Unsupervised Learning

K-Means, GMMs

Machine Learning Course - CS-433

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Supervised Learning

We are given labeled training data $\mathcal{D} = \{(x_n, y_n)\}_{n \in [N]}$

MNIST Dataset

Image(X)	Label(y)
	“5”
	“7”
	“3”

The training objective is usually the alignment of the model predictions and the given labels

X

Model

Prediction ($\hat{y}$)

“7”

Ground truth (y)

“5”

training objective

$loss(y, \hat{y})$

Supervised Learning

We are given labeled training data $\mathscr{D} = \{(x_n, y_n)\}_{n \in [N]}$

Labeled data is **costly** and **time-consuming** to obtain, but unlabeled data is **abundant** (e.g. text and images online)

MNIST Dataset

Image(X)	Label(y)
	“5”
	“7”
	“3”

The training objective is usually the alignment of the model predictions and the given labels

X

Model

Prediction ($\hat{y}$)

“7”

Ground truth (y)

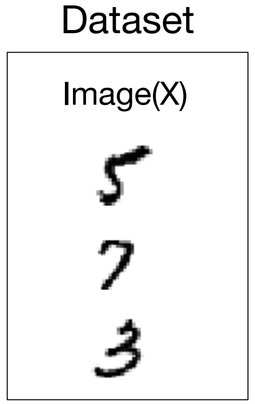
“5”

training objective

$loss(y, \hat{y})$

Unsupervised Learning

We are given only unlabeled training data $\mathscr{D} = \{x_n\}_{n \in [N]}$



What can we still learn from this data?

Main learning goals are

- Learning a compact and useful representation of the data
- Density estimation and generative modelling

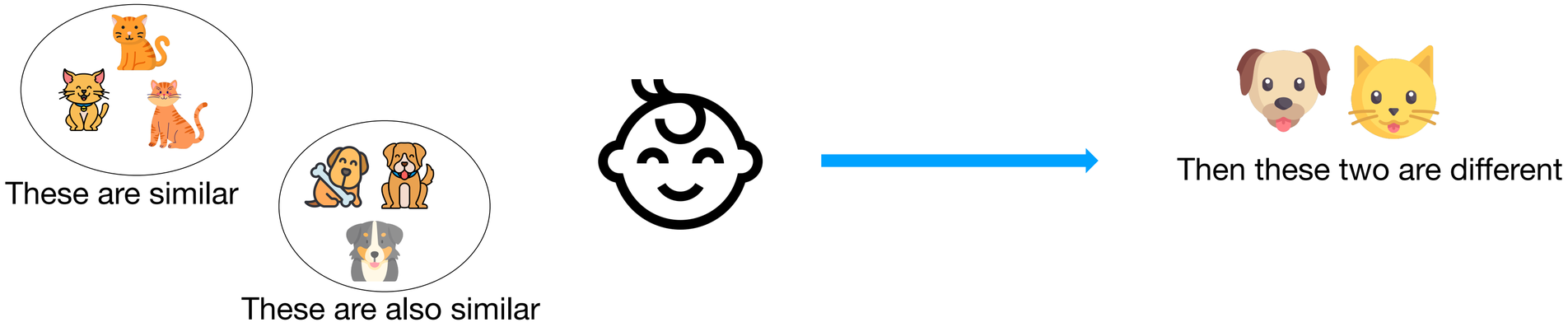
Useful for

- Exploratory data analysis (finding patterns in the data) and anomaly detection
- Learning good features/embeddings for various tasks
- Generate new observations

Unsupervised Learning

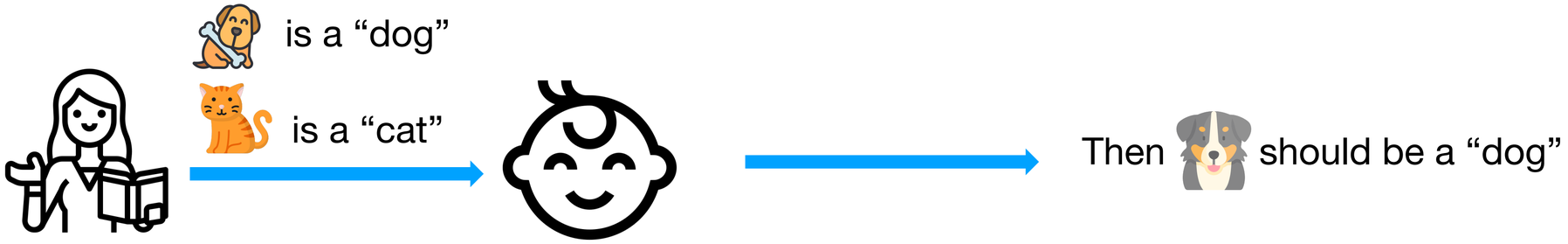
Supervised Learning: The Teacher-Guided Approach

Unsupervised Learning: The Self-Discovery Approach

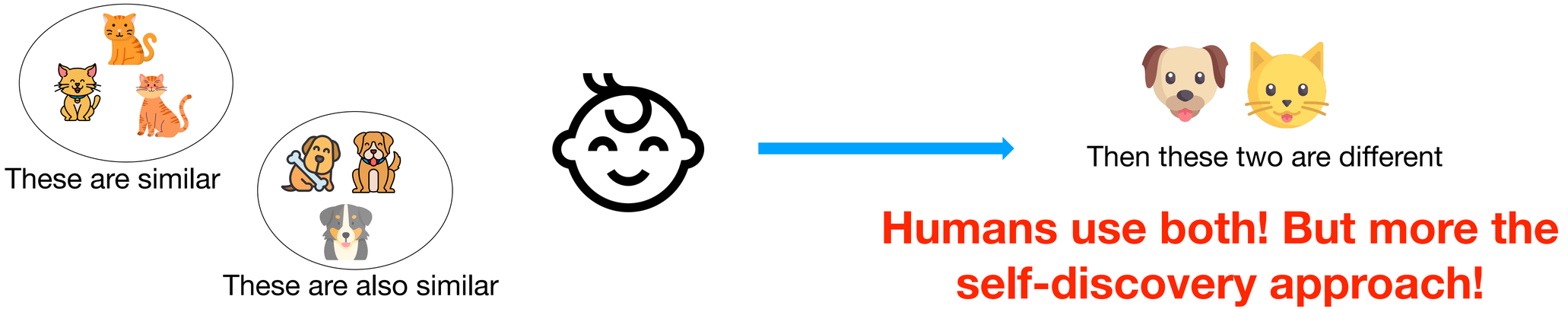


Unsupervised Learning

Supervised Learning: The Teacher-Guided Approach



Unsupervised Learning: The Self-Discovery Approach



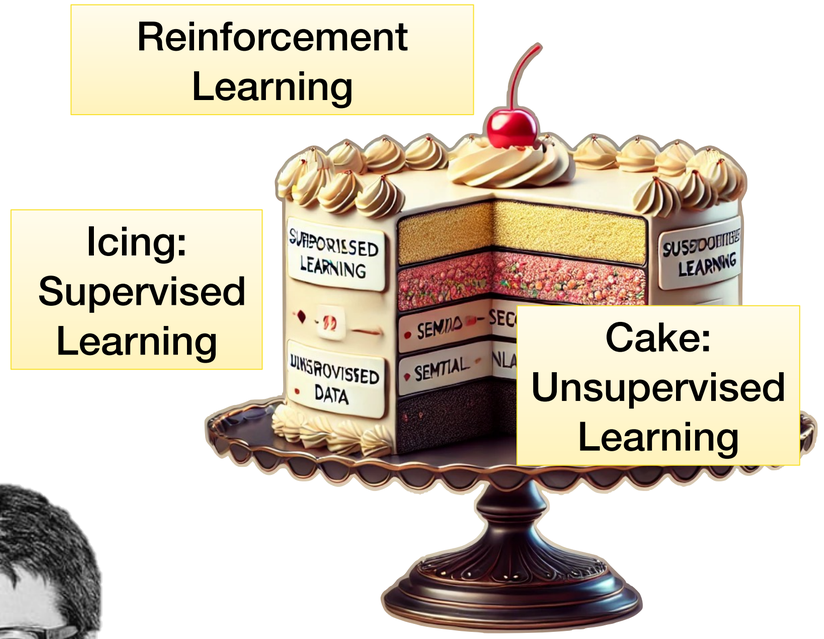
Humans use both! But more the self-discovery approach!

Deep Learning and Cake Analogy

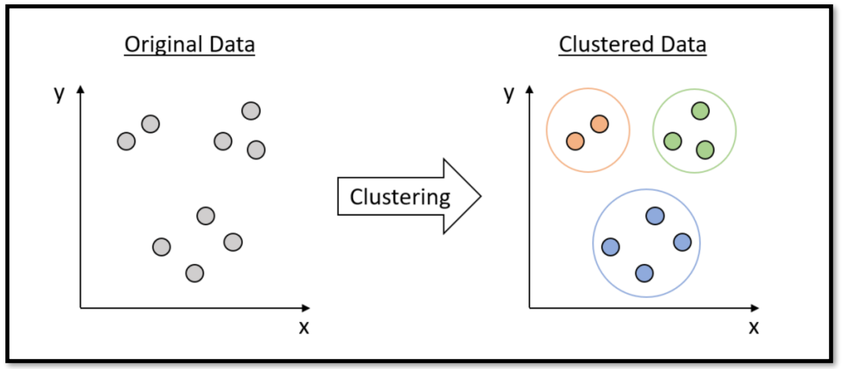
Unsupervised learning leverages vast amounts of unstructured data without the need for labeled examples

"Most of human and animal learning is unsupervised learning. If intelligence was a cake, unsupervised learning would be the cake, supervised learning would be the icing on the cake, and reinforcement learning would be the cherry on the cake."

NeurIPS 2016



Unsupervised Learning Examples

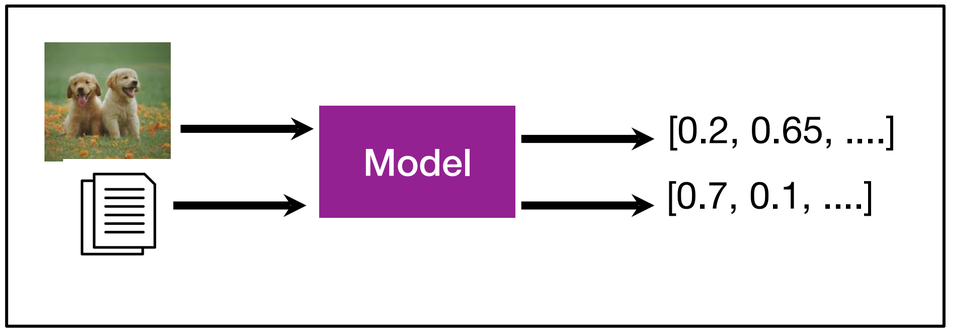


Clustering: Group the data points into clusters based on their similarities

- K-means, Gaussian Mixture Models (GMMs)

Representation Learning: Converting raw data into good numerical features

- Matrix factorization, GloVe, FastText
- BERT
- Contrastive learning (CLIP, SimCLR)



Generative Modelling

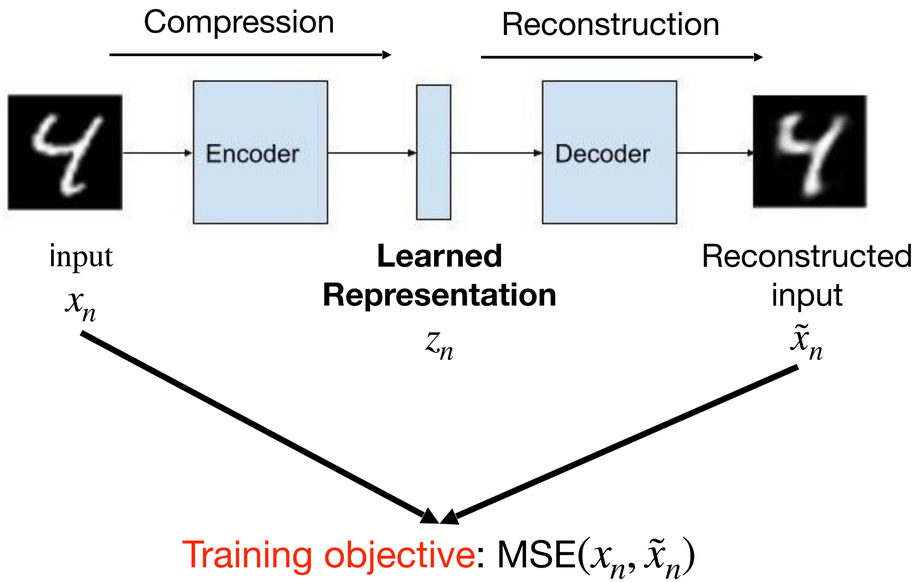
- Gaussian Mixture Models (GMMs)
- Large Language Models (LLMs) for text generation (e.g. GPT)
- GANs and Diffusion models for image generation

Unsupervised Learning

We can seek many ideas to find a training objective.

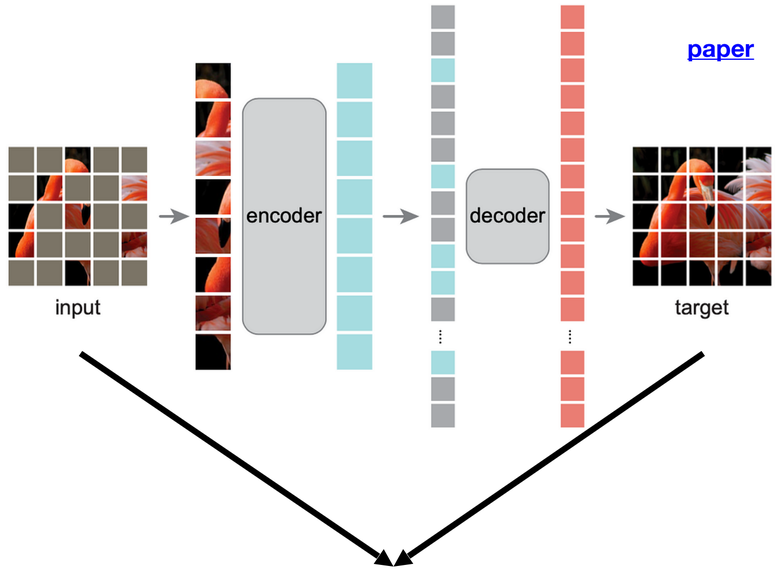
Two examples:

AutoEncoders



Training objective: MSE$(x_n, \tilde{x}_n)$

Masked AutoEncoders



Training signal: MSE$(target, reconstructed)$

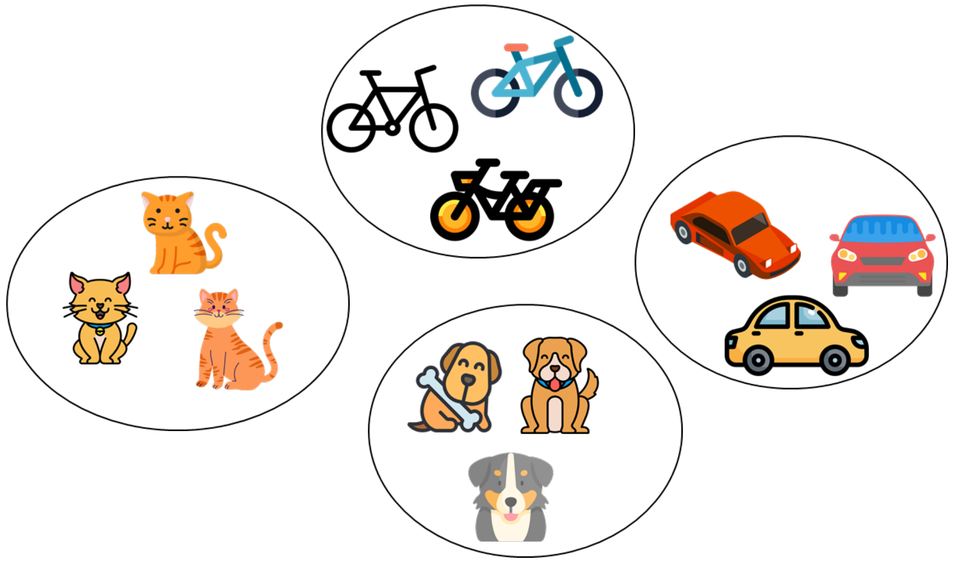
Clustering

Clustering

One of the most widely used techniques for exploratory data analysis

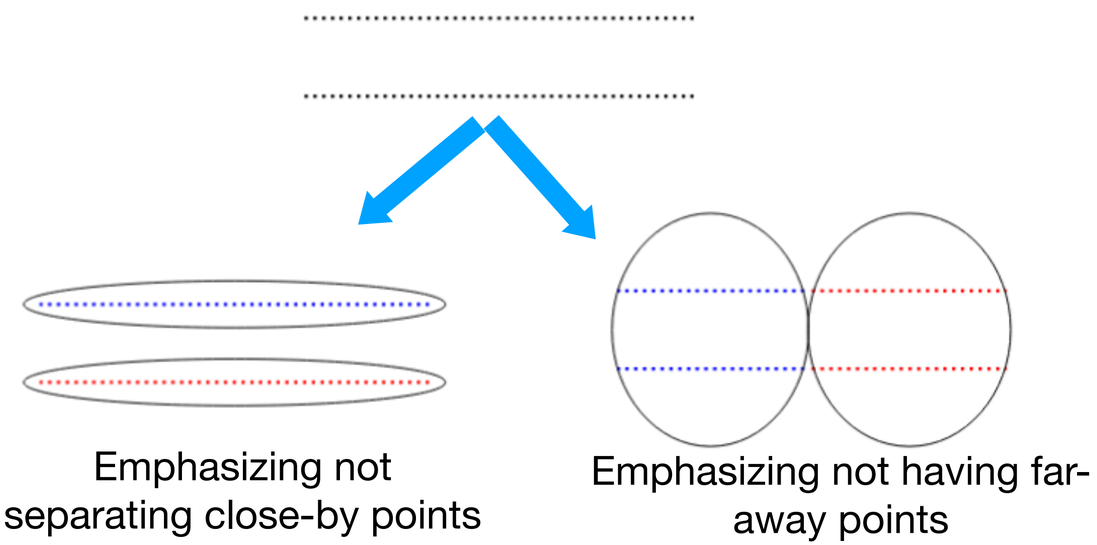
Clustering is the task of grouping a set of objects such that:

- *Similar* objects end up in the same group
- *Dissimilar* objects are separated into different groups



Challenges in Clustering

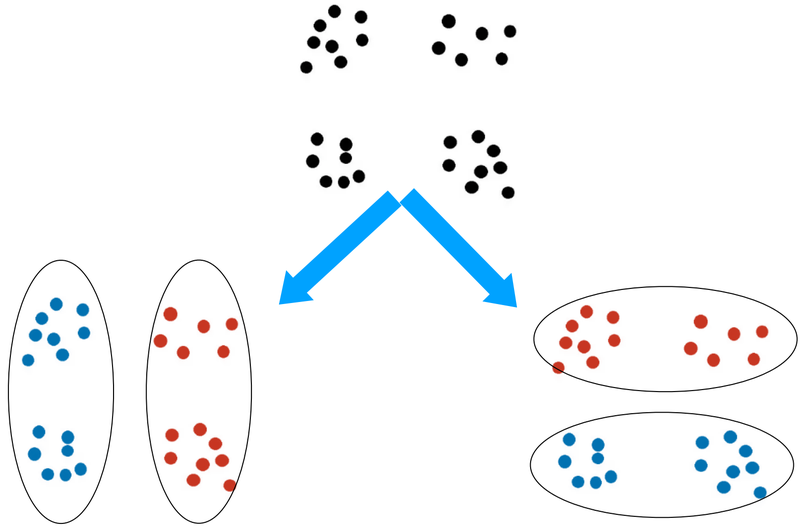
Ambiguity of what is a cluster



Emphasizing not separating close-by points

Emphasizing not having far-away points

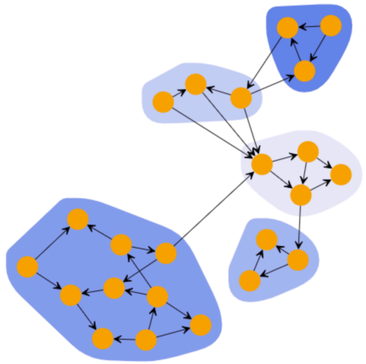
Lack of “ground truth”



It is difficult to evaluate the success

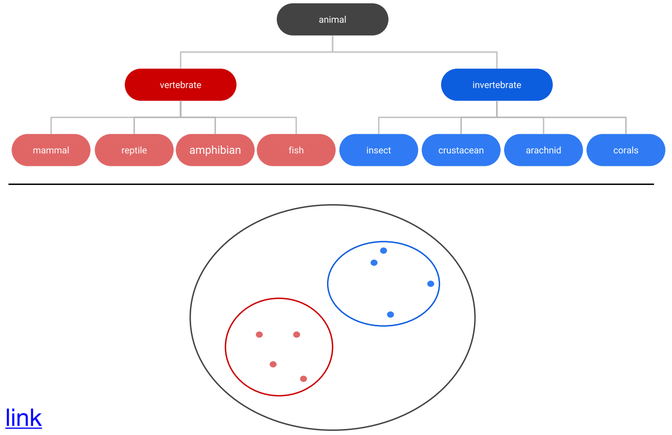
Different Approaches for Clustering

Graph-based clustering
Graph partition to minimize inter-cluster weights and maximize intra-cluster weights



Examples: Spectral clustering, graph-cut based approaches

Hierarchical clustering
Build a tree (bottom-up or top-down), representing distances among data points



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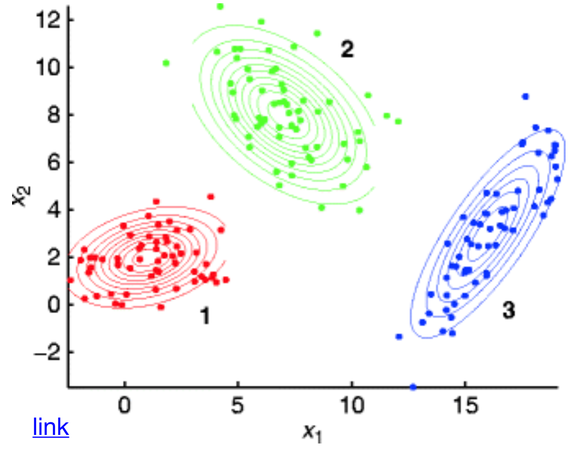
Examples: Linkage-based approaches

Model-based clustering
Maintain cluster models and infer memberships based on them



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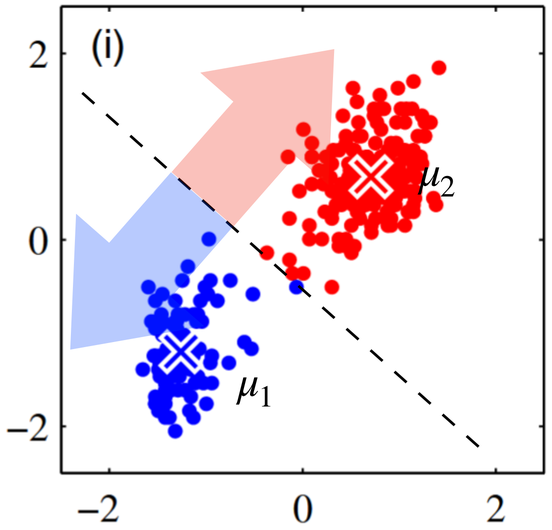
Examples: K-means, GMMS

K-Means

K-Means is an **unsupervised learning algorithm** used for **clustering**

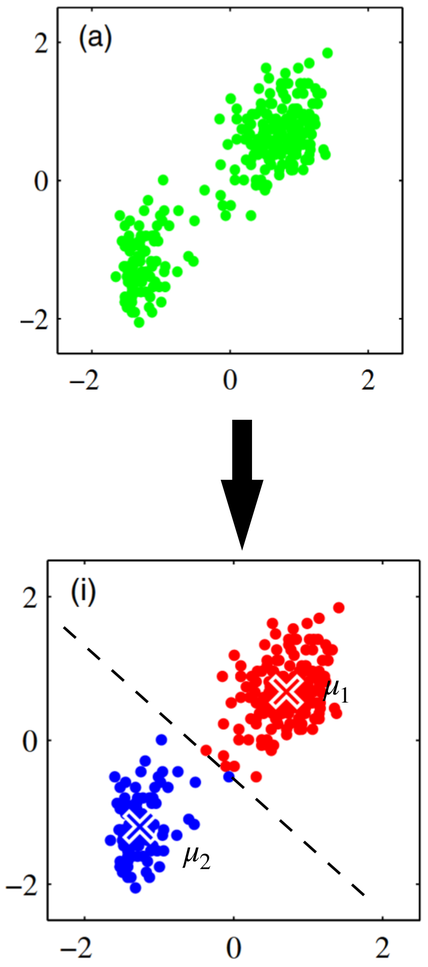
It aims to partition data into K clusters, where each point belongs to the cluster with the closest mean



Key Concepts:

- **Clusters**: Groups of data points with similar characteristics
- **Centroids**: The center of each cluster, representing the "mean" position of data points in the cluster (μ_1, μ_2)

K-Means



Input:

- A dataset $\mathscr{D} = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N\}$ with N datapoints, each in $\mathbb{R}^D$
- Number of clusters K

Output:

- Cluster centroids $\mu_1, \mu_2, \ldots, \mu_K$
- Cluster assignments $z_{nk} \in \{0,1\}$ for each datapoint

Objective function: Within-cluster sum of squares (WCSS)

$$\min_{\mathbf{z},\mu} \; \mathscr{L}(\mathbf{z}, \mu) = \sum_{n=1}^{N} \sum_{k=1}^{K} z_{nk} \|\mathbf{x}_n - \mu_k\|_2^2$$

$$\text{s.t. } \mu_k \in \mathbb{R}^D, z_{nk} \in \{0,1\}, \; \sum_{k=1}^{K} z_{nk} = 1,$$

where $\mathbf{z}_n = [z_{n1}, z_{n2}, \ldots, z_{nK}]^\top$, $\mathbf{z} = [\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_N]^\top$, and $\mu = [\mu_1, \mu_2, \ldots, \mu_K]^\top$

K-Means Objective

$$\min_{\mathbf{z},\mu} \; \mathcal{L}(\mathbf{z},\mu) = \sum_{n=1}^{N}\sum_{k=1}^{K} z_{nk}\|\mathbf{x}_n - \mu_k\|_2^2$$

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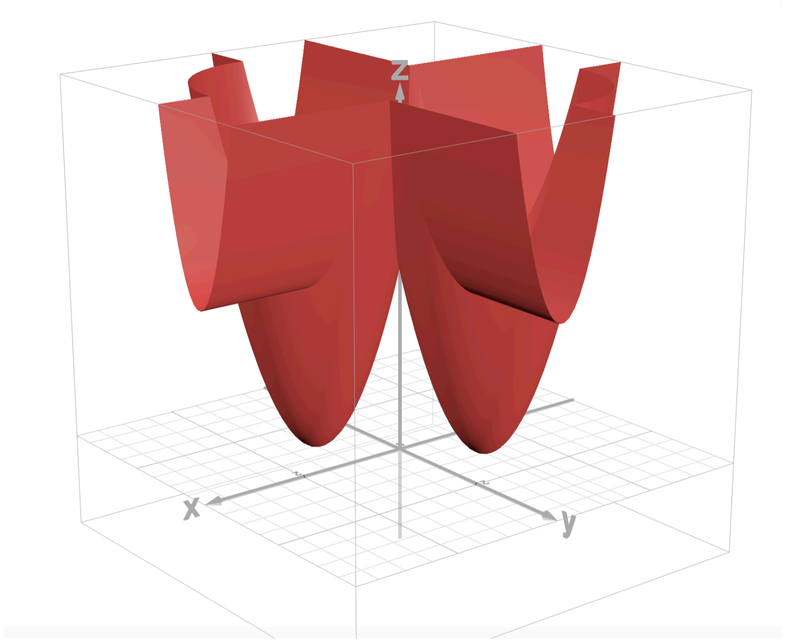
where $\mathbf{z}_n = [z_{n1}, z_{n2}, \ldots, z_{nK}]^\top, \mathbf{z} = [\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_N]^\top,$
and $\mu = [\mu_1, \mu_2, \ldots, \mu_K]^\top$

- **The objective is non-convex** and there are multiple local minima.
- Some of the optimization variables are **discrete**



TODO: figure description

K-Means Algorithm

Input: dataset $\mathscr{D}$; Number of clusters K

Initialize: Randomly choose initial centroids

$\mu_1, \mu_2, \ldots, \mu_K$

Repeat until convergence:

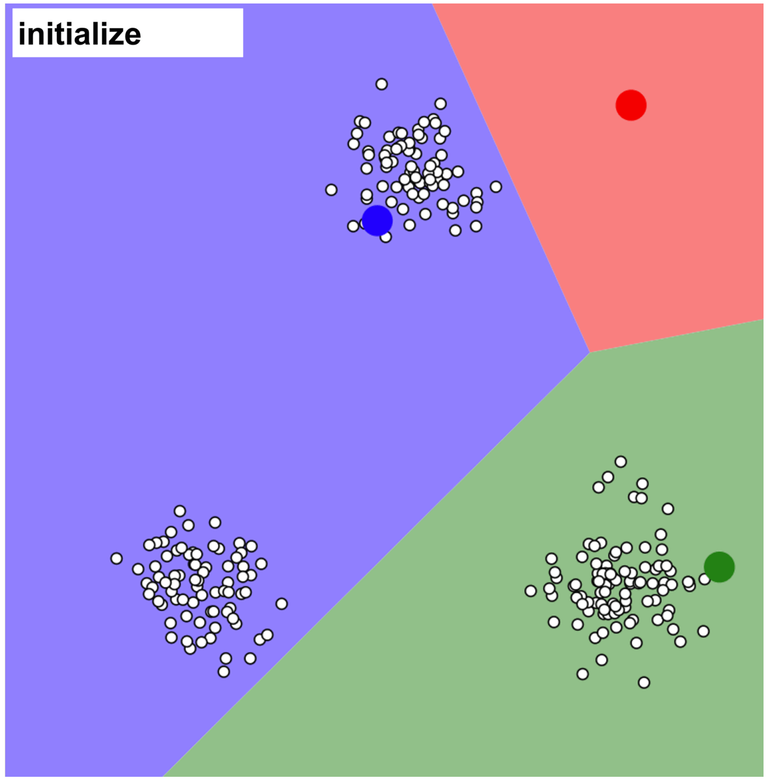
- Assignment step:
  - $\forall n \in [N]$ compute $z_{nk} = \begin{cases} 1 & \text{if } k = \arg\min_j \|\mathbf{x}_n - \mu_j\|_2^2 \\ 0 & \text{otherwise} \end{cases}$

Optimal assignment maps each point to its nearest center

Break ties arbitrarily!

- Update step:
  - $\forall k \in [K]$ update $\mu_k = \frac{\sum_{n=1}^{N} z_{nk}\mathbf{x}_n}{\sum_{n=1}^{N} z_{nk}}$

Optimal centers are the means of each cluster

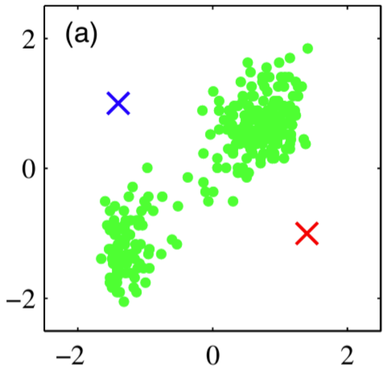


Demo

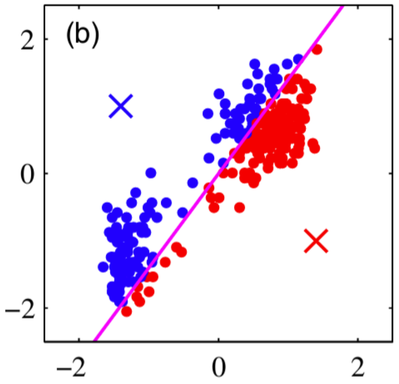
Iteration cost: $O(NKd)$

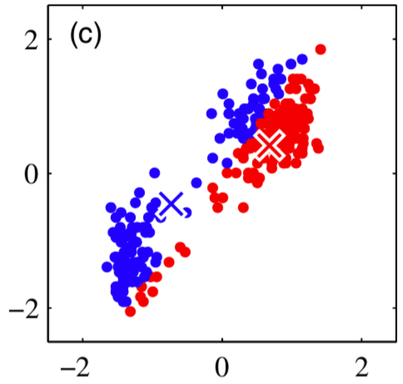
K-Means Algorithm

Initialize

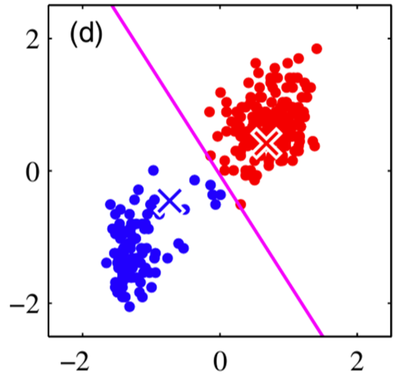


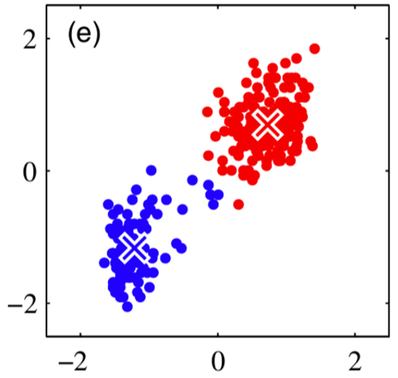
Iteration=0



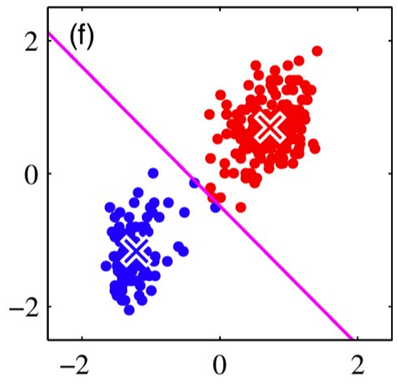


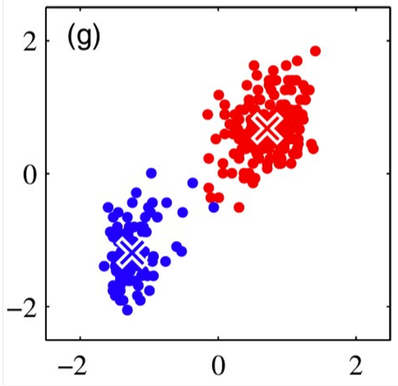
Iteration=1



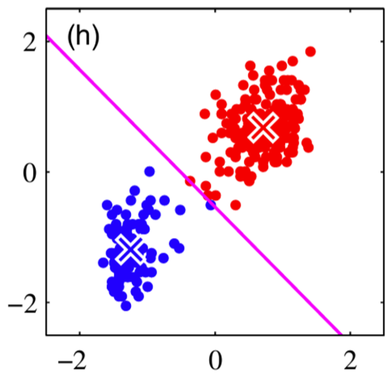


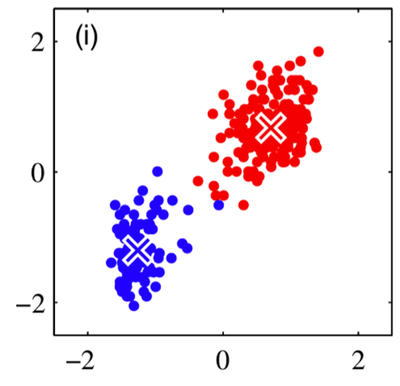
Iteration=2





Iteration=3





Assignment step

Update step

Assignment step

Update step

Monotonic Decrease of K-Means Objective

Proposition: Each iterations of the K-means algorithm decreases the K-mean objective function:

$$\mathscr{L}(\mathbf{z}^{(\mathbf{t})}, \mu^{(\mathbf{t})}) \leq \mathscr{L}(\mathbf{z}^{(\mathbf{t-1})}, \mu^{(\mathbf{t-1})})$$

Proof:

Assignment step: Each data point is assigned to its nearest centroid (centroids are fixed)

$$\sum_{n=1}^{N} \sum_{k=1}^{K} z_{nk}^{(t-1)} \|\mathbf{x}_n - \boldsymbol{\mu}_k^{(t-1)}\|_2^2 \geq \sum_{n=1}^{N} \sum_{k=1}^{K} z_{nk}^{(t)} \|\mathbf{x}_n - \boldsymbol{\mu}_k^{(t-1)}\|_2^2$$

Update step: The mean minimizes the sum of squared Euclidean distances to the points in the cluster (assignments are fixed)

$$\sum_{n=1}^{N} \sum_{k=1}^{K} z_{nk}^{(t)} \|\mathbf{x}_n - \boldsymbol{\mu}_k^{(t-1)}\|_2^2 \geq \sum_{n=1}^{N} \sum_{k=1}^{K} z_{nk}^{(t)} \|\mathbf{x}_n - \boldsymbol{\mu}_k^{(t)}\|_2^2$$

Convergence of K-Means Algorithm

K-means is a **coordinate descent algorithm**:

$$\mathbf{z}^{(t+1)} = \arg\min_{\mathbf{z}} \mathscr{L}(\mathbf{z}, \mu^{(t)})$$
$$\mu^{(t+1)} = \arg\min_{\mu} \mathscr{L}(\mathbf{z}^{(t)}, \mu)$$

K-means converges in a finite number of steps (due to monotonic decrease of the lower-bounded objective function and a finite number of possible assignments)

No guarantee on the number of iterations needed for convergence (can be exponential)

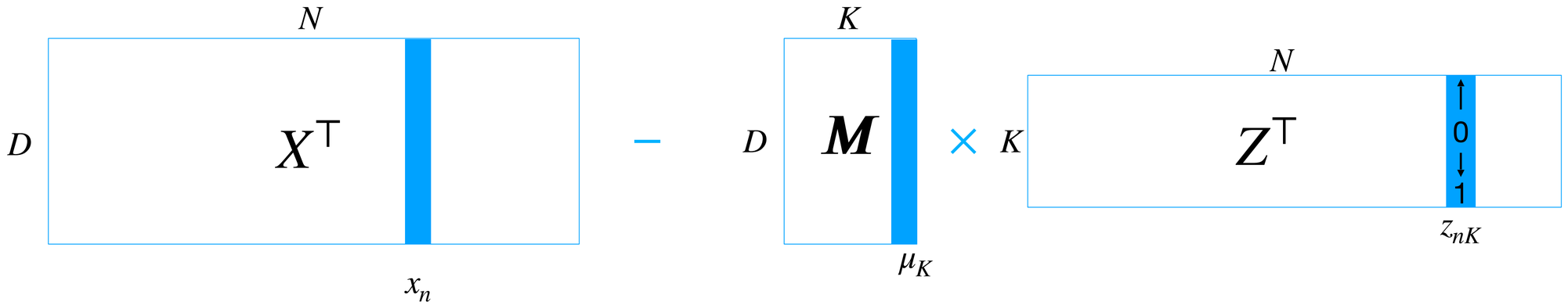
No nontrivial lower bound on the gap between the final objective value and the global minimum

May fail to find the global optimum (might even converge to a point which is not a local minimum)

K-Means as Matrix Factorization

We can interpret K-Means as Matrix Factorization:

$$\begin{aligned}\min_{\mathbf{z},\boldsymbol{\mu}} \ \mathscr{L}(\mathbf{z},\mu) &= \sum_{n=1}^{N}\sum_{k=1}^{K} z_{nk}\|\mathbf{x}_n - \mu_k\|_2^2 \\ &= \|X^\top - MZ^\top\|_{\text{Frob}}^2\end{aligned}$$

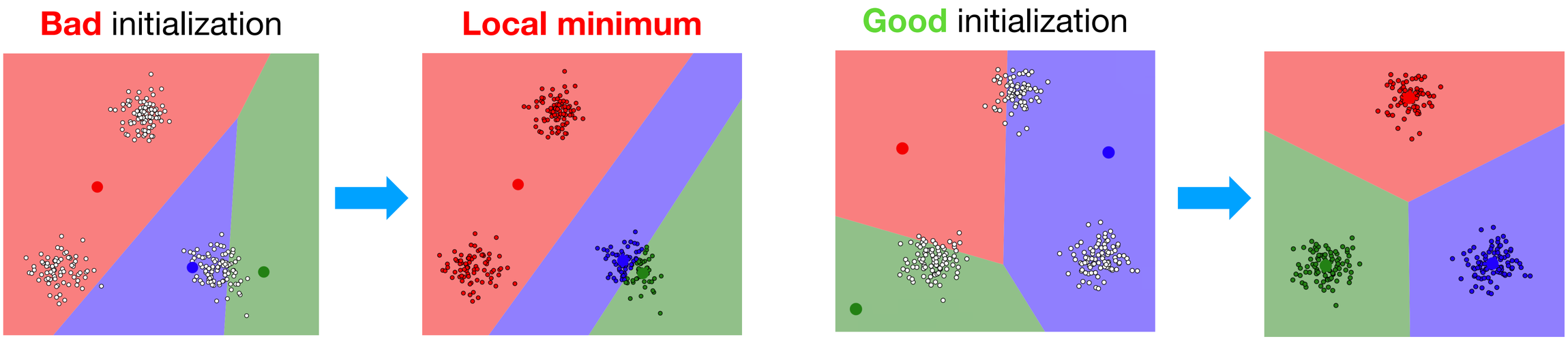


x_n is reconstructed by the mean of closest centroid μ_k

K-Means Challenges

Challenge 1: Performance strongly depends on the initialization

Try here!



Solutions:

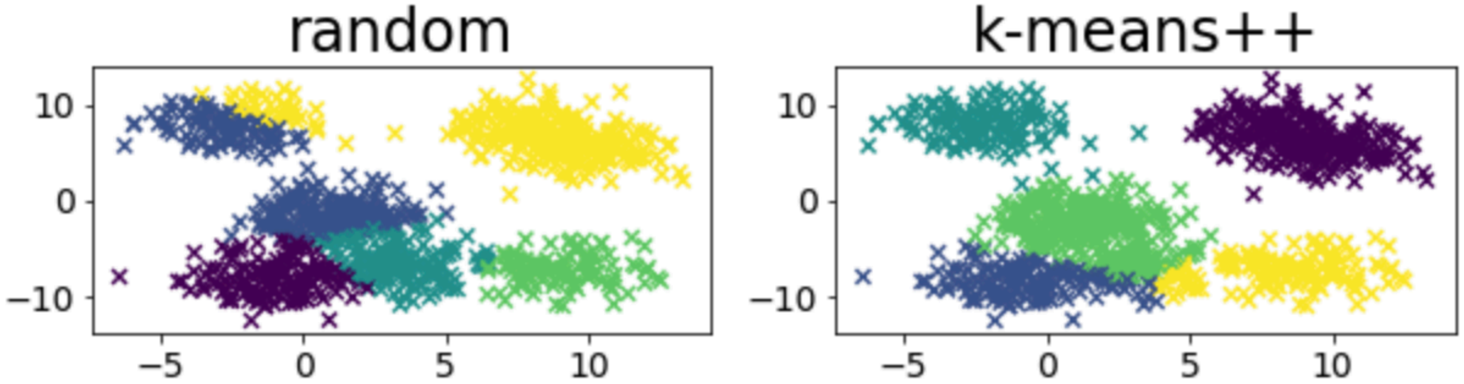
- Multiple random restarts
- Seeding with K-means++

K-Means++

An improved initialization method for the K-means that helps to avoid poor initial centroid placements

The basic idea is to spread out the initial centroids so that they are more representative of the data distribution, rather than choosing them randomly

Benefits: Avoids poor local minima, faster convergence, and lower K-means objective (expected cost $O(\log K)$ of the optimal solution)



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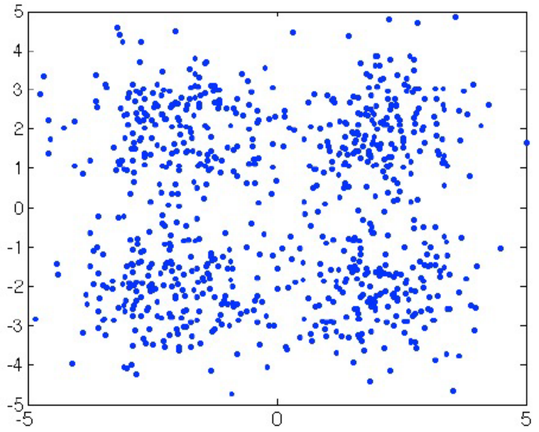
K-Means++

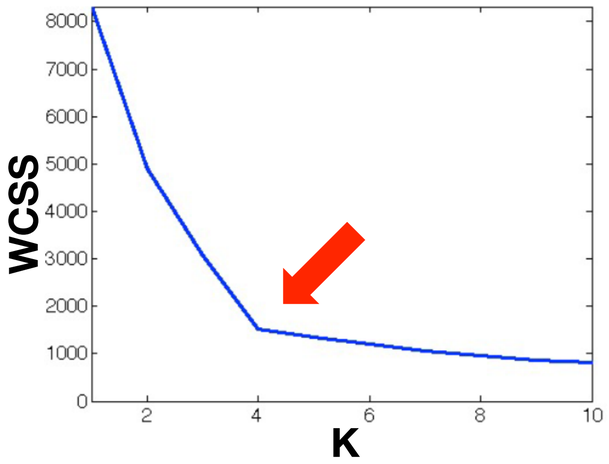
1. Select the first centroid μ_1 randomly from the data points in $\mathscr{D}$
2. Select subsequent centroids probabilistically:
    1. For each point x, calculate the distance $D(\mathbf{x}) = \min_{j \in \{1,\dots,m\}} \|\mathbf{x} - \mu_j\|_2^2$, where $\{\mu_1, \cdots, \mu_m\}$ represents the centroids that have already been chosen
    2. Select the next centroid μ_{m+1} by choosing a point x from $\mathscr{D}$ with probability: $P(\mathbf{x}) = \frac{D(\mathbf{x})}{\sum_{x \in \mathscr{D}} D(\mathbf{x})}$
3. Repeat Step 2 until K centroids have been chosen
4. Run standard K-means

Challenge 2: How to define the number of clusters?

Test loss typically keeps decreasing with increasing K so we cannot use cross-validation to determine the number of clusters

- Domain knowledge
- Elbow method



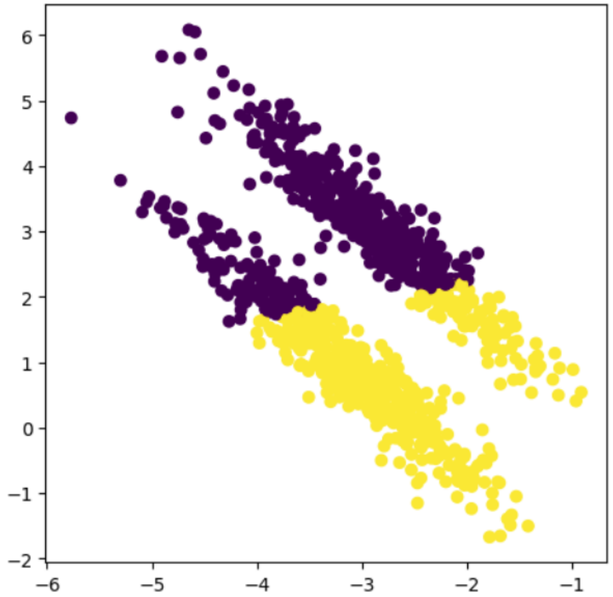


1. Run K-means for different values of K (e.g., 1, 2, ..., 10) and calculate the within-cluster sum of squares (WCSS) for each K
2. Plot K vs the WCSS, and look for the **elbow point** where the rate of decrease sharply slows

Diminishing returns: A new cluster significantly reduces loss when there are too few clusters, but offers little improvement once the optimal number is reached

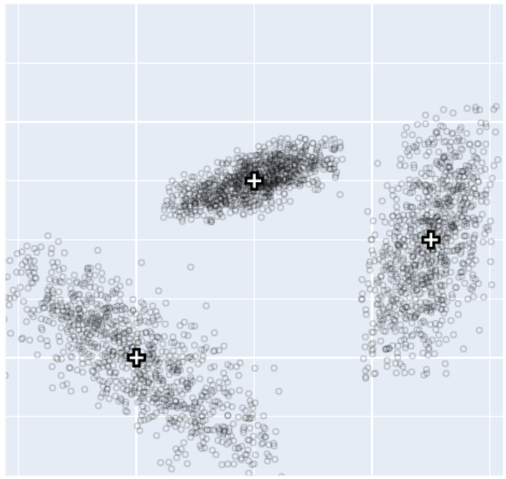
Challenge 3: It cannot model well clusters of arbitrary shape

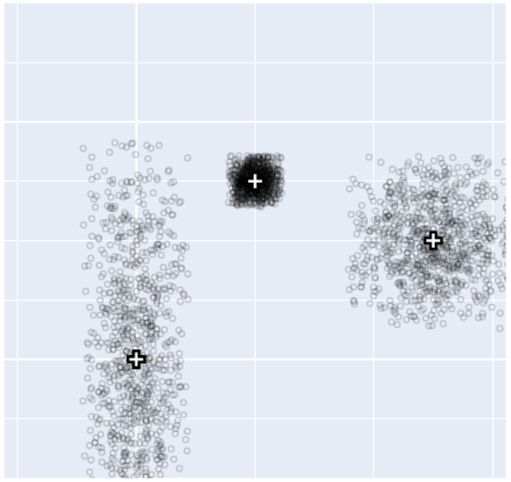
K-Means forces the clusters to be spherical (e.g., not elliptical) and of equal size

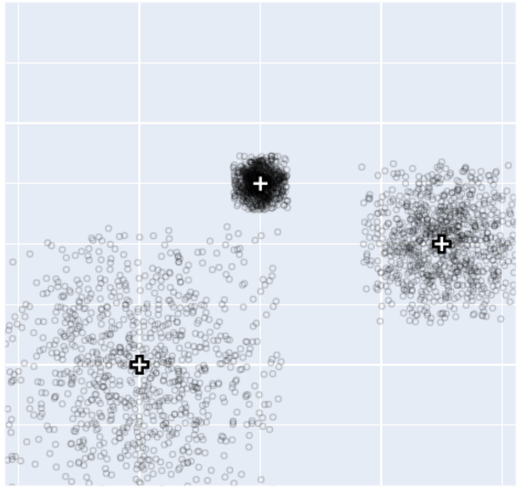


K-means struggles with elliptical clusters

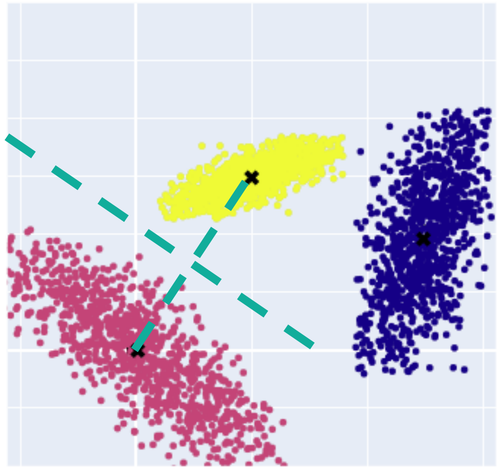
When Does K-Means Fail?



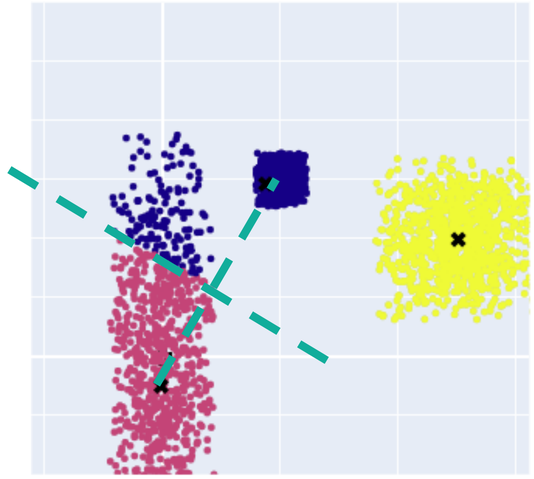




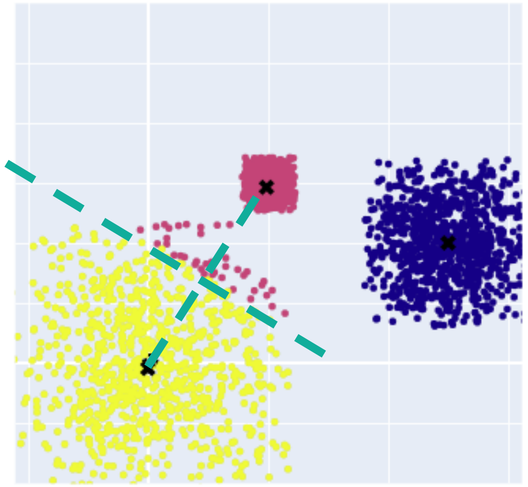
When Does K-Means Fail?



Works!



Fails!

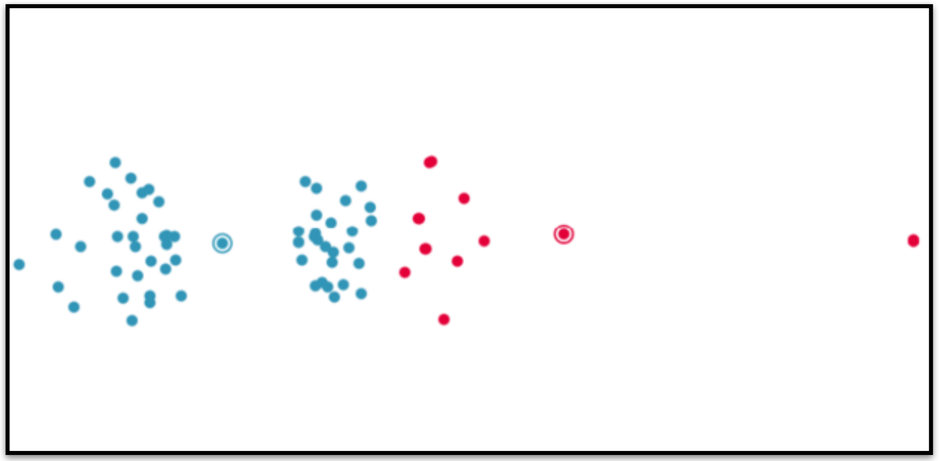


Fails!

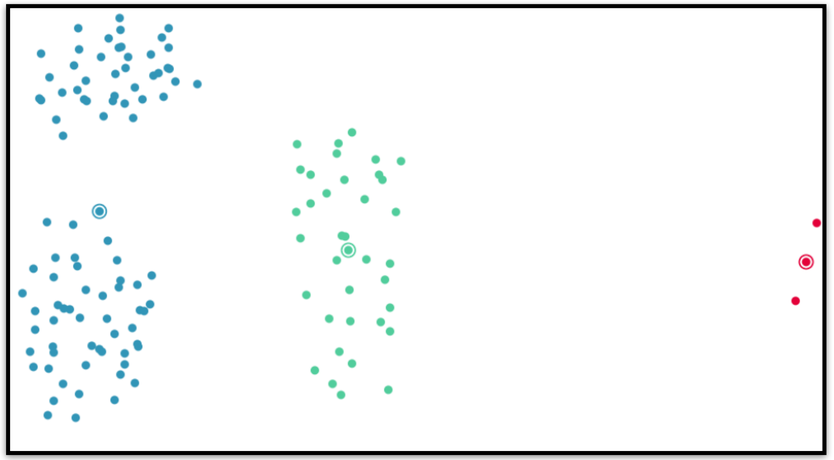
K-Means fails when clusters are not separated by the bisectors of the lines connecting their centers

Challenge 4: Sensitivity to outliers

Outliers can drag the centroids away from the actual dense areas, causing clusters to become stretched or less representative of the majority of data points



Outliers can lead to suboptimal results

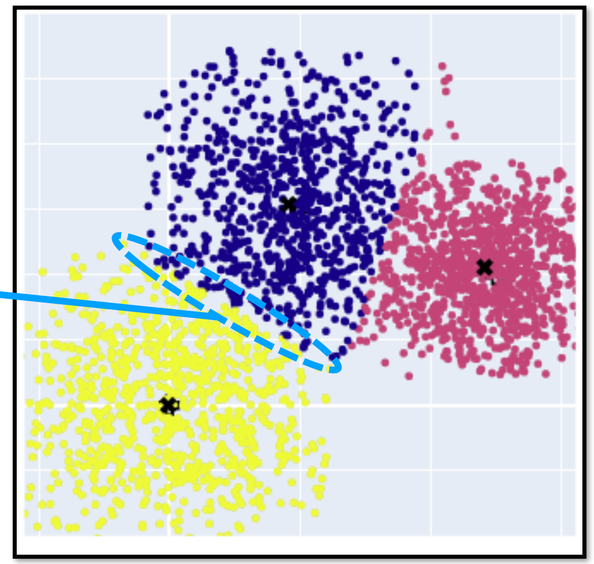


Outliers can lead to undesirable clusters

Challenge 5: Hard assignments in overlapping clusters

In many cases, data has overlapping clusters or points that don't clearly belong to any single cluster

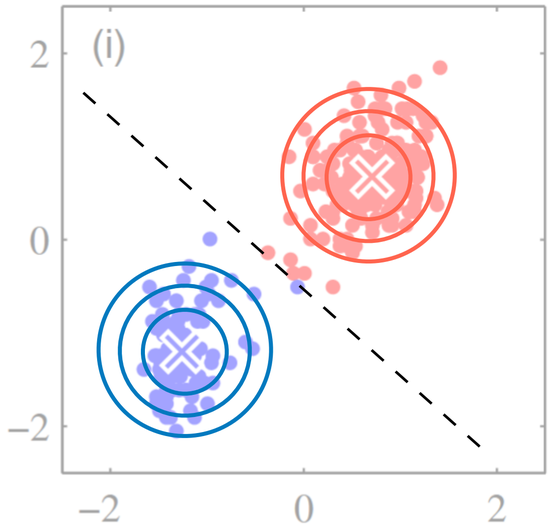
Very similar (close) datapoints belong to different clusters



Probabilistic view on K-Means

Consider each cluster as an isotropic Gaussian:

$$P(\mathbf{x}_n \,|\, \mu, \mathbf{z}_n) = \prod_{k=1}^{K} \mathcal{N}(\mu_k, I_D)^{z_{nk}}$$
$$= \prod_{k=1}^{K} c \exp\left(-\frac{1}{2}\|\mathbf{x}_n - \boldsymbol{\mu}_k\|_2^2 z_{nk}\right)$$



Dataset likelihood will be:

$$\log \prod_{n=1}^{N} P(\mathbf{x}_n \,|\, \mu, \mathbf{z}_n) = \log \prod_{n=1}^{N} \prod_{k=1}^{K} c \exp\left(-\frac{1}{2}\|\mathbf{x}_n - \boldsymbol{\mu}_k\|_2^2 z_{nk}\right)$$
$$= -\sum_{n=1}^{N} \sum_{k=1}^{K} z_{nk} \|\mathbf{x}_n - \boldsymbol{\mu}_k\|_2^2 + c'$$
$$= -\mathcal{L}(\mathbf{z}, \boldsymbol{\mu}) + c'$$

K-means can be interpreted as **maximizing the log-likelihood of the data** with this data model

GMM

Gaussian Mixture Models

Data is modeled as a mixture of K Gaussian distributions

Instance space is $\mathcal{X} = \mathbb{R}^d$ and each sample x is generated as follows:

1. Choose a random component $k \in \{1,2,...,K\}$, i.e., let Z be a multinomial r.v. with $P(Z = k) = \pi_k$
2. Sample X, given the value of $Z = k$, from a Gaussian distribution:

$$\mathbb{P}[X = \mathbf{x} \,|\, Z = k] = \frac{1}{(2\pi)^{d/2} \,|\, \Sigma_k \,|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{x} - \mu_k)^T \Sigma_k^{-1} (\mathbf{x} - \mu_k)\right)$$

Gaussian Mixture Models

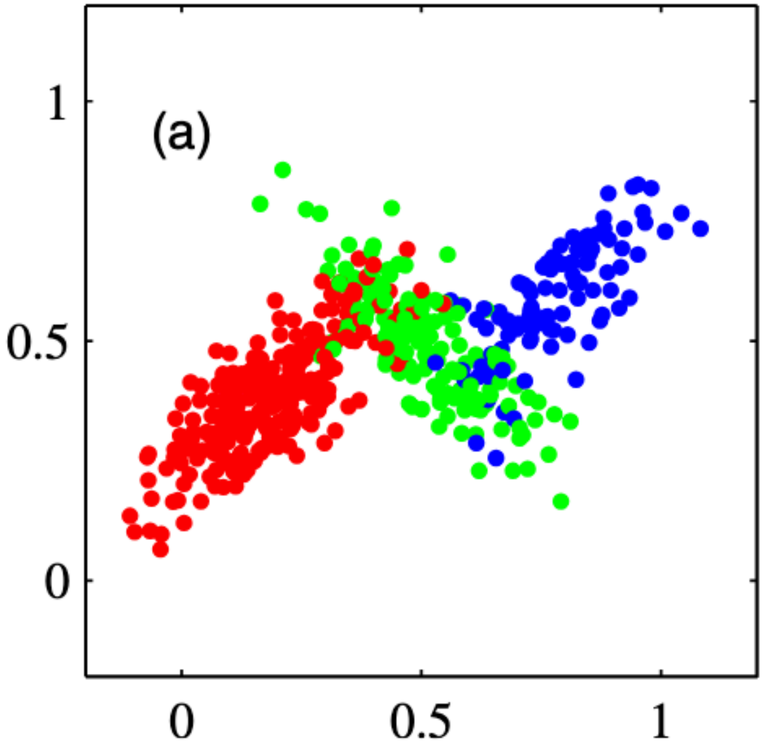
Then we can write the distribution of X as:

$$\begin{aligned}\mathbb{P}[X = \mathbf{x}] &= \sum_{k=1}^{K} \mathbb{P}[Z = k]\mathbb{P}[X = \mathbf{x} \,|\, Z = k] \\ &= \sum_{k=1}^{K} \pi_k \mathcal{N}\left(x \,|\, \mu_k, \Sigma_k\right) \\ &= \sum_{k=1}^{K} \frac{\pi_k}{(2\pi)^{d/2} |\,\Sigma_k\,|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{x} - \mu_k)^T \Sigma_k^{-1} (\mathbf{x} - \mu_k)\right)\end{aligned}$$

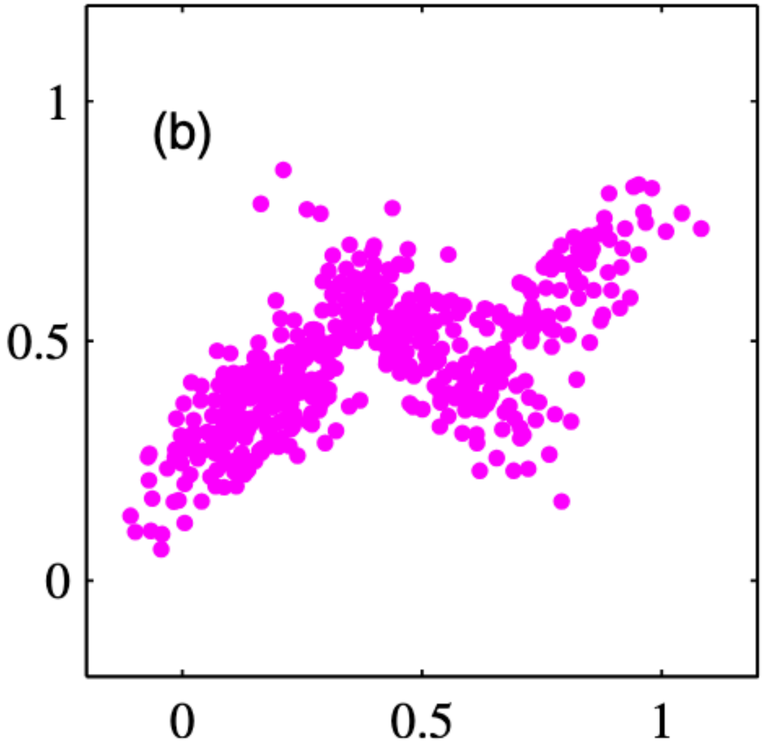
Z is a latent (hidden) variable that is not directly observed

We introduce Z because it helps us describe a simple parametric form

Visualizing the Joint and Marginal Distributions of GMM



Samples from the joint distribution $P(X, Z)$, with Z represented by colors



Samples from the marginal distribution $P(X)$

Recap

Unsupervised Learning: Learns patterns from unlabeled data to discover hidden structures

K-Means Clustering: Partitions data into K clusters by minimizing the distance between points and cluster centroids

K-Means is simple and efficient but assumes well-separated clusters and requires a predefined K

GMM: Data is modeled as a mixture of K Gaussian distributions. Offers great flexibility in modeling as you can freely choose $\{\pi_k, \mu_k, \Sigma_k\}_{k \in K}$

Our objective is to maximize the log-likelihood of the data to get estimates of the model parameters but this brings new challenges (next week)