Unsupervised Learning and K-Means Clustering

Data Science Dojo

Unsupervised Learning (1/5)

- Trying to find hidden structure in unlabeled data
- No error or reward signal to evaluate a potential solution
- Common techniques: K-Means clustering, hierarchical clustering, hidden Markov models, etc.
  - It has a long history, and used in almost every field, e.g., medicine, psychology, botany, sociology, biology, archeology, marketing, insurance, libraries, etc.

Unsupervised Learning (2/5)

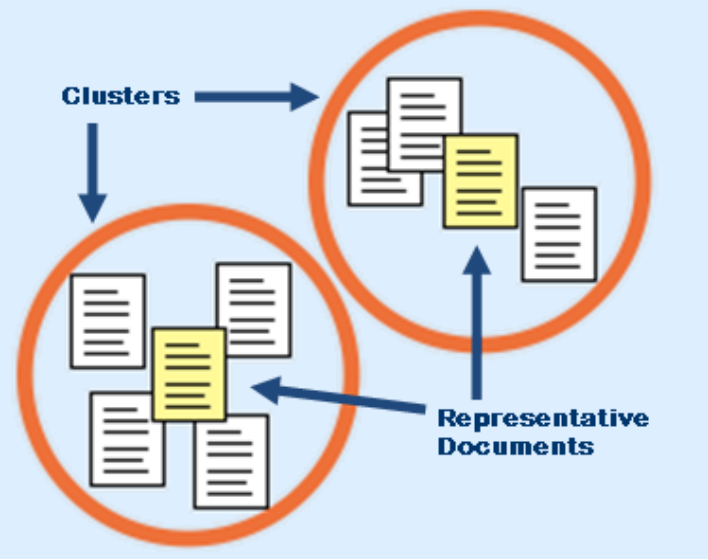
Example 1: Clothing size

- Tailor-made for each person is too expensive
- One-size-fits-all: does not work!
- Groups people of similar sizes together to make “small”, “medium”, and “large” t-shirts

Unsupervised Learning (3/5)

Example 2: Text document organization

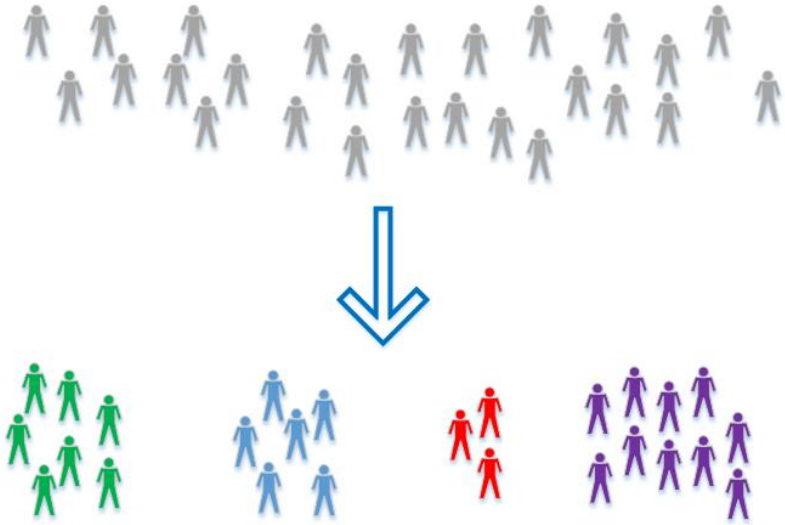
- To find groups of documents that are similar to each other based on the important terms appearing in them



Unsupervised Learning (4/5)

Example 3: Target Marketing

- Subdivide market into distinct subsets of customers where any subset may conceivably be selected as a segment to be reached with a particular offer



Unsupervised Learning (5/5)

Example 4: Social network graphs

- Subdivide social network into distinct subsets of user groups (Facebook friends, LinkedIn contacts…)

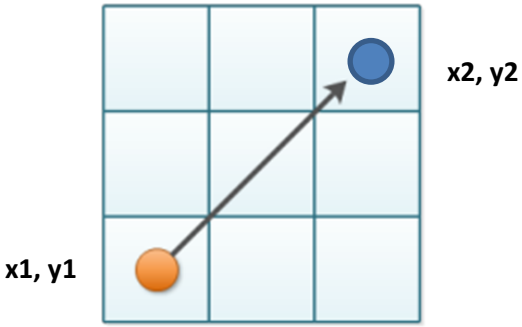
K-Means Clustering

- Partitions data points into similarity clusters
- Unsupervised technique
- Only works for numeric data

Age	Pclass_1	Pclass_2	Pclass_3	Gender_F	Gender_M
19	0	1	0	0	1
28	1	0	0	1	0
64	0	0	1	0	1

Euclidean Distance

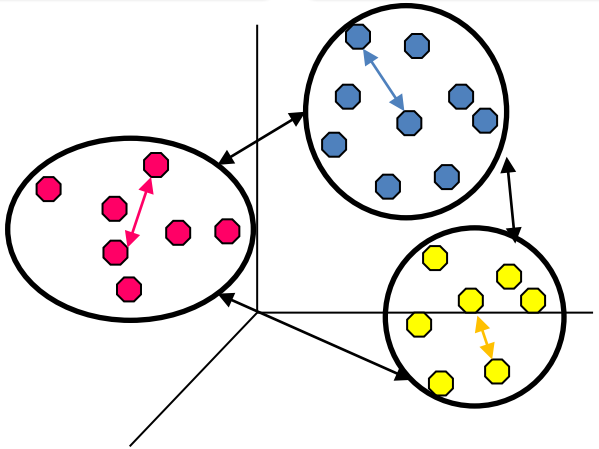
points in a two-dimensional space to determine intra- and inter-cluster similarity



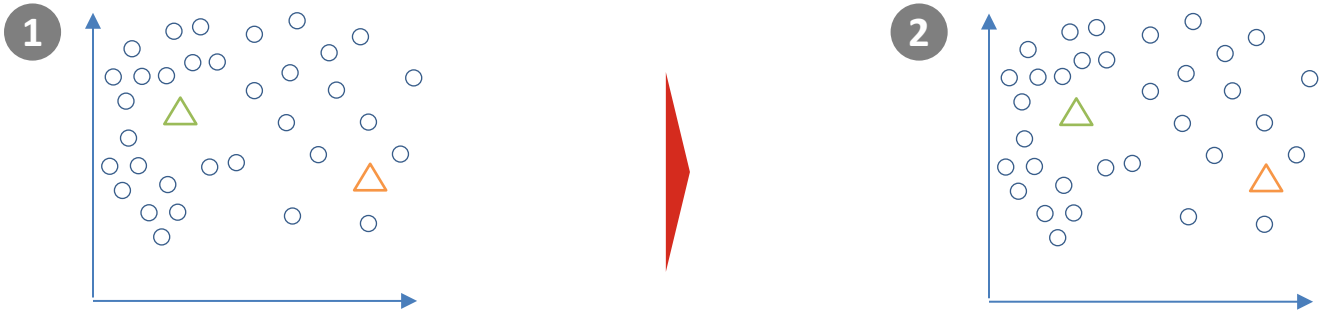
$$\sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2}$$

Intra-cluster distances are minimized

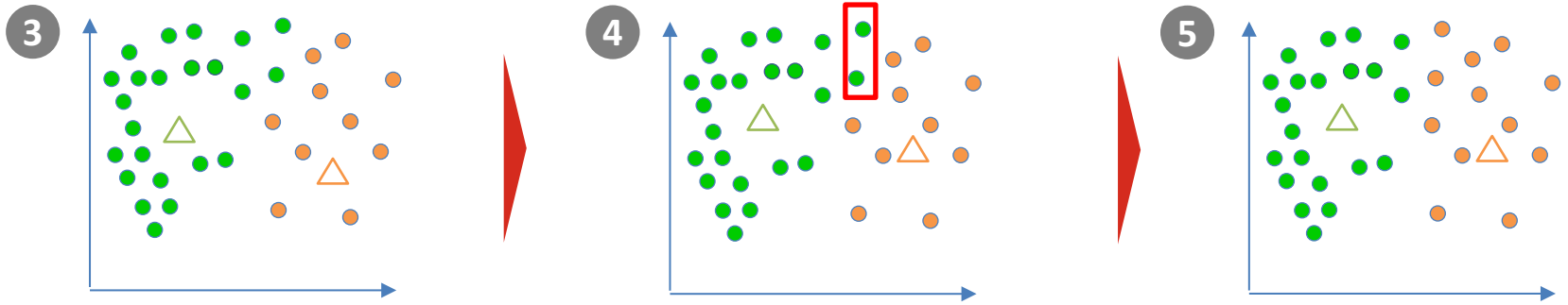
Inter-cluster distances are maximized



K-means Clustering (1/2)



K-means Clustering (2/2)

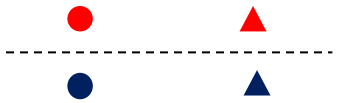


K-Means Clustering

- Minimizes aggregate intra-cluster distance
  - Measure squared distance from point to center of its cluster.

$$\sum_{j=1}^{K} \sum_{x \in g_j} D(c_j, x)^2$$

- Could converge to local minimum
  - Different starting points → very different results
  - Run many times with random starting points
- Nearby points may not be assigned to the same cluster



K-means Clustering

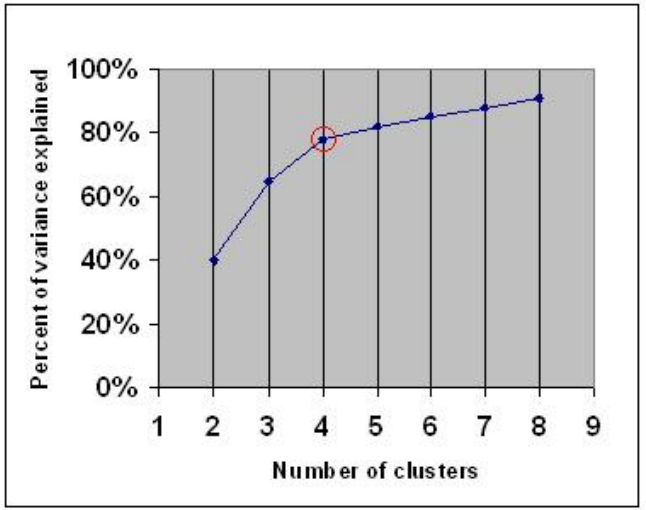
- Strengths
  - Simple: easy to understand and to implement
  - Efficient: linear time, minimal storage
- Weaknesses
  - Mean must be well defined
  - The user needs to specify k
  - Algorithm is sensitive to outliers

How many clusters?

Elbow method

- percentage of variance explained as a function of the number of clusters

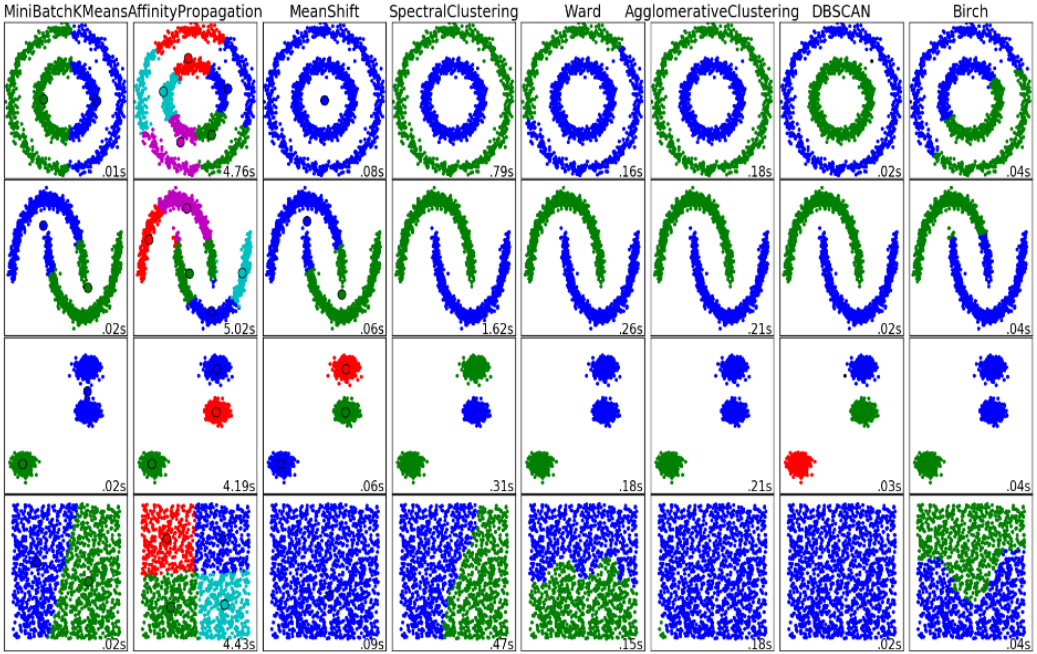
- choose a number of clusters so that adding another cluster doesn't give much better modeling of the data.



Other K Optimization Techniques

- Silhouette
- Calinsky criterion
- Bayesian Information Criterion
- Affinity propagation (AP) clustering
- Gap statistic

Other K Optimization Techniques



A comparison of the clustering algorithms in scikit-learn

QUESTIONS