K-means clustering

Definition and Purpose

K-means is a method to **partition n observations into k clusters** in which each observation belongs to the cluster with the nearest **mean (cluster centers or cluster centroid), serving as a prototype of the cluster**. It minimizes with-cluster variances (squared Euclidean distance), but not regular Euclidean distance (can be solved using k-medians or k-medoids).

In the mathematic expression, given a set of observations $(x_1, x_2, \dots, x_n)$, where each observation is d-dimensional real vector, it aims to partition the n observations into k cluster $S = \{S_1, S_2, \dots, S_k\}$

$$\arg_S \min \sum_{i=1}^{k} \sum_{X \in S_i} \left|\left|X - \mu_i\right|\right|^2 = \arg_S \min \sum_{i=1}^{k} |S_i| \, Var S_i$$

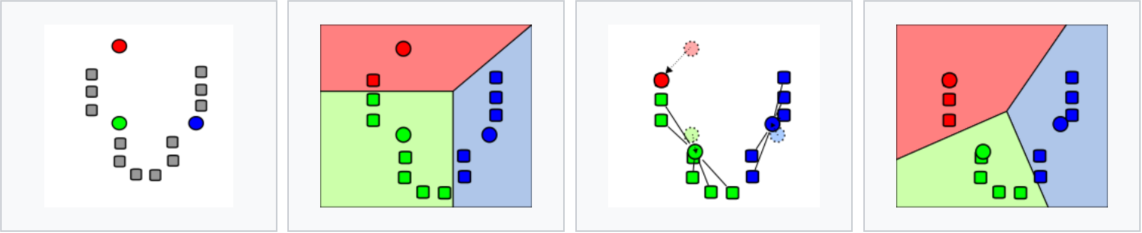
μ_i is the mean of points in S_i,

Algorithms

Given an initial set of k-means $m_1^{(1)}, \dots, m_k^{(1)}$, the algorithm proceeds by alternating between two steps:

1. **Assignment step:** Assign each observation to the cluster with the nearest mean: with the squared Euclidean distance (Mathematically, this means **partitioning the observations according to the Voronoi diagram** centered by the means).
2. Update Step: Recalculate means (centroids) for observations assigned to each cluster.

Demonstration of the standard algorithm



1. *k* initial "means" (in this case *k*=3) are randomly generated within the data domain (shown in color).

2. *k* clusters are created by associating every observation with the nearest mean. The partitions here represent the Voronoi diagram generated by the means.

3. The centroid of each of the *k* clusters becomes the new mean.

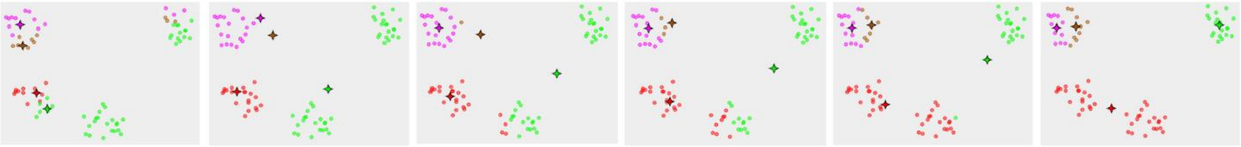
4. Steps 2 and 3 are repeated until convergence has been reached.

The algorithm has converged when the assignments no longer change. **The algorithm is not guaranteed to find the optimum**. Various modifications of k-means such as spherical k-means and k-medoids have been proposed to allow using other distance measures.

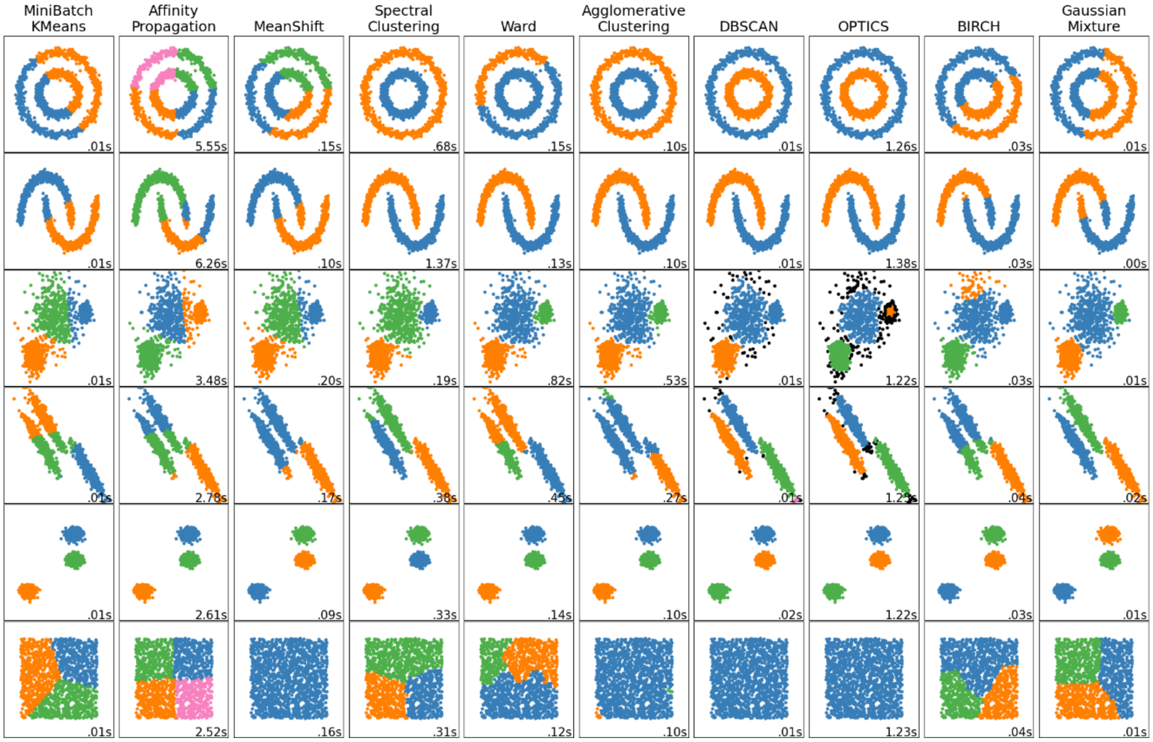
Properties

Three key features of *k*-means that make it efficient are **often regarded as its biggest drawbacks**:

1. The number of clusters k is an input parameter: **an inappropriate choice of k may yield poor results**. That is why, when performing k-means, it is important to run diagnostic checks for determining the number of clusters in the data set.
2. Convergence to a **local minimum may produce counterintuitive ("wrong") results** (**wrong initial position**)



3. Euclidean distance is used as a metric and variance is used as a measure of cluster scatter.


MiniBatch KMeans
Affinity Propagation
MeanShift
Spectral Clustering
Ward
Agglomerative Clustering
DBSCAN
OPTICS
BIRCH
Gaussian Mixture
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