# Unsupervised ML

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# Objective

- Discover information from data without labeled examples
- Extract some hidden organisation, patterns, relation between element
- There are three cases in unsupervised learning:
  - Clustering
  - Dimensional reduction
  - Association rule

# Unsupervised learning

# Unsupervised learning

- Unsupervised learning is a paradigm in machine learning where, in contrast to supervised learning and semi-supervised learning, algorithms learn patterns exclusively from unlabeled data.
- `https://en.wikipedia.org/wiki/Unsupervised_learning`

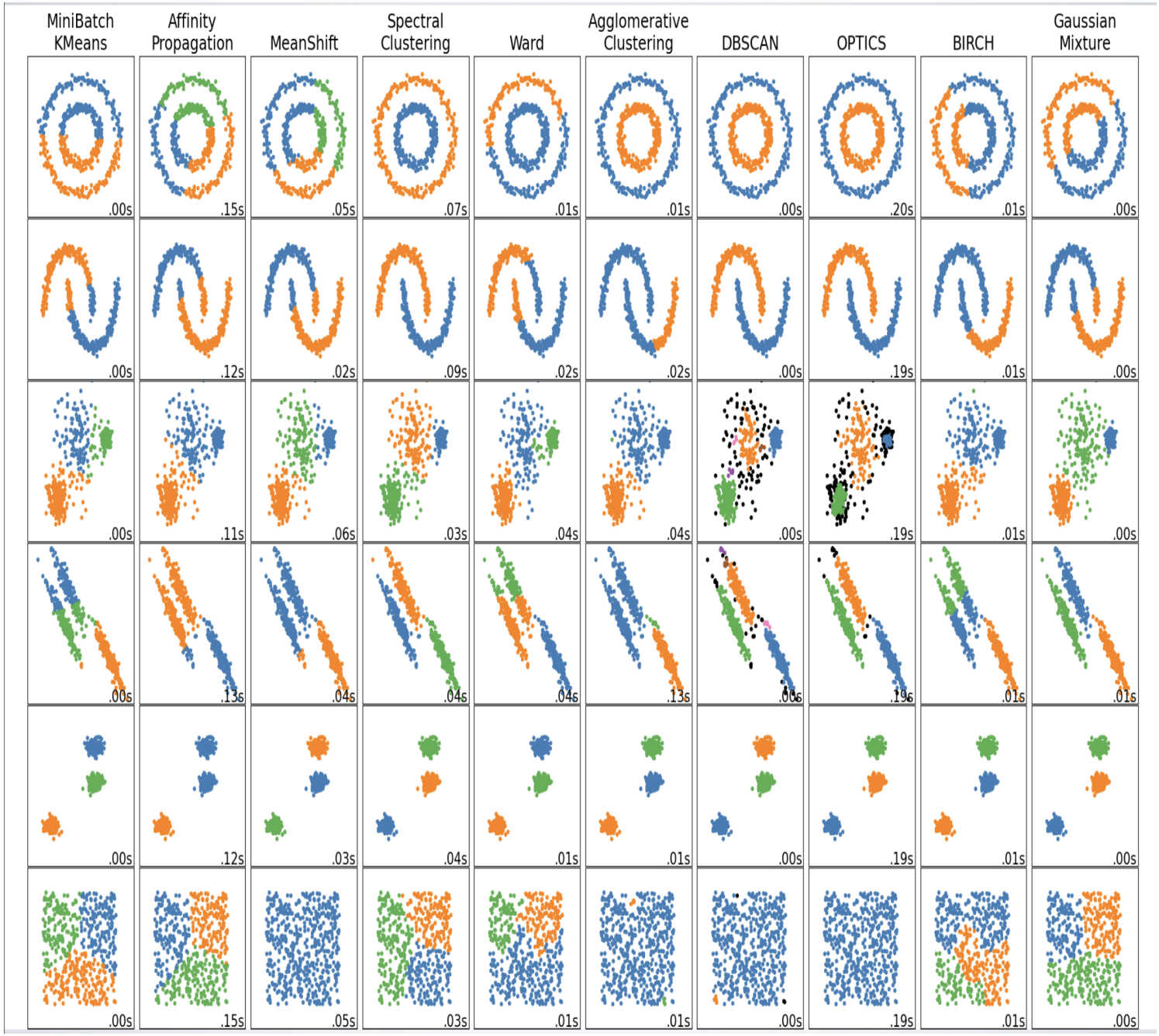
# CLUSTERING

# Clustering

- The most famous unsupervised ML problem
- Most people use "good old" methods: k-means(1967), DBSCAN(1996)
- Part of the problem: clustering is not well defined

# Clustering

- How would you define a good cluster?
- A good partition in clusters?


MiniBatch KMeans
Affinity Propagation
MeanShift
Spectral Clustering
Ward
Agglomerative Clustering
DBSCAN
OPTICS
BIRCH
Gaussian Mixture
.00s .15s .05s .07s .01s .01s .00s .20s .01s .00s
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# K-Means

Definition

- For a target number of cluster K
- Find the item assignment minimizing
  - The inter-cluster variance (weighted by cluster size)
  - The squared distance from points to their cluster center
  - The squared distance between cluster elements

# K-Means

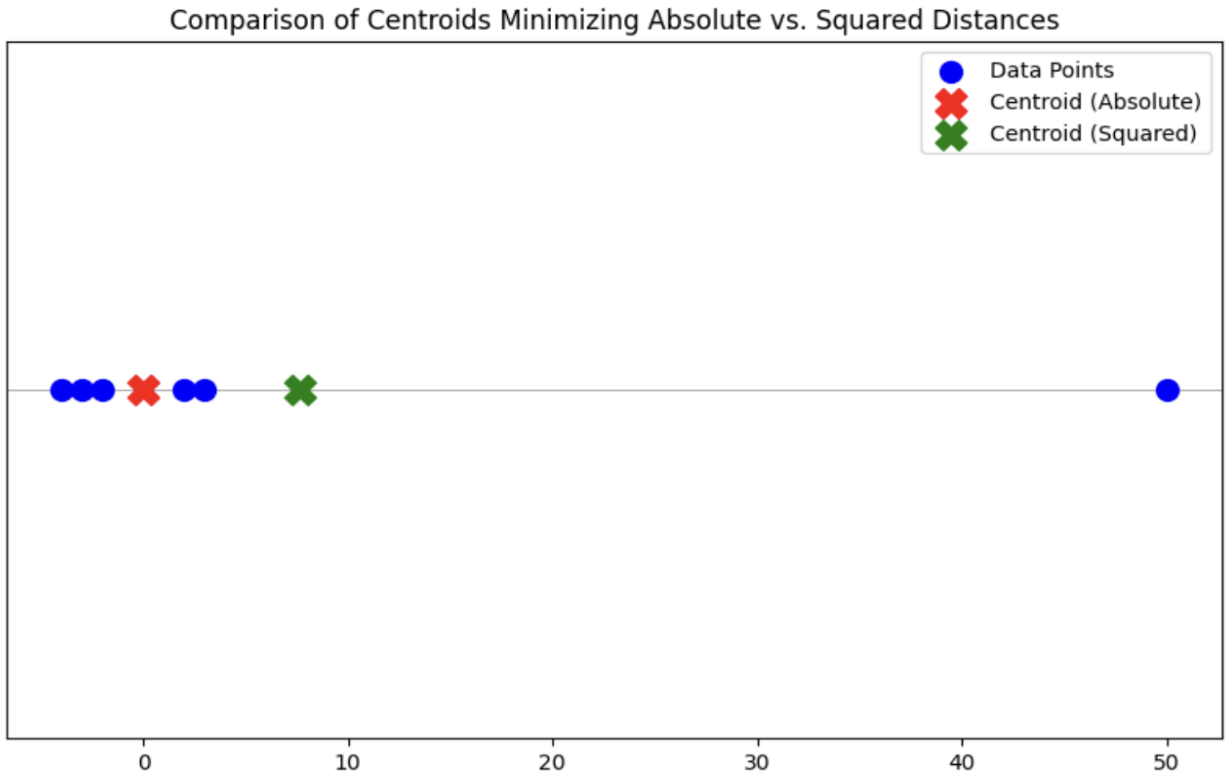
$$\arg\min_{S} \sum_{i=1}^{k} \sum_{x \in S_i} \| x - \mu_i \|^2 = \arg\min_{S} \sum_{i=1}^{k} \| S_i Var(S_i)$$

- S a cluster assignment
- k a number of cluster
- x a dimensional item

# K-Means

Consequence: outliers penalized more (pros and cons)

- Squared distance minimized by the **mean**
- Absolute distance minimized by the **median**



# K-Means

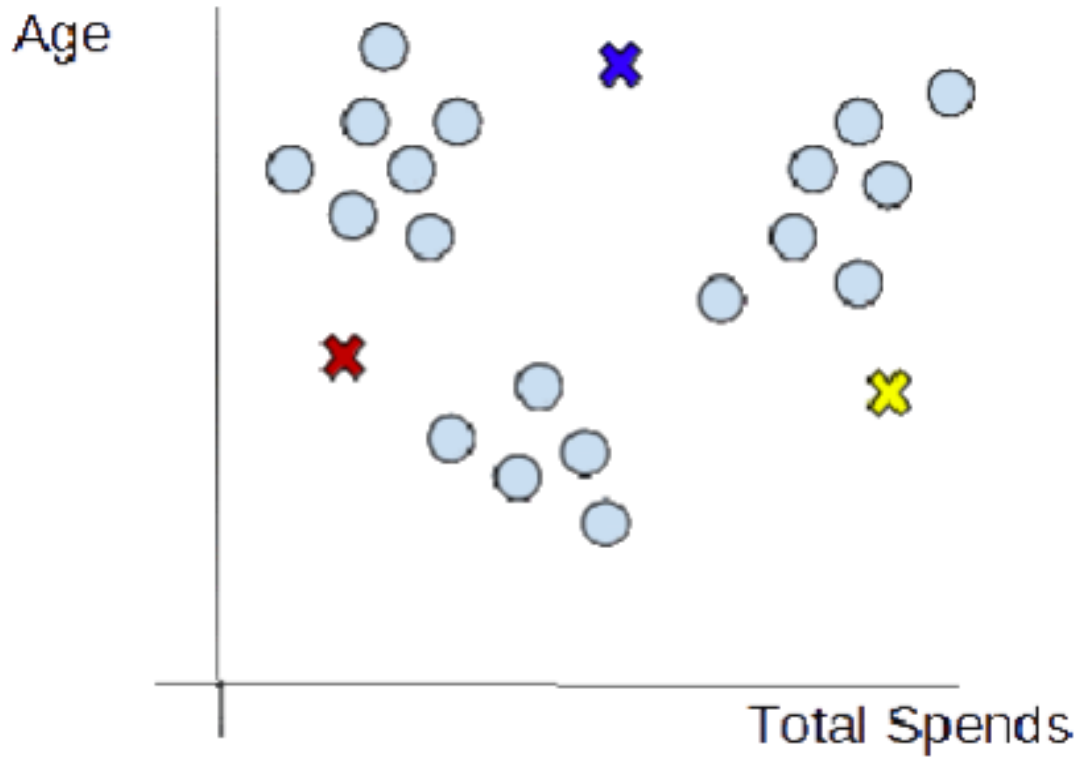
$$\arg\min_{S} \sum_{i=1}^{k} \sum_{x \in S_i} \| x - \mu_i \|^2 = \arg\min_{S} \sum_{i=1}^{k} \| S_i Var(S_i)$$

Note that without fixing k, there is a trivial solution with each item alone in its own cluster.

# K-Means

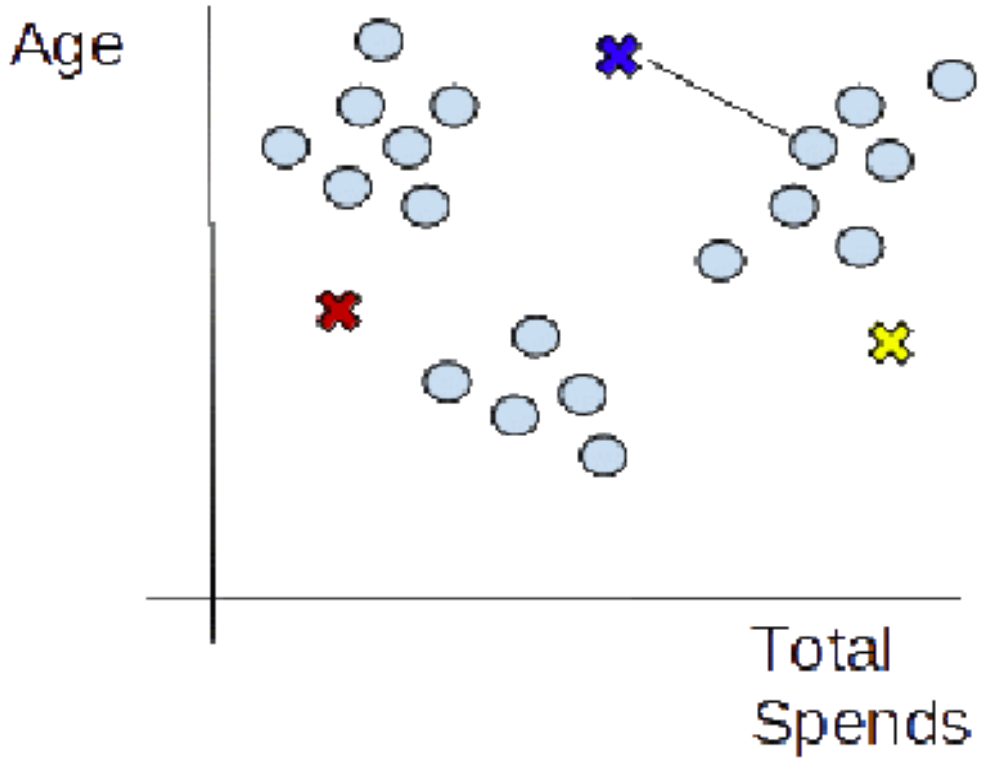
How does K-Means work?

1. Choosing the number of clusters
2. Initializing centroids (the center of a cluster)



# K-Means

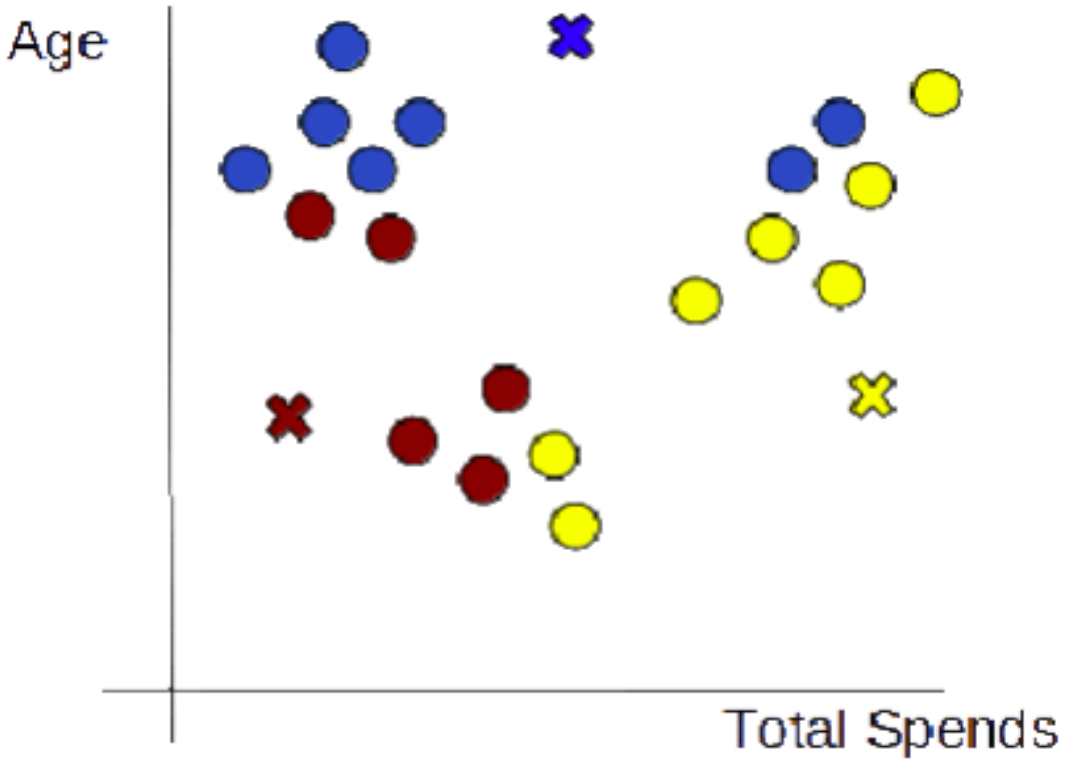
3. Assign data points to the nearest cluster




In this step, we will first calculate the distance between data point X and centroid C using Euclidean Distance metric.

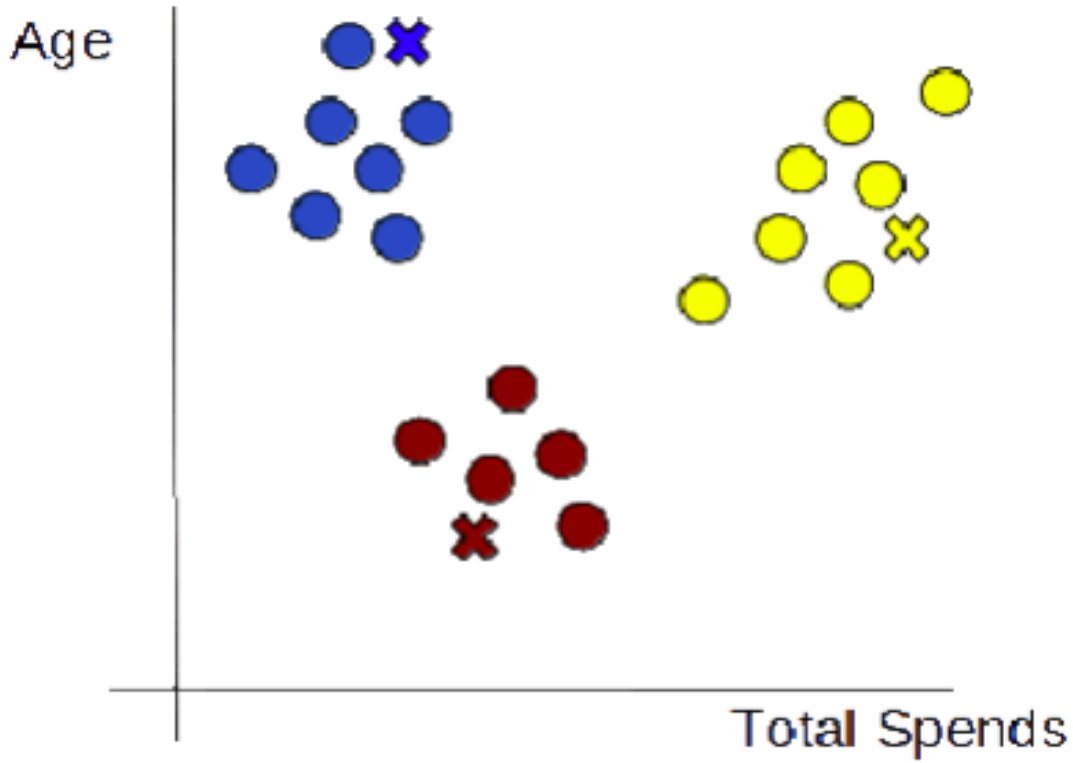
# K-Means

Then choose the cluster for data points where the distance between the data point and the centroid is minimum.



# K-Means

4. Re-initialize centroids
5. Repeat steps 3 and 4



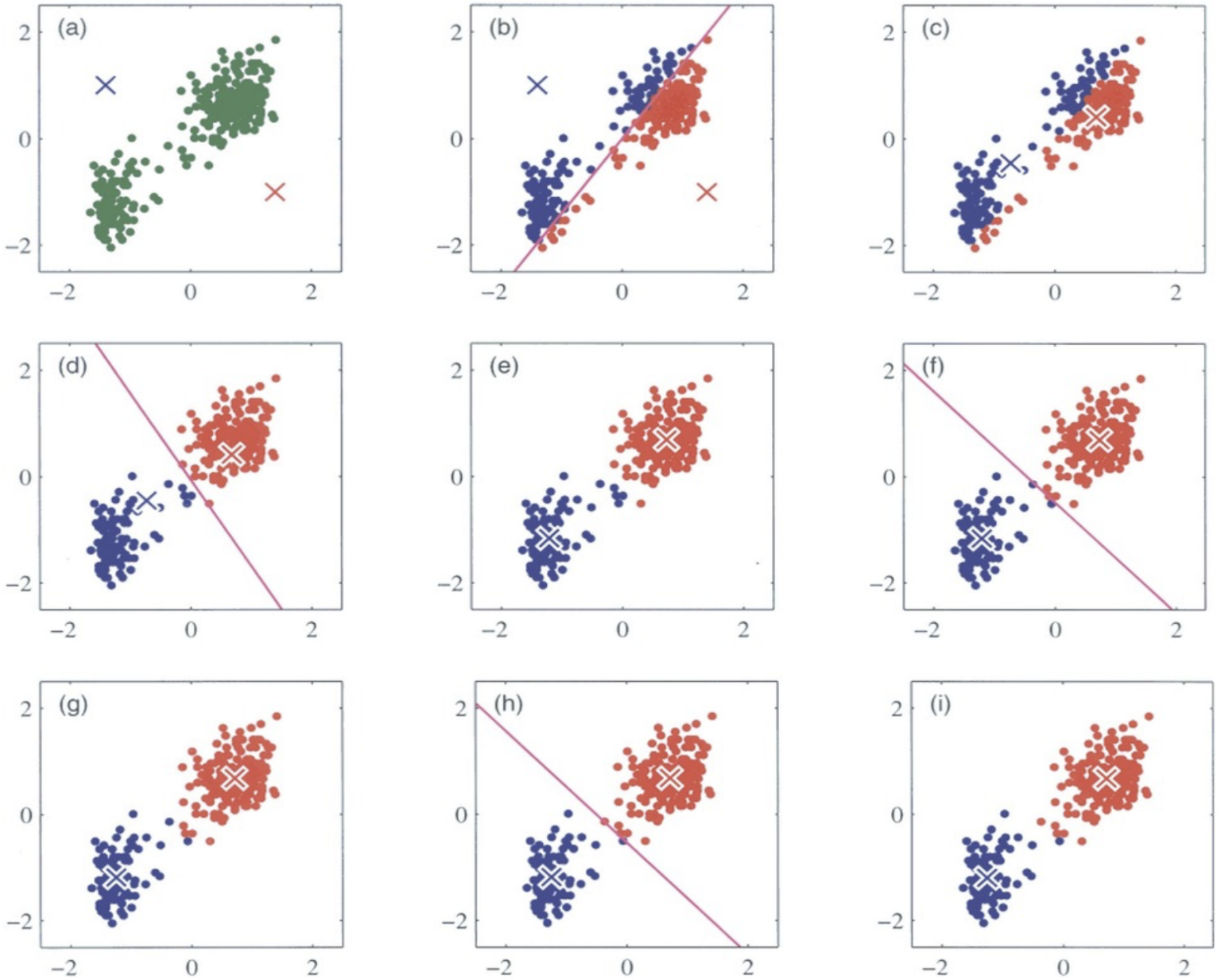
# K-Means

- Discovering the global minimum is NP-hard
- How to find quickly a good solution?
  - Naive k-means
  - K-means ++ (used in most current implementations)
  - Use optimized data structure

# Naive K-Means

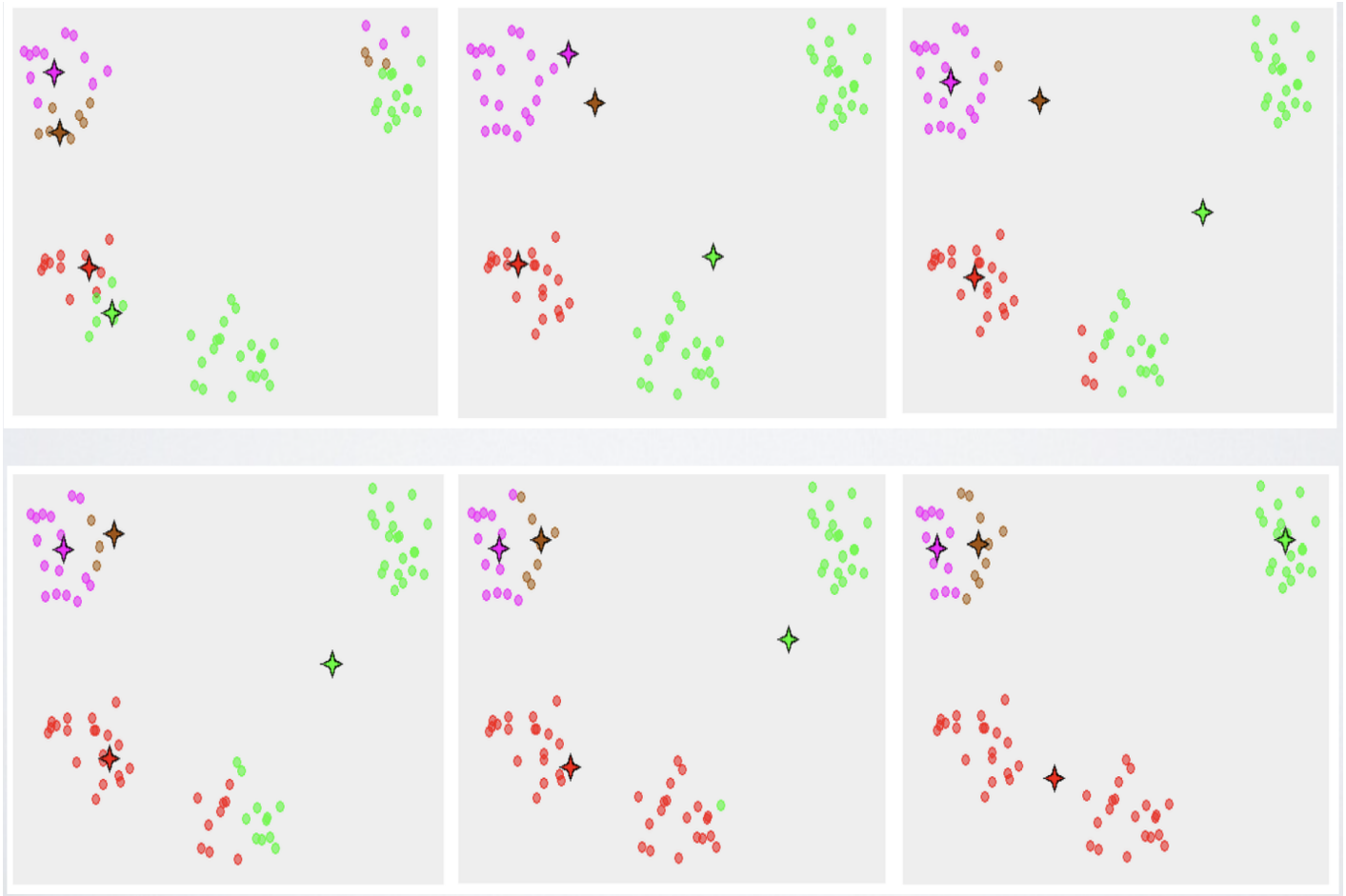
- Assignment: assign each item to its closest cluster center
- Update: recompute the center of each cluster as the mean (centroid) of items that compose that cluster
- Start with random centroid

# Naive K-Means



# Naive K-Means

Known limit: convergence to poor local minimum if poor initial centroids



# K-Means++

- Several variants to choose wisely the initial centroids
- K-means++ is proven to improve the results, statistically.
  - Not always, but improves more often than deteriorate the results.

# K-Means++

1. Choose one center uniformly at random among the data points
2. For each data point x not chosen yet, computer D(x), the distance between x and the nearest center that has already been chosen.
3. Choose one new data point at random as a new center, using a weighted probability distribution where a point x is chosen with probability proportional to

$$D(x)^2$$

4. Repeat steps 2 and 3 until k centers have been chosen.

# Weakness

We can identify some clear weaknesses:

- K-means has a tendency to search for clusters of equal sizes (minimize overall cluster variance)
- Clusters tend to be circular, since all directions are worth the same

# Normalization

Important point: k-means is based on Euclidean distance

- We minimize the inter-cluster Eclidean distance between points
- We could adapt the method to other distances

Data nees to be normalized/standardized

- Clustering based on age in years
- Remember: normalization/standardization are not fixing magically problems (outlier).

# Experiments

- Go to the webpage of the class and do today's experiments
- The "advance" section is not mandatory, you can do it if you have time