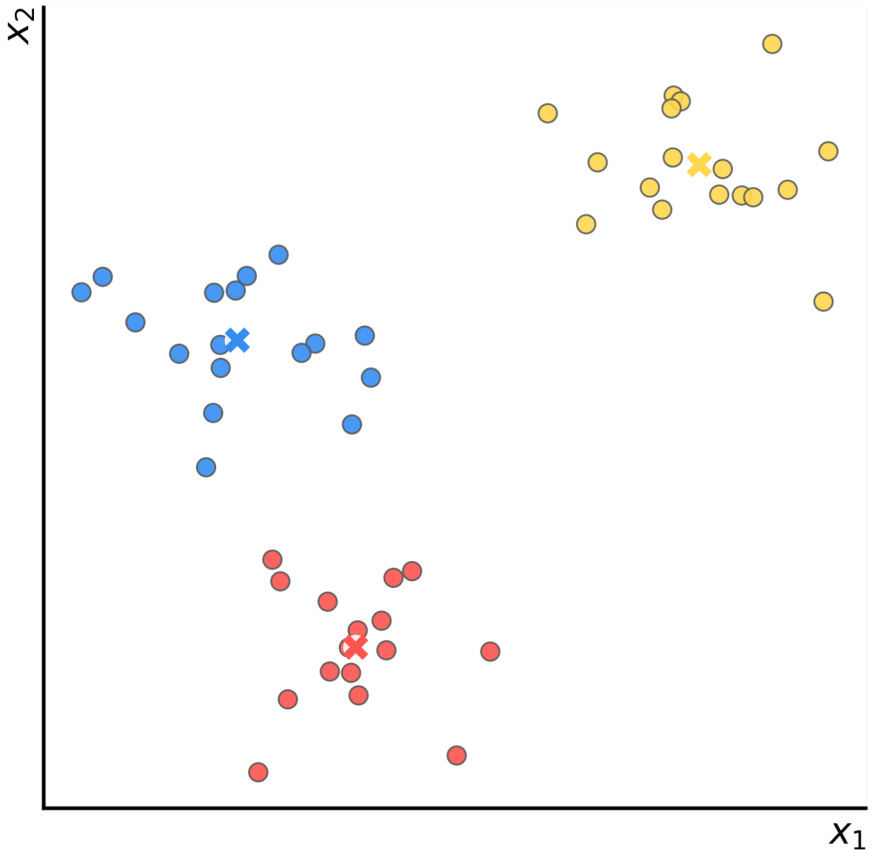
This depends on the **centroid initialization**.



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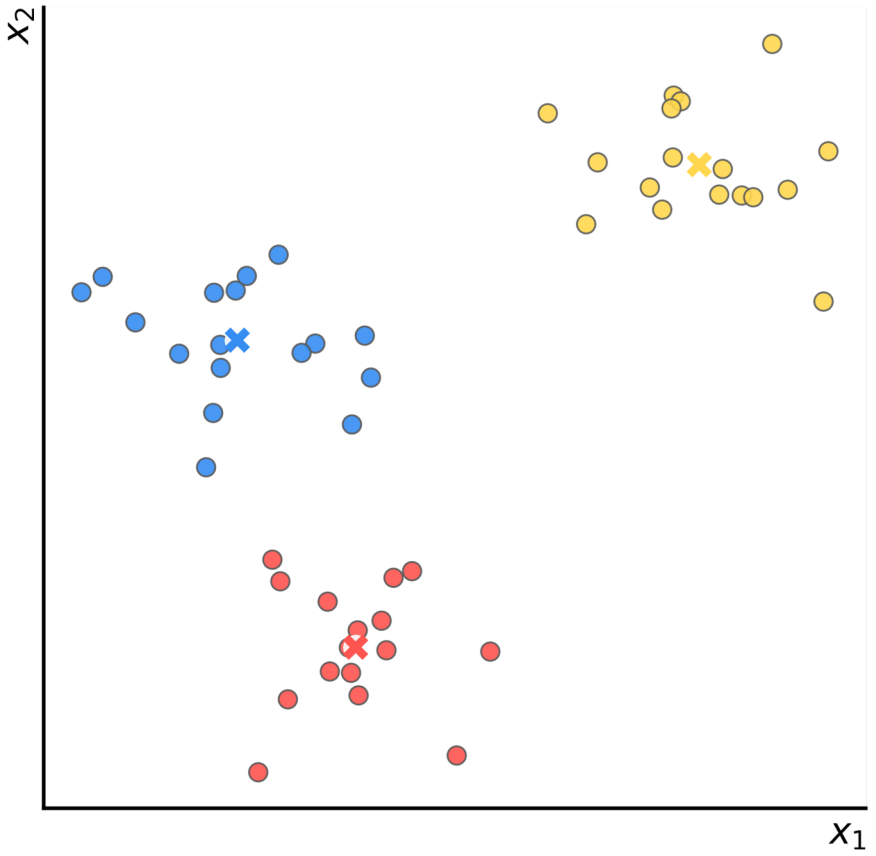
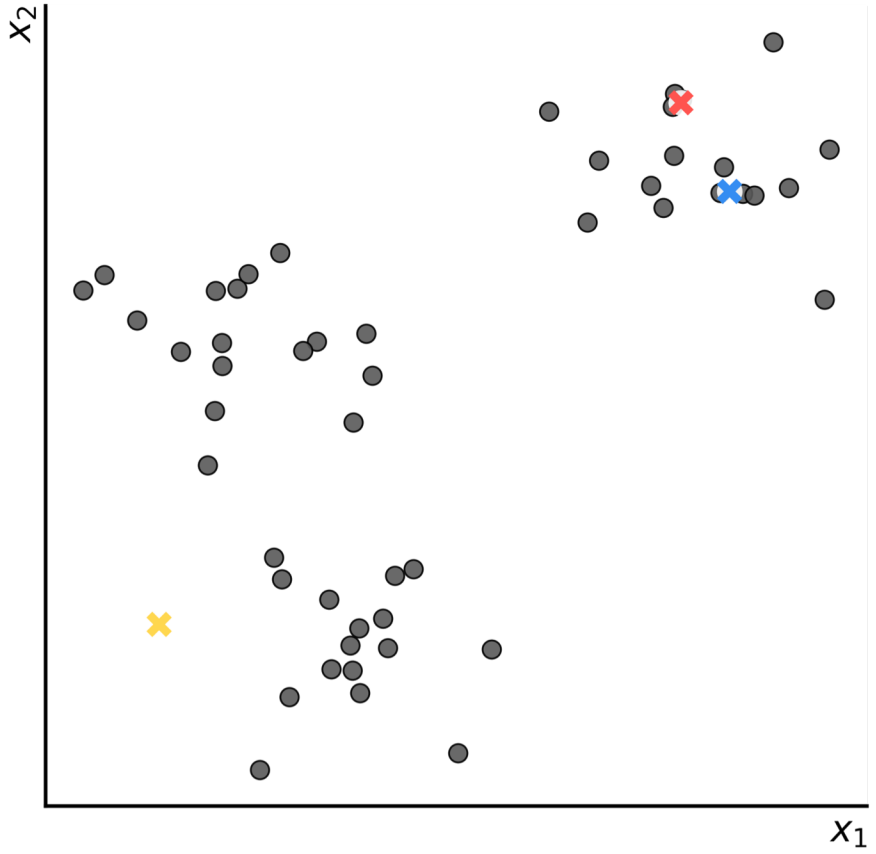
Poor initial centroids result to **poor clusters**.



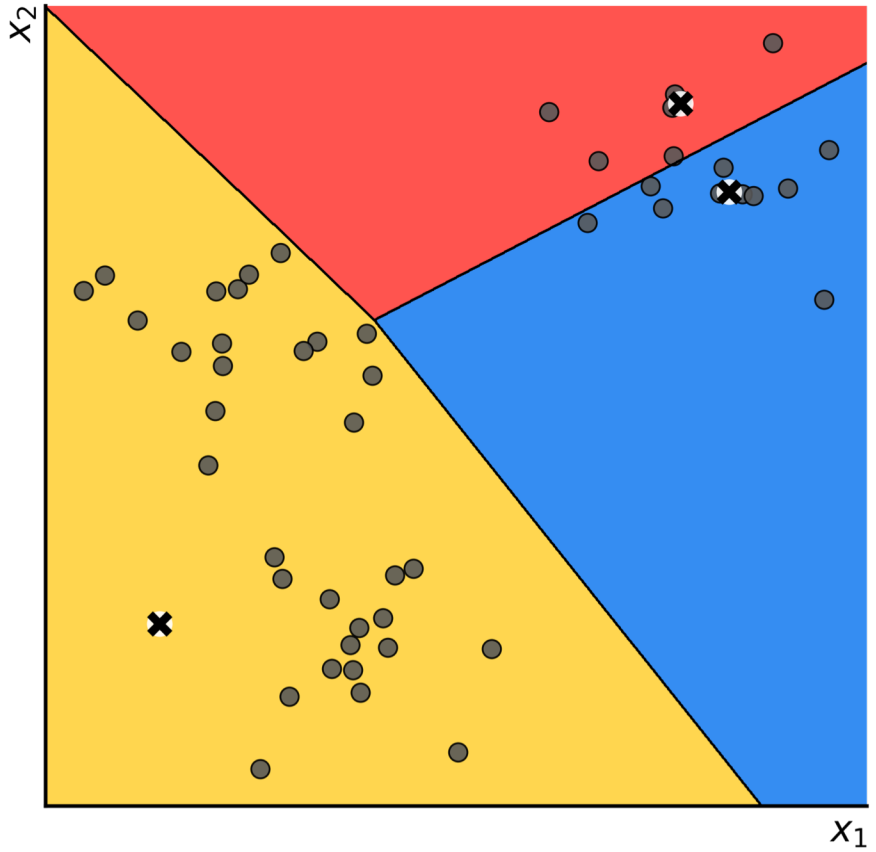
Example with poor initial centroids



initial centroids

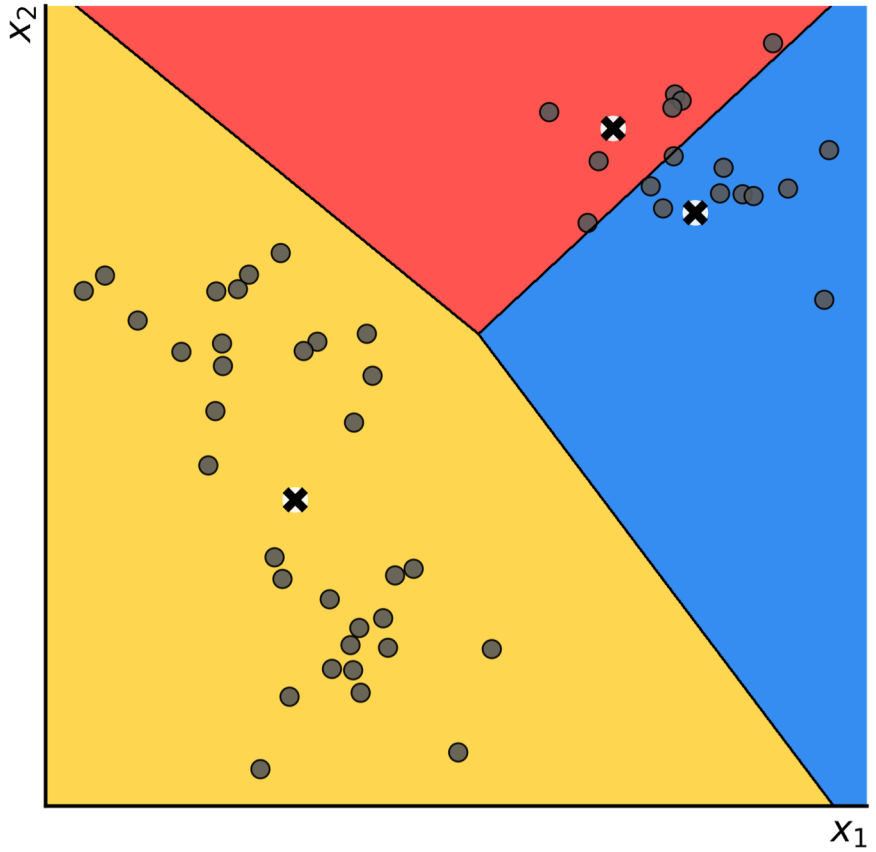
Example with poor initial centroids

Iteration 1



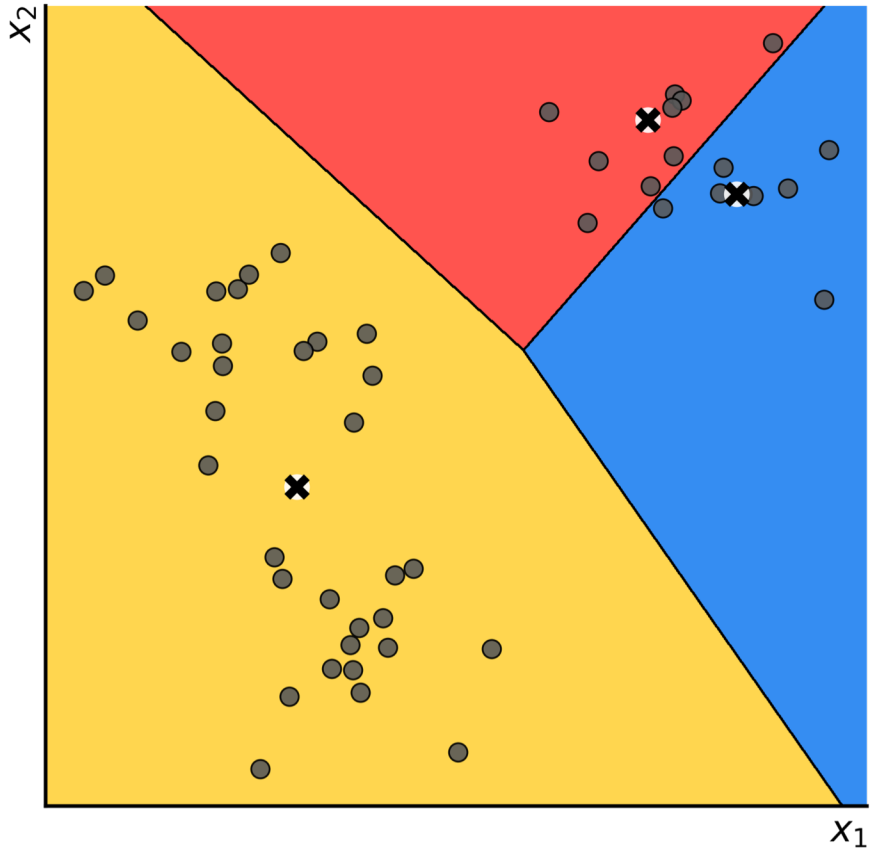
Example with poor initial centroids

Iteration 2



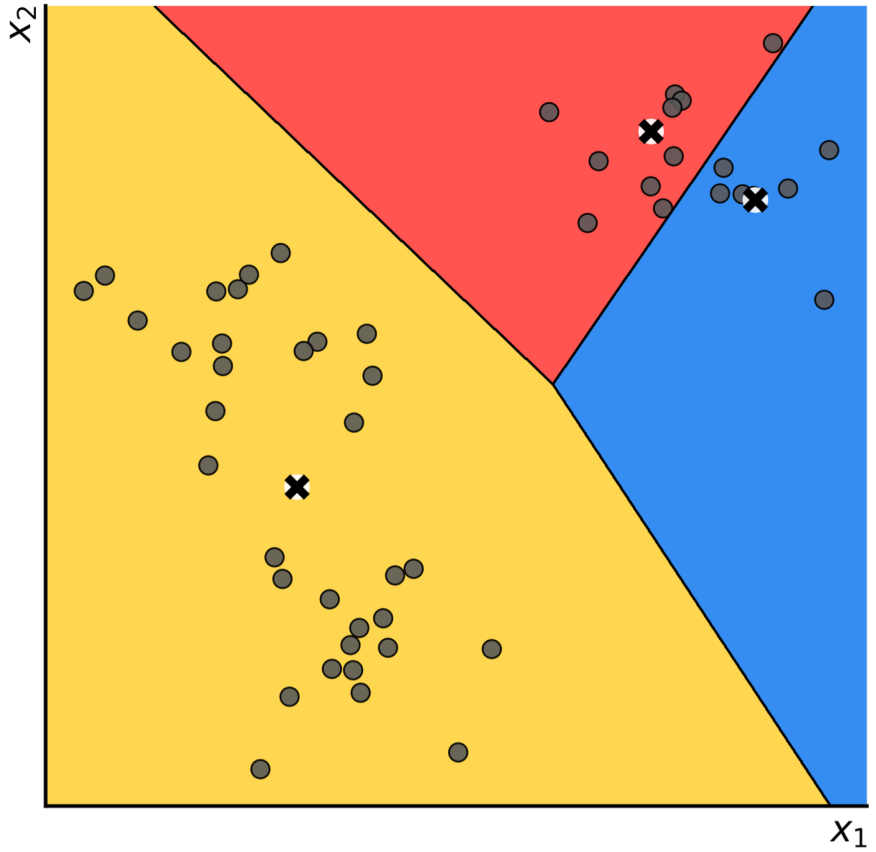
Example with poor initial centroids

Iteration 3



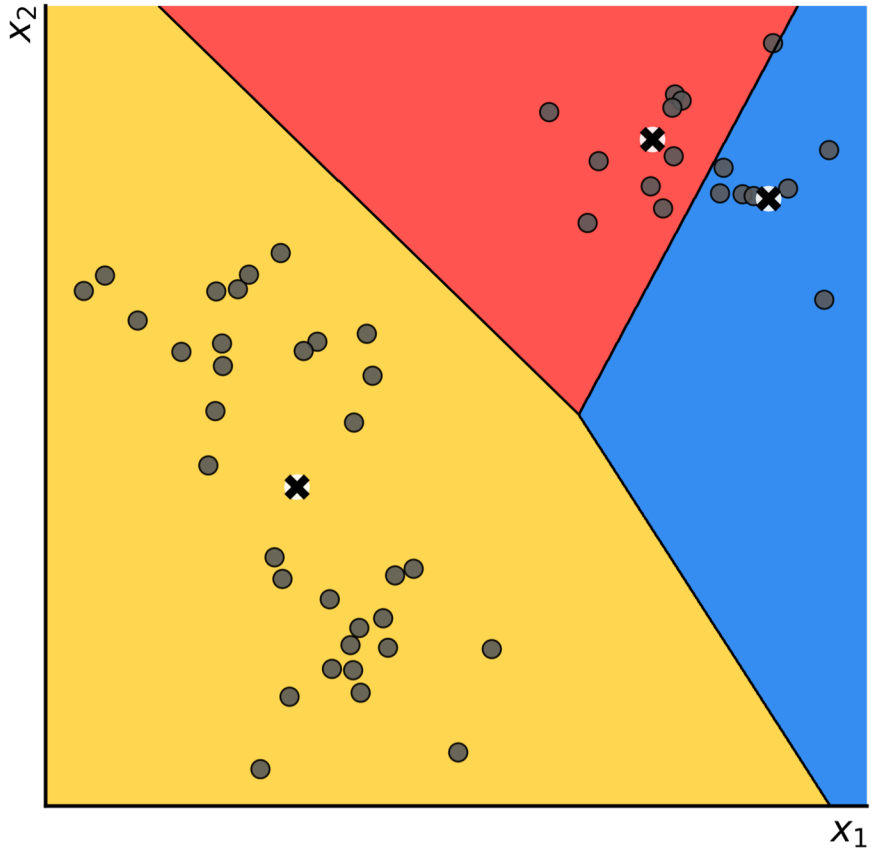
Example with poor initial centroids

Iteration 4

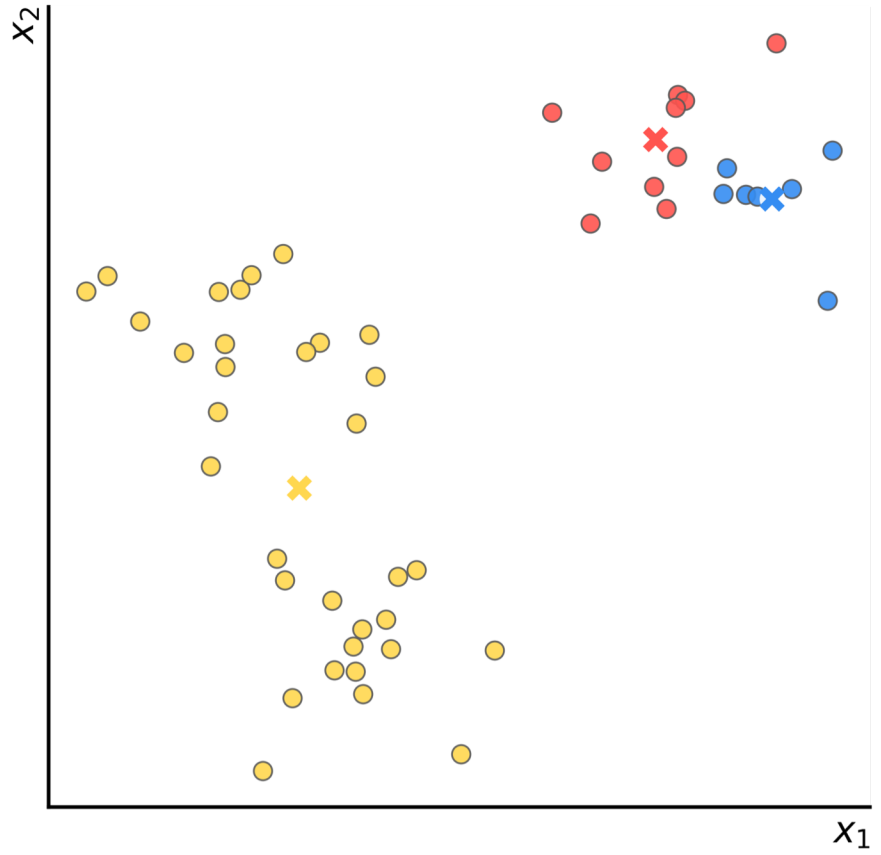


Example with poor initial centroids

Final
Decision Boundary

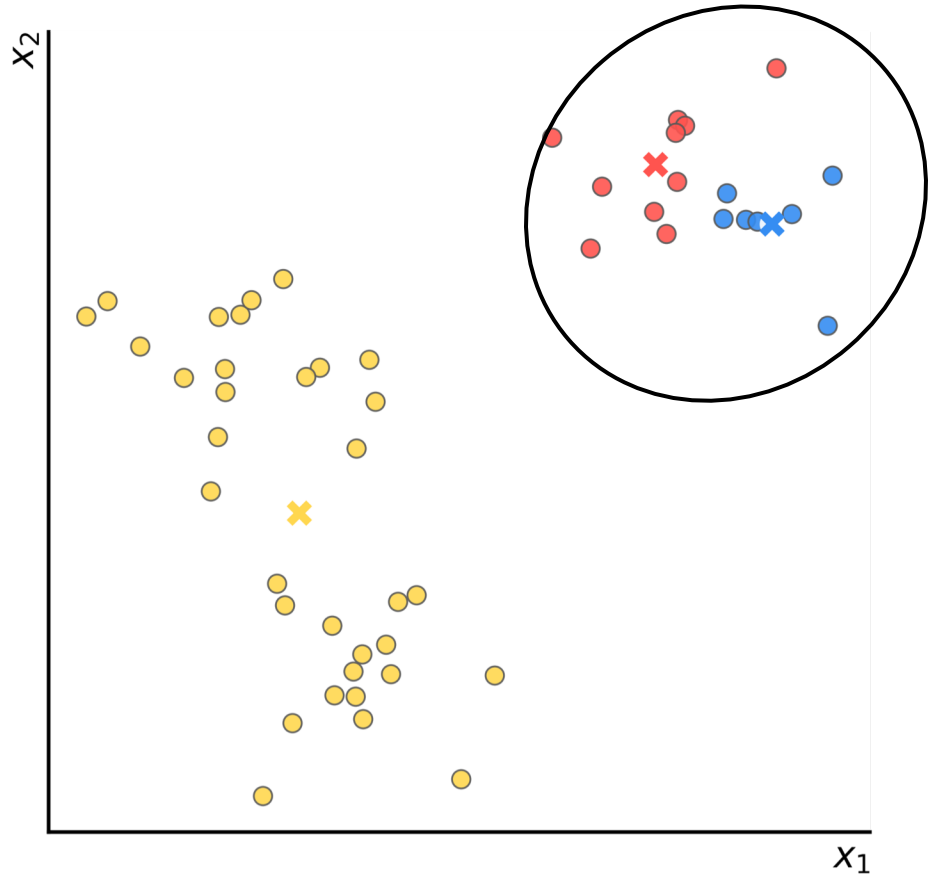


Example with poor initial centroids



Final
Clusters and Centroids

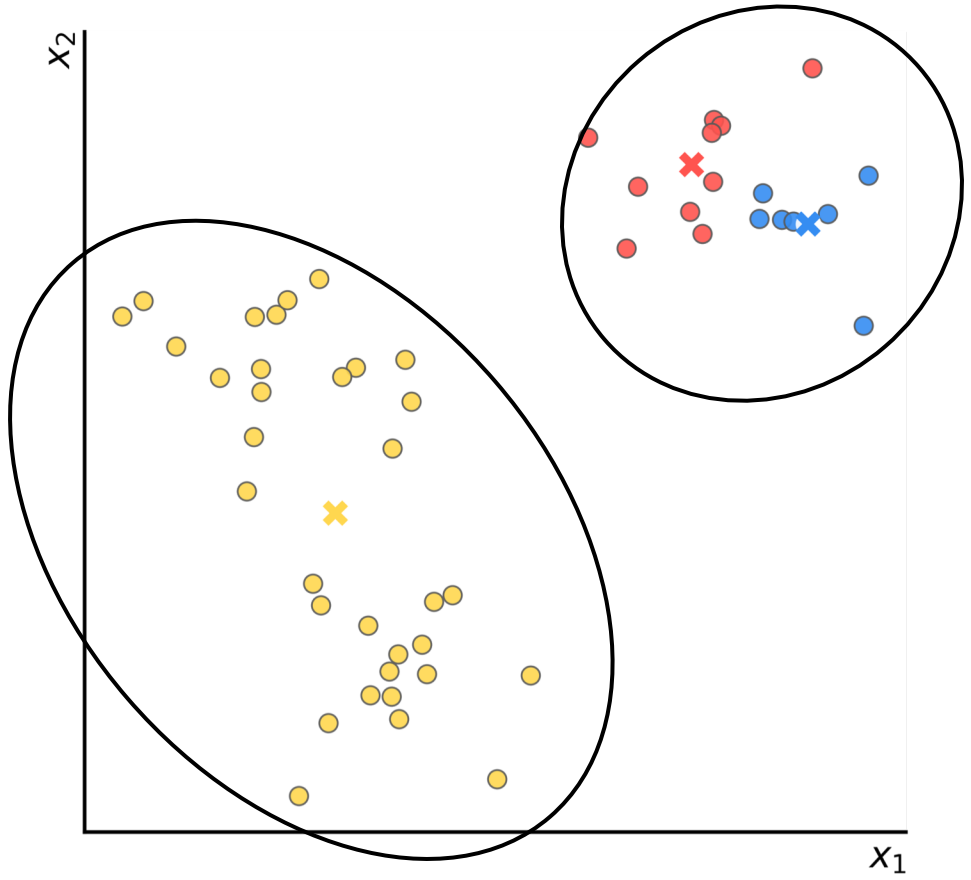
Example with poor initial centroids



A **cluster** is overpartitioned into two clusters

Example with poor initial centroids

Two **clusters** is underpartitioned into a single cluster



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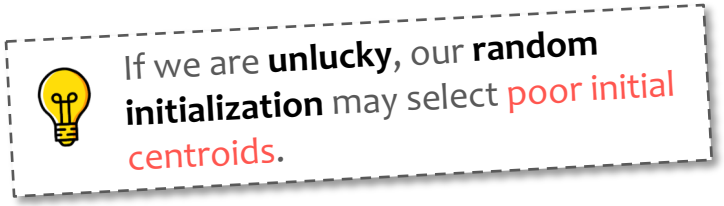
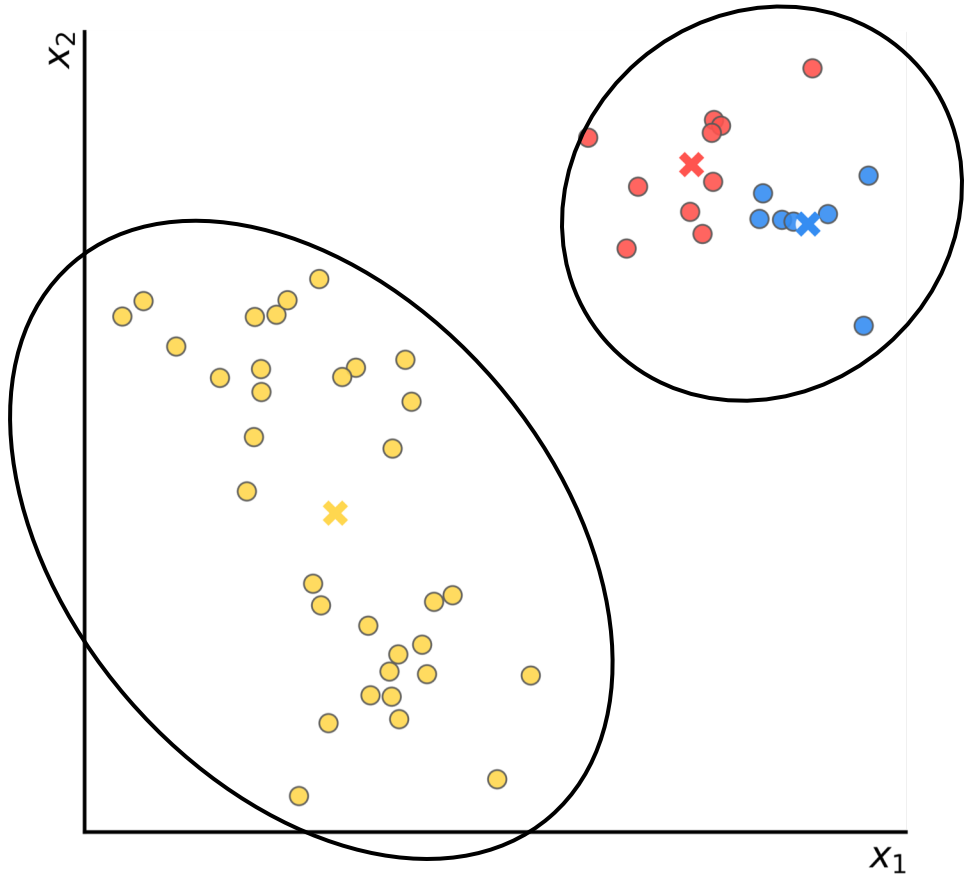


If we are **unlucky**, our **random initialization** may select poor initial centroids.



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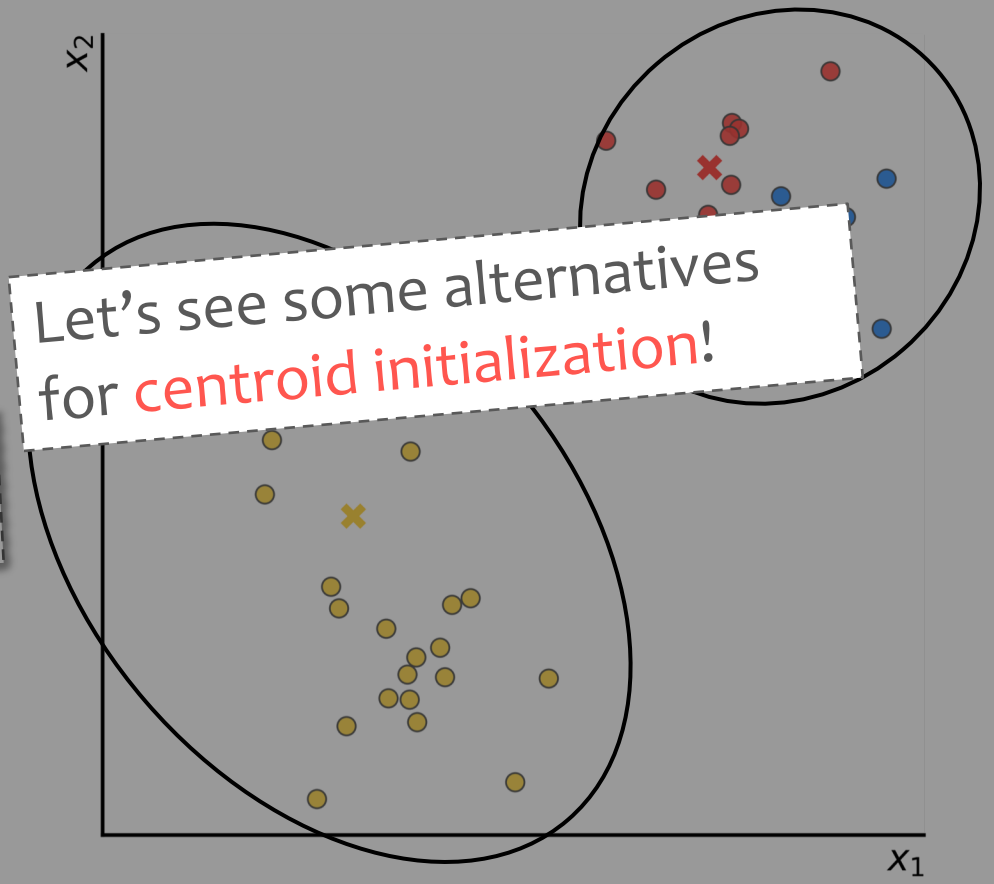

Let's see some alternatives for centroid initialization!

If we are **unlucky**, our **random initialization** may select poor initial centroids.

KMeans++

Initialization:

1) Take one centroid $\boldsymbol{c^{(1)}}$, chosen uniformly at random from the dataset $\mathbf{X}$;

2) Take a new centroid $\boldsymbol{c^{(l)}}$, choosing an instance $\boldsymbol{x^{(i)}} \in \mathbf{X}$ with probability $\frac{D(\boldsymbol{x^{(i)}})^2}{\sum_{j=1}^{m} D(\boldsymbol{x^{(j)}})^2}$;

- where $D(\boldsymbol{x^{(i)}})$is the distance between the instance $\boldsymbol{x^{(i)}}$ and **the nearest centroid** that **was already chosen**;
- This probability distribution ensures that instances farther away from already chosen centroids are much more likely be selected as centroids.

3) Repeat the previous step until all k centroids have been chosen;

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3) Repeat the previous step until all k centroids have been chosen;

This is the **default initialization** for `KMeans` in Scikit-learn, but we can also force to use the **the original method** (*i.e.*, picking k instances randomly as initial centroids).

Optimization Strategy

Another solution to get proper initial centroids and, consequently, good **resulting clusters** is **to run KMeans** multiple times with different random initializations and **keep the best model**, which is that with **the lowest inertia**.

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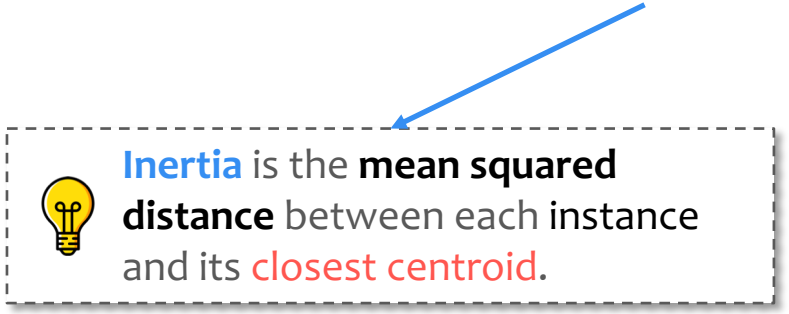

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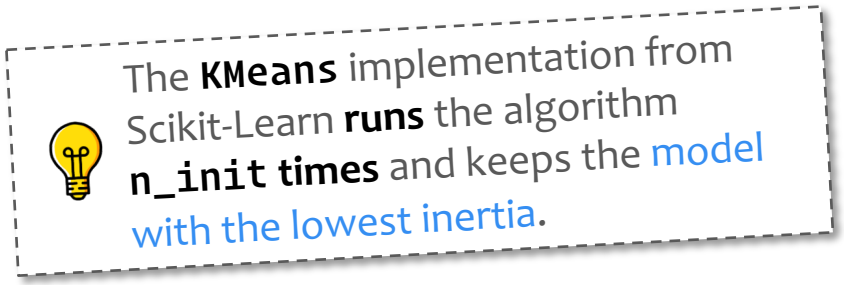
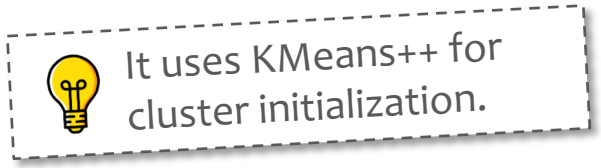
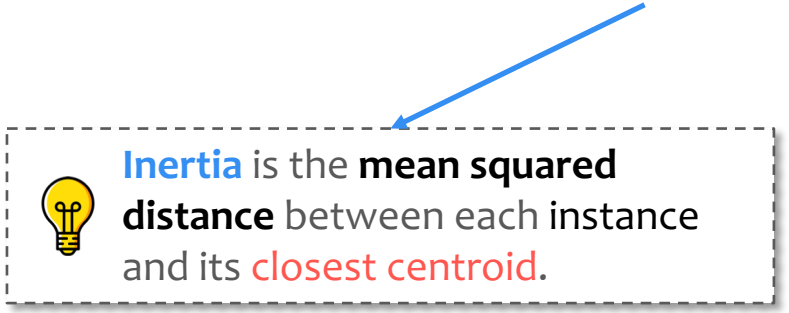






Codes

Finding the optimal number of clusters

Finding the optimal number of clusters

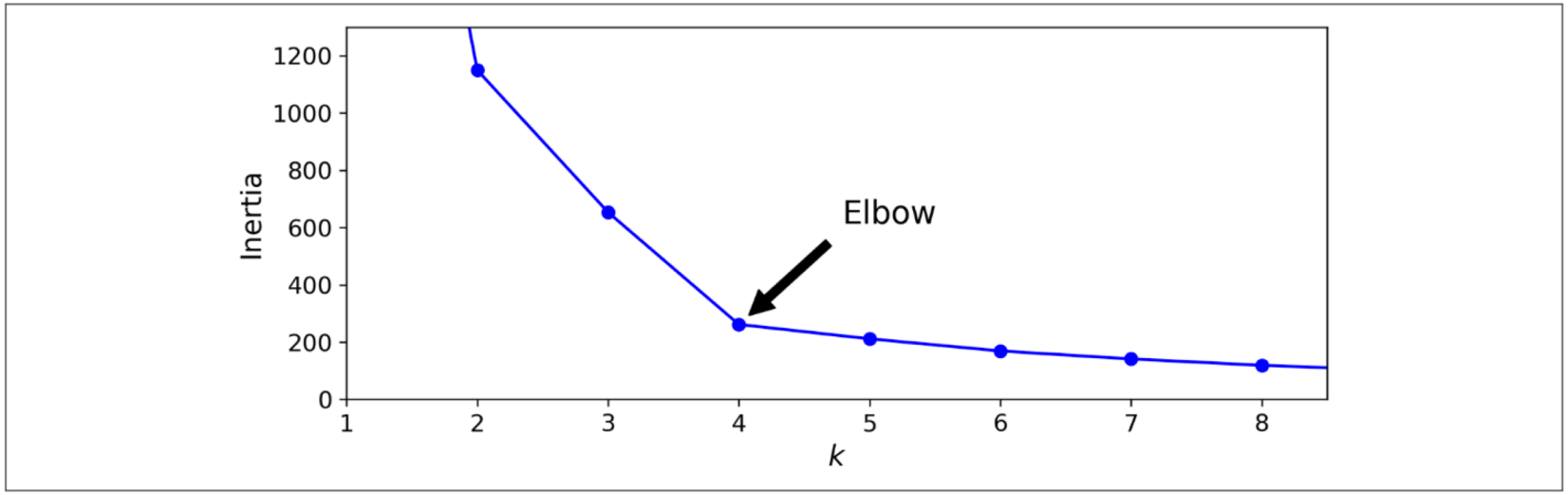
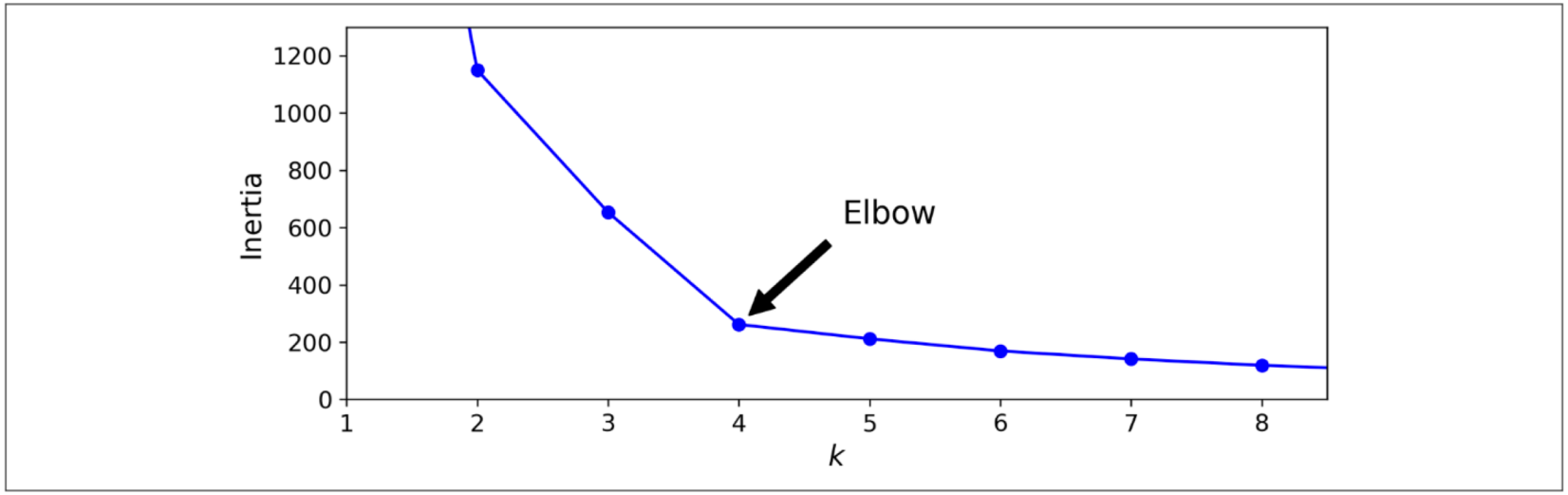


Figure 9-8. When plotting the inertia as a function of the number of clusters k, the curve often contains an inflexion point called the "elbow"

https://github.com/ageron/handson-ml2/blob/master/09_unsupervised_learning.ipynb

Finding the optimal number of clusters

This technique for choosing the best value for the number of clusters is rather coarse.



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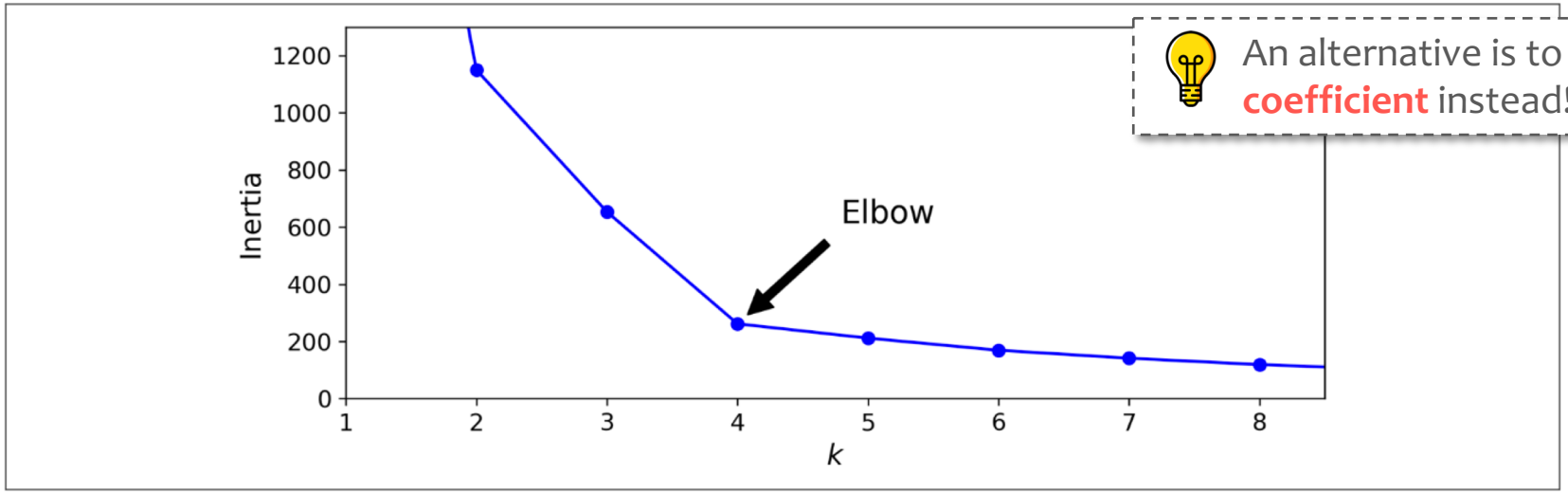
This technique for choosing the best value for the number of clusters is rather coarse.

An alternative is to use the **silhouette coefficient** instead!



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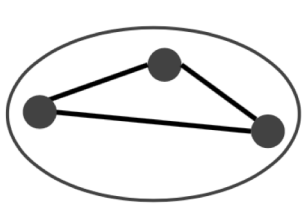
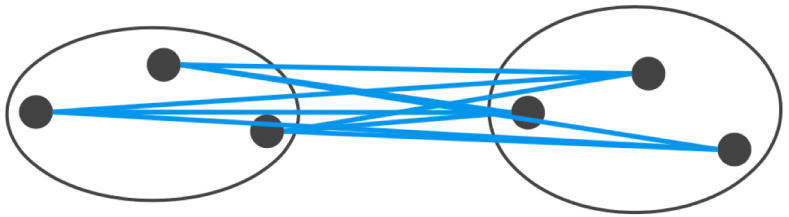
Silhouette Coefficient

The silhouette value is a measure of how similar a sample is to its own cluster (**cohesion**) compared to other clusters (**separation**)



Cohesion



Separation

Silhouette Coefficient

- The silhouette value is a measure of how similar a sample is to its own cluster (**cohesion**) compared to other clusters (**separation**)
- The silhouette ranges from −1 to +1
  - High value = the clustering configuration is appropriate
  - Low value = the clustering configuration may have too many or too few clusters

Silhouette Coefficient

- The Silhouette Coefficient is defined for each sample and is composed of two scores:
  - **a:** The mean distance between **a sample** and all other points in **the same cluster**
  - **b:** The mean distance between **a sample** and all other points in **the next nearest cluster**
- The Silhouette Coefficient s for a single sample is given as:

$$s = \frac{b - a}{\max(a, b)}$$

- The score is bounded between -1 for incorrect clustering and +1 for highly dense clustering (a $\ll$ b).
- Scores around zero indicate overlapping clusters

Silhouette Coefficient

```
>>> from sklearn.metrics import silhouette_score
>>> silhouette_score(X, kmeans.labels_)
0.655517642572828
```

Let's compare the silhouette scores for different numbers of clusters (see Figure 9-9).

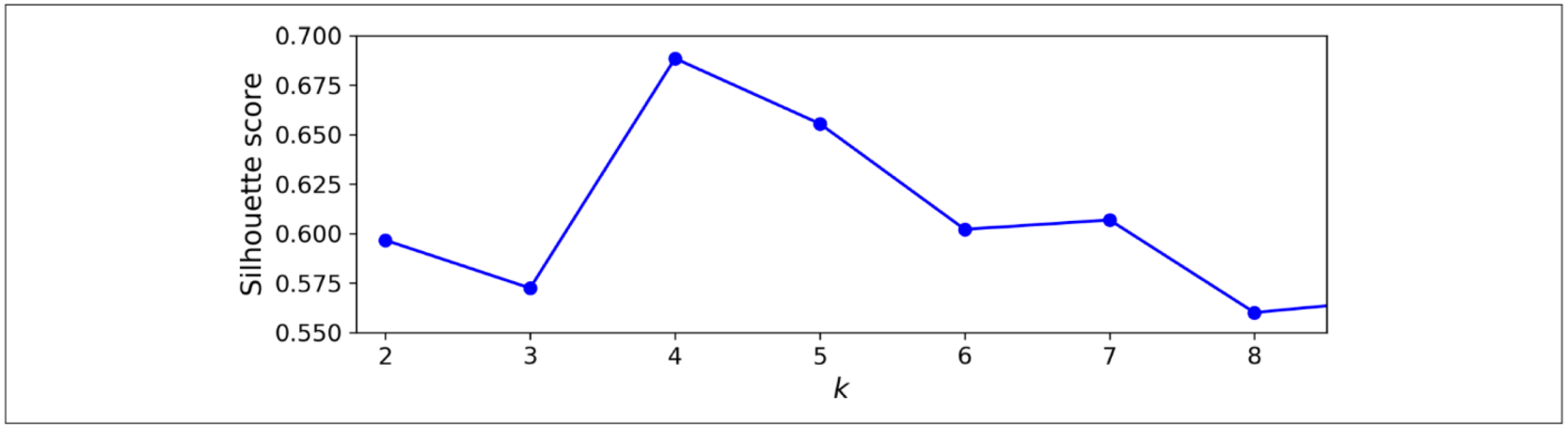


Figure 9-9. Selecting the number of clusters k using the silhouette score

Silhouette Coefficient

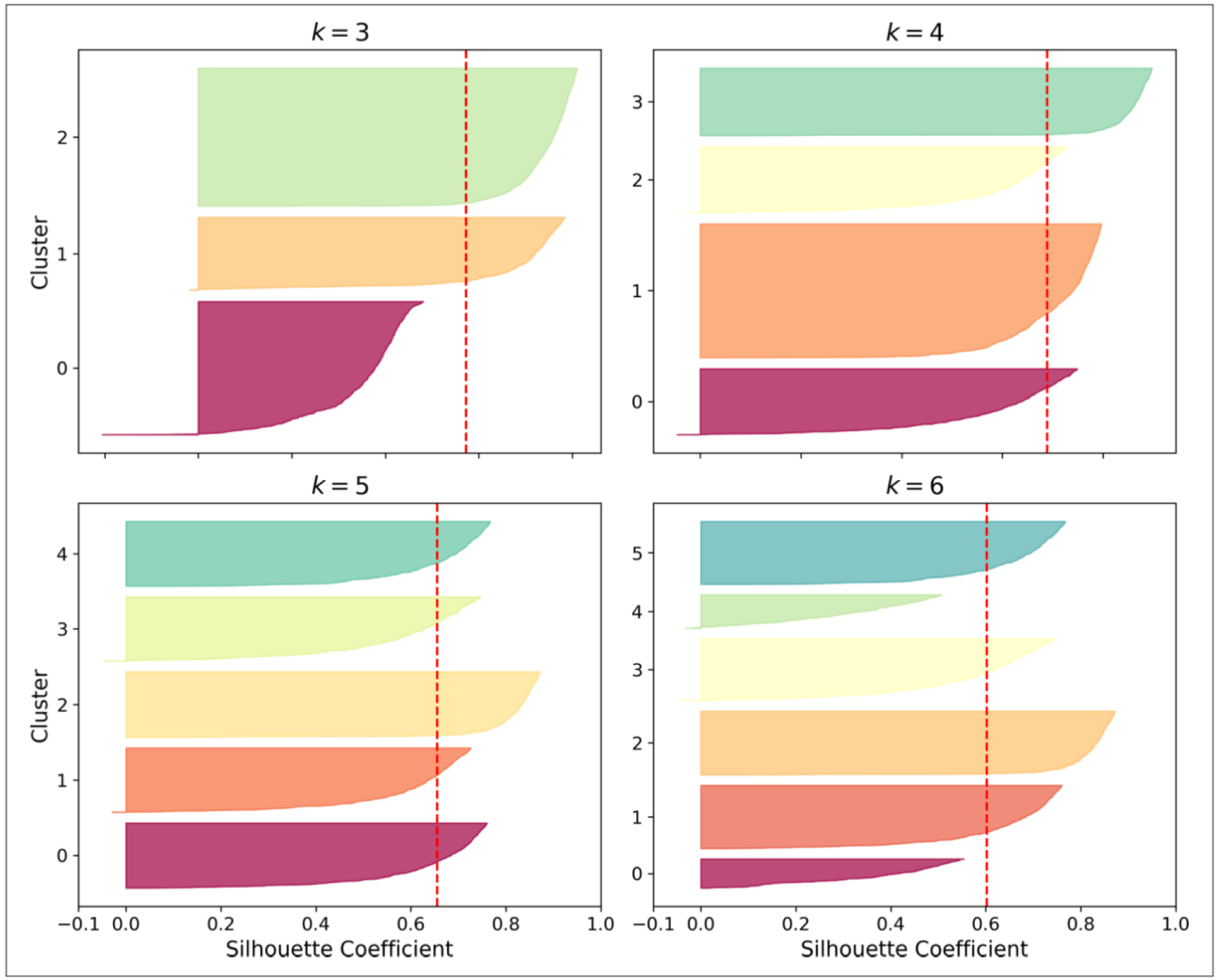


Figure 9-10. Analyzing the silhouette diagrams for various values of k

Aprendizado de Máquina e Reconhecimento de Padrões

Kmeans

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