T6: Unsupervised learning

Fundamentos del Aprendizaje Automático

Curso 2025/2026

Structure

Outline

Problem statement

- **Supervised learning**: target to *guide* the learning process $\Rightarrow P(\omega|\mathbf{x})$

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- **Unsupervised learning**: No specific target is provided
  - $\rightarrow$ Data assortment $\mathcal{D} = \{\mathbf{x}_i\}_{i=1}^{|\mathcal{D}|}$
  - $\rightarrow$ Related to Exploratory Data Analysis

Main tasks

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   - Visualization purposes

3. **Outlier/anomaly detection**:
   - Identify elements that *differ* for the rest in the assortment
   - Removenoise in assortments
   - Track unexpected behaviours

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Definition

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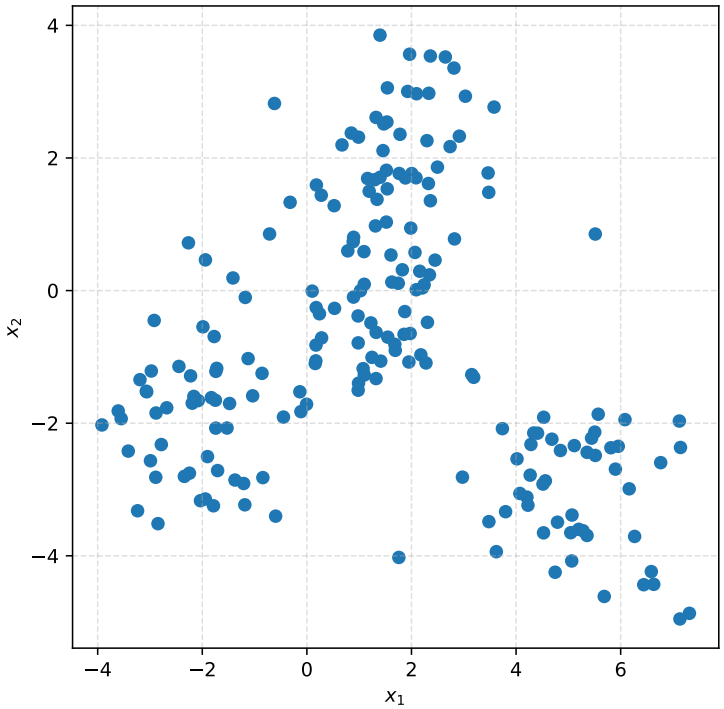

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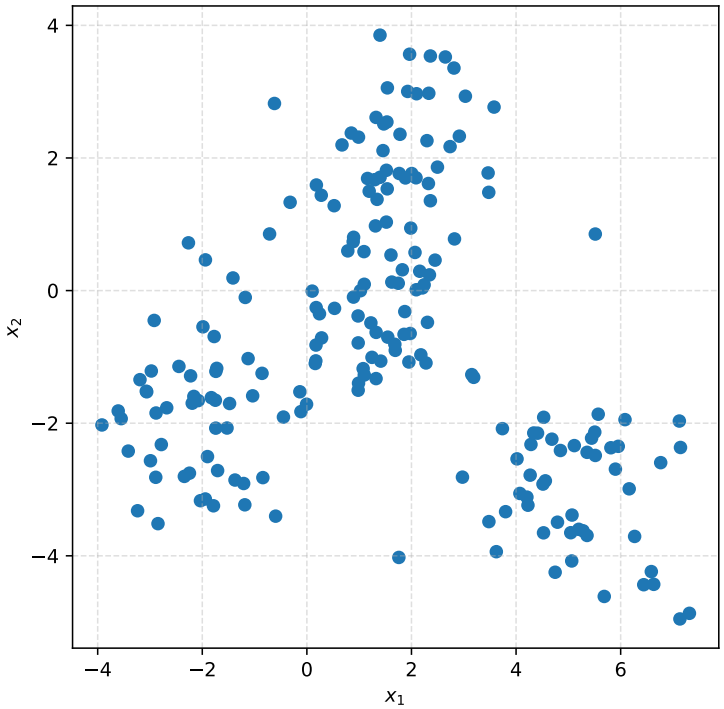
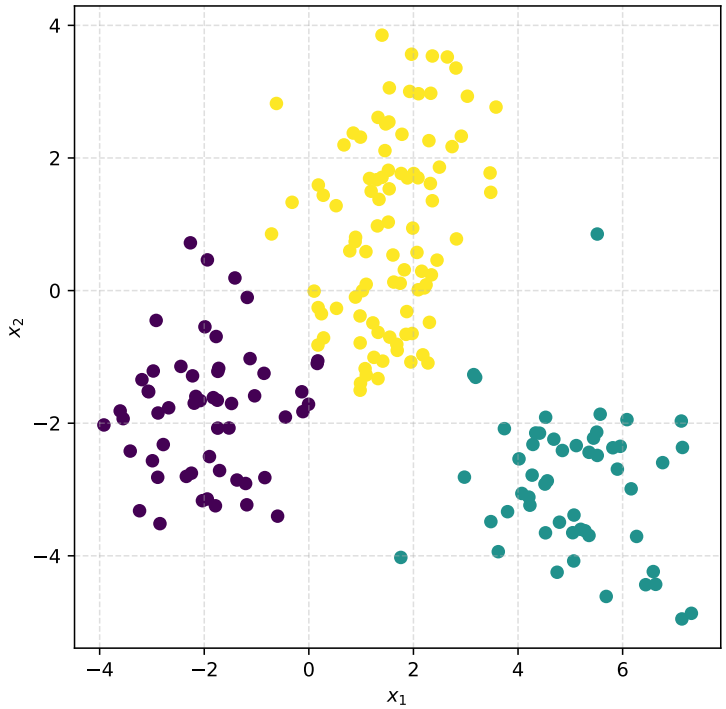
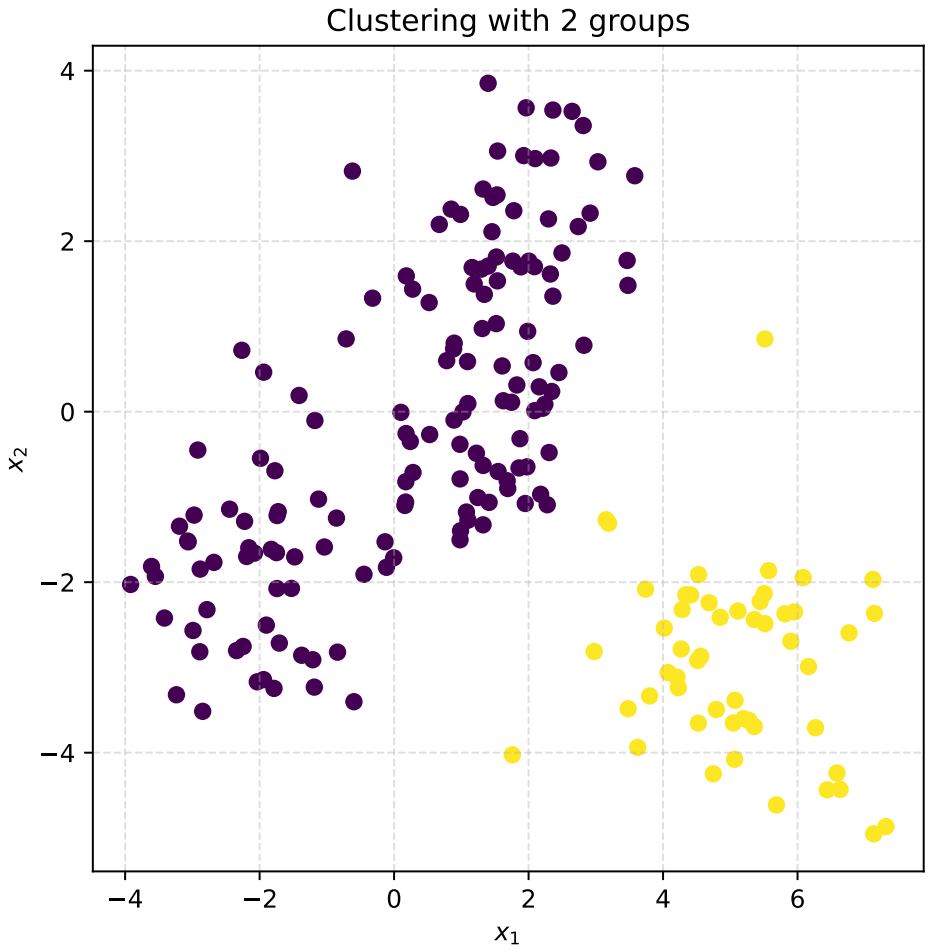




Example



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   - Data is organized in a plain structure without hierarchy
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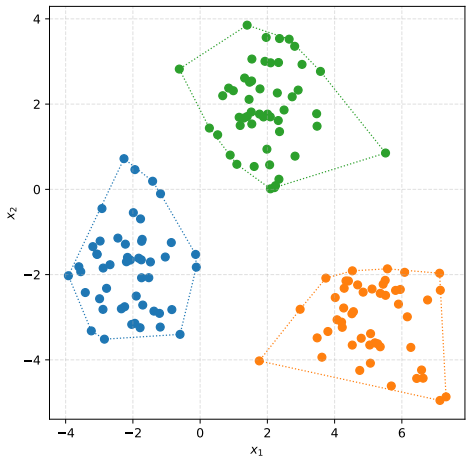

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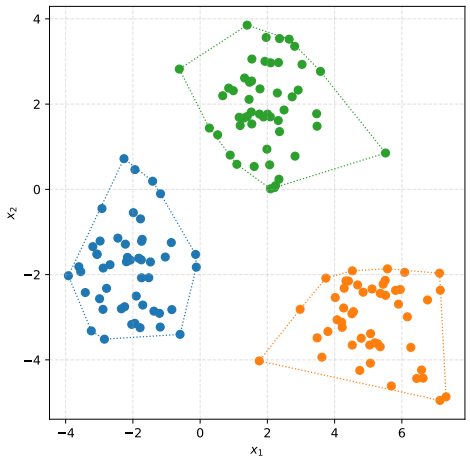
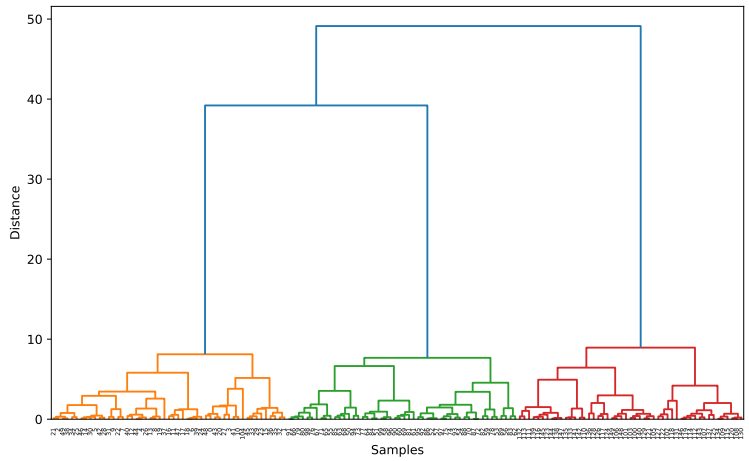
2. Hierarchical clustering
   - $\mathcal{D}$ is partitioned into levels in a hierarchical format $\Rightarrow$ Dendrogram
     - $\rightarrow$ Tree-like diagram that shows how items are grouped
   - Two main approaches:
     - $\rightarrow$ **Top-down** or divisive
     - $\rightarrow$ **Bottom-up** or agglomerative





Partitional clustering

1.1 Hard clustering

1.2 Mixture resolving

1.3 Fuzzy clustering

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1.3 Fuzzy clustering

- Clusters are defined as *fuzzy* sets
- Elements may belong to more than one cluster: $\cap_{j=1}^{|\mathcal{C}|} \mathcal{C}_j \neq \emptyset$

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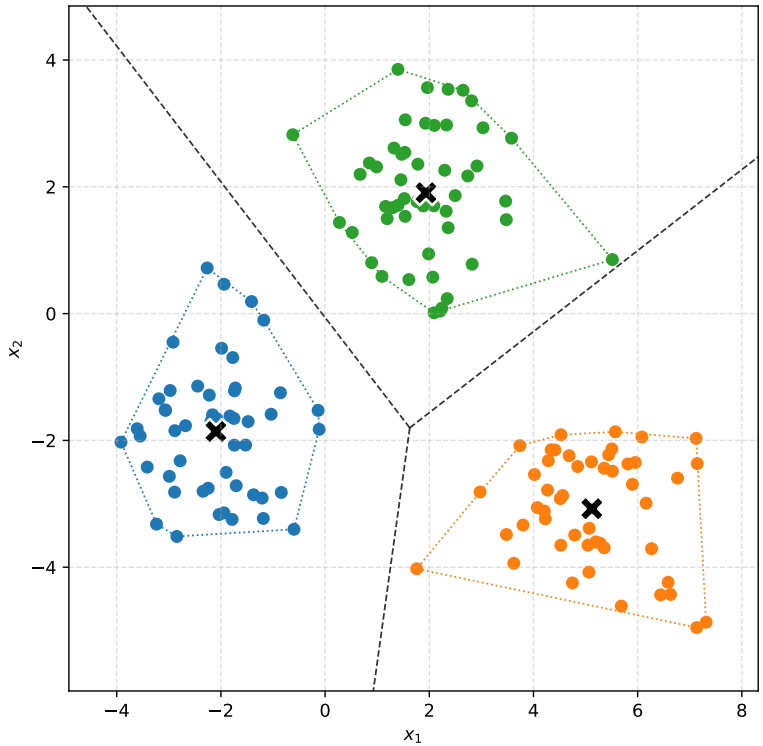

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Elements from $\mathcal{D}$ associated to a given cluster $\mathcal{C}_j$:

$$\mathcal{C}_j = \left\{ \mathbf{x}_i \in \mathcal{D} : \underset{1 \leq m \leq |\mathcal{C}|}{\arg\min}\, d\left(\mathbf{x}_i, \boldsymbol{\mu}_m\right) \right\}$$

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The exact solution to this equation is NP-hard

- The iterative Lloyd's algorithm provides a suboptimal solution

Lloyd's algorithm

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1. **Assignment** step:

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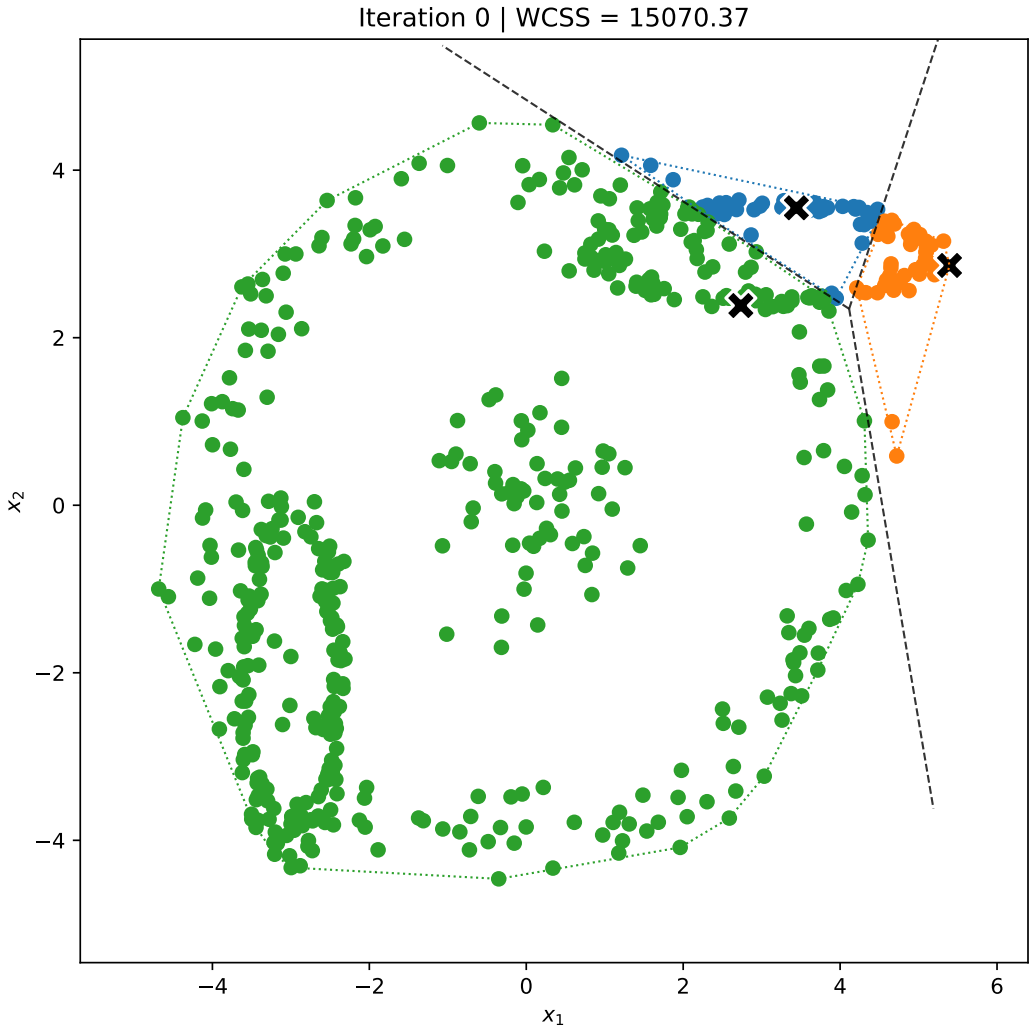
Process seeks to minimize *Within-Cluster Sum of Squares*:

- No changes in the cluster assigment between iterations

Lloyd's algorithm



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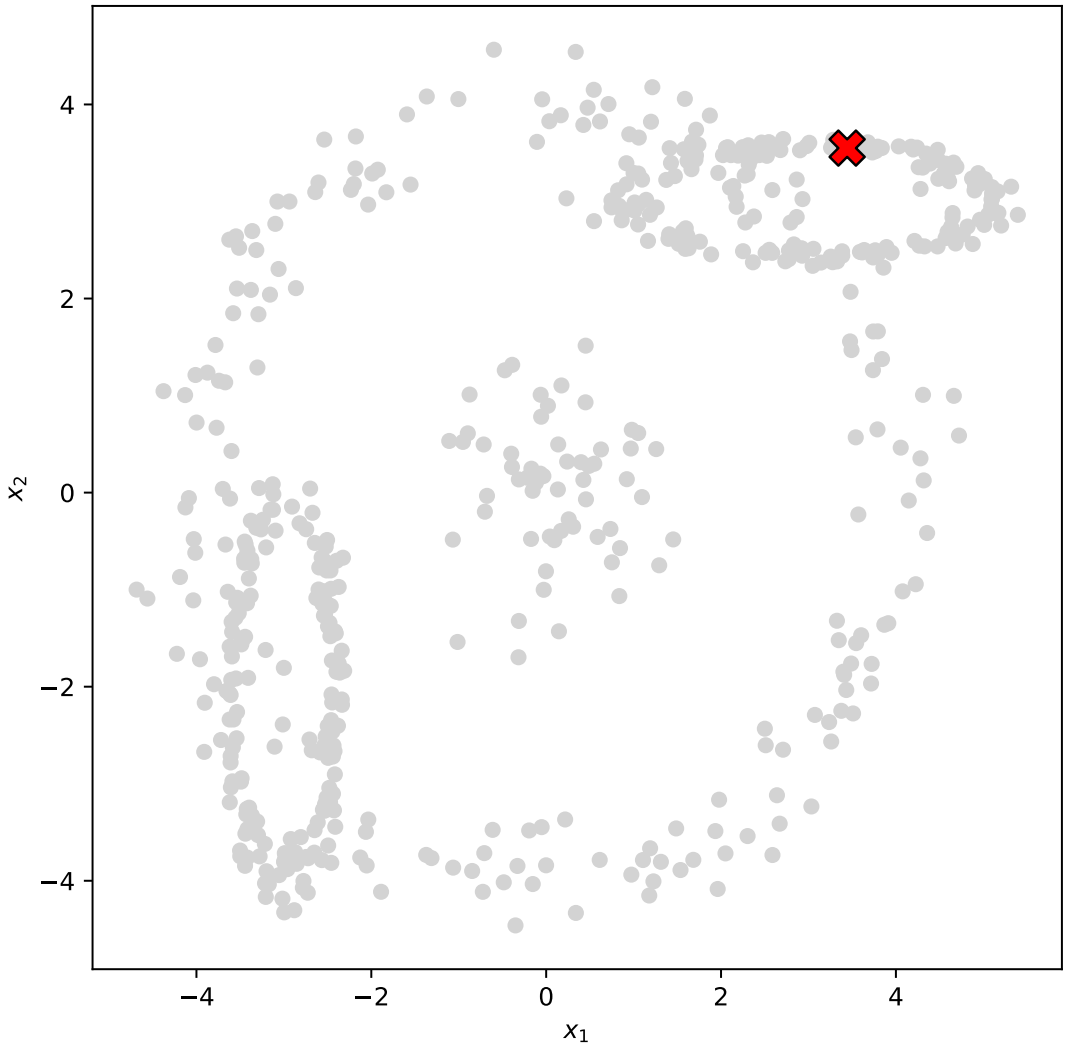
k-means++ initialization method

Input: Number of clusters $|\mathcal{C}|$
Result: Set of centroids $\{\boldsymbol{\mu}_j\}_{j=1}^{|\mathcal{C}|}$
$K = 1$, $\boldsymbol{\mu}_1 \in_R \mathcal{D}$;
while $K < |\mathcal{C}|$ **do**
  $\mathcal{P} = \left\{\min_{k=1}^{K} ||\mathbf{x}_i - \boldsymbol{\mu}_k||^2\right\} \forall \mathbf{x}_i \in \mathcal{D}$;
  $\boldsymbol{\mu}_{K+1} = \mathcal{D}_{\text{Categorical}(\mathcal{P}/\sum \mathcal{P})}$;
  $K = K + 1$;
end

Example of k-means++



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✓ Alternative approach: k-Medoids
- *In-set mean* $\Rightarrow$ Closest element in cluster $\mathcal{C}_j$ to mean $\boldsymbol{\mu}_j$ $(1 \leq j \leq |\boldsymbol{\mathcal{C}}|)$

$$\boldsymbol{\mu}_j^s = \arg\min_{\mathbf{x} \in \mathcal{C}_j} d\left(\mathbf{x}, \boldsymbol{\mu}_j\right)$$

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Two representative strategies to perform this estimation:

1. Elbow method
2. Silhoutte method

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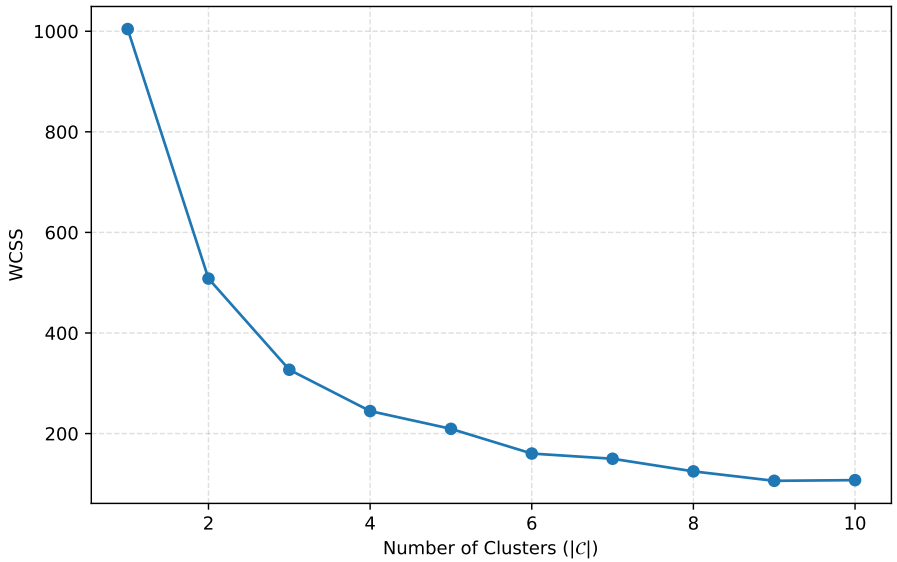

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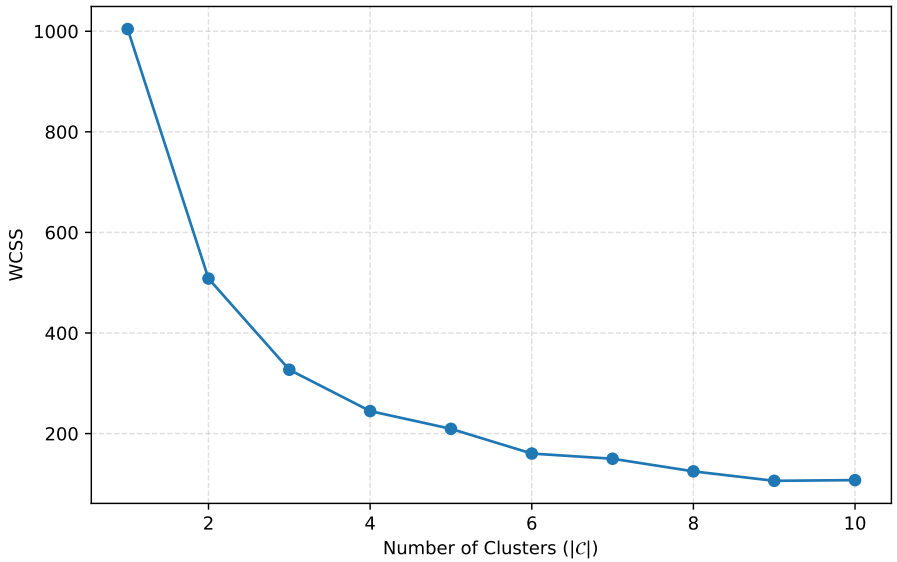
  - $\rightarrow$ *Turning* point $\Rightarrow$ Elbow of the curve



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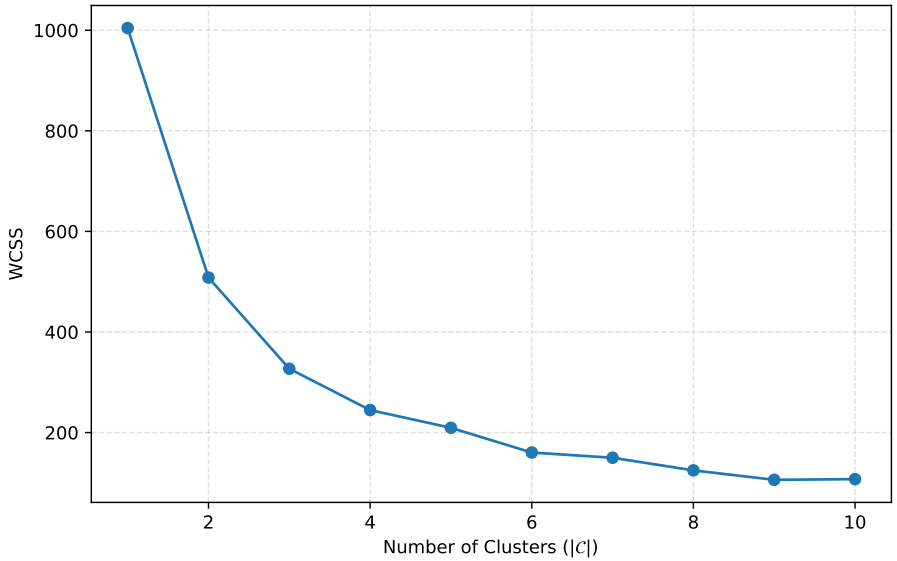
  - → Graphically, this relation resembles a negative exponential curve
- After a certain point: more clusters ⇔ small WCSS improvements
  - → *Turning* point ⇒ Elbow of the curve
- The elbow is assumed to be the optimal number of clusters $|\mathcal{C}|$



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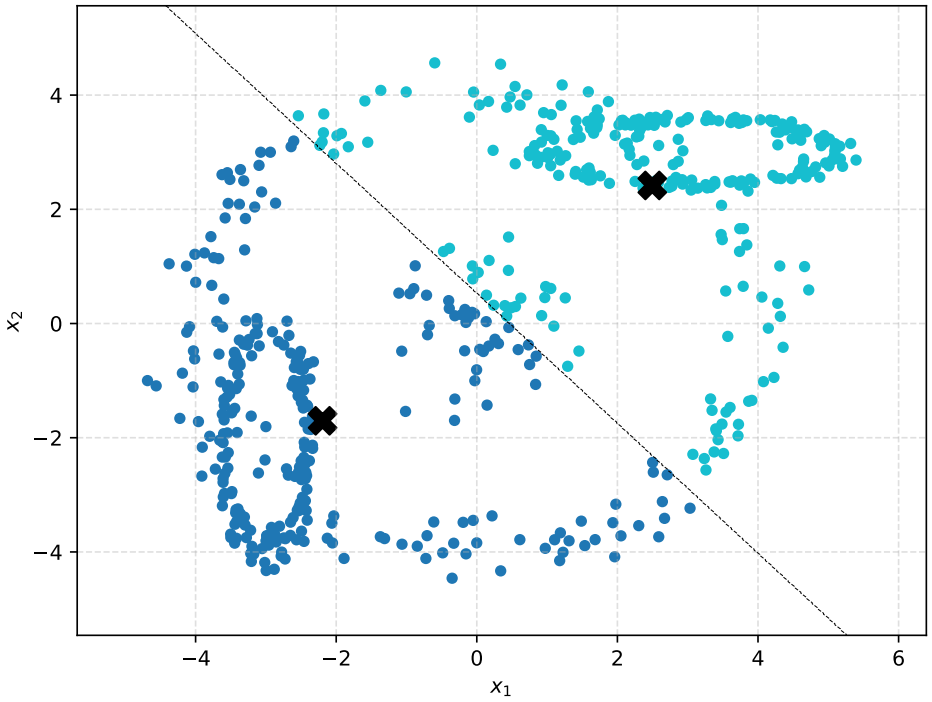

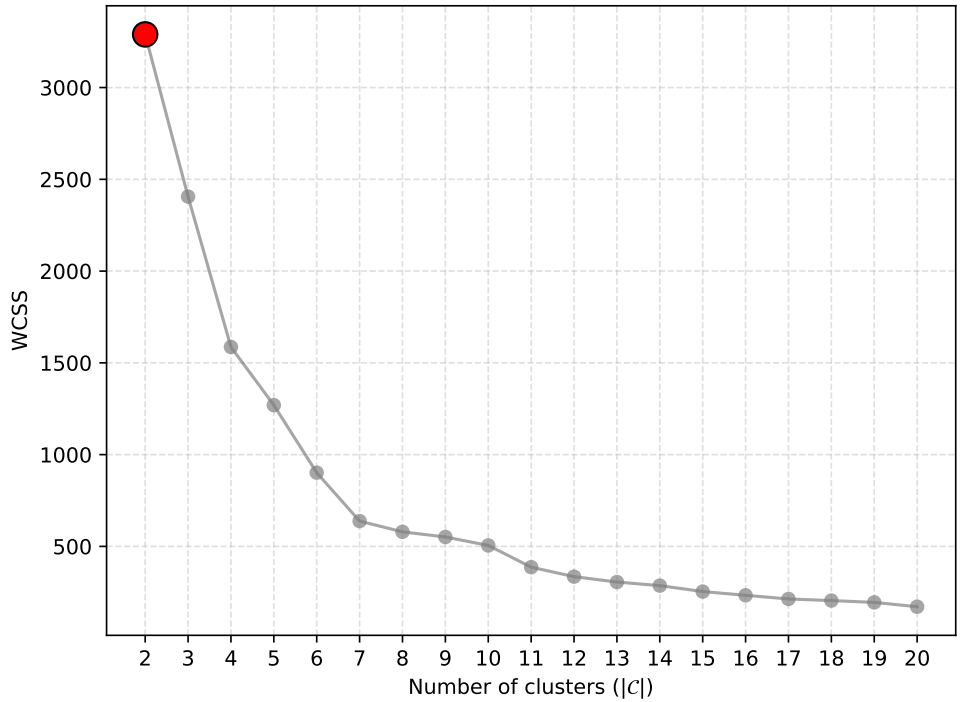

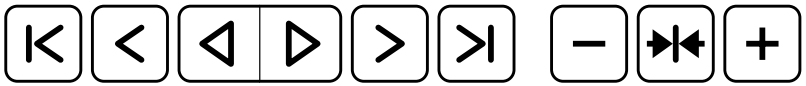

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Measures how well each sample $\mathbf{x}_i$ fits into its assigned cluster $\mathcal{C}_j$ compared to other clusters

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Considers two aspects for assessing the *quality* of the clustering:

1. Compactness: how tight a cluster is
2. Separation: how far apart clusters are

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- Silhouette score $s(\mathbf{x}_m)$:

$$s(\mathbf{x}_m) = \frac{b(\mathbf{x}_m) - a(\mathbf{x}_n)}{\max\left\{a(\mathbf{x}_m), b(\mathbf{x}_m)\right\}} \in [-1, +1]$$

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The Silhouette indicator exhibits three situations:

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Since the indicator is individual, a global Silhouette may be derived as:

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Silhouette method

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$\rightarrow$ Can be used as alternative metric for the Elbow method

Silhouette method