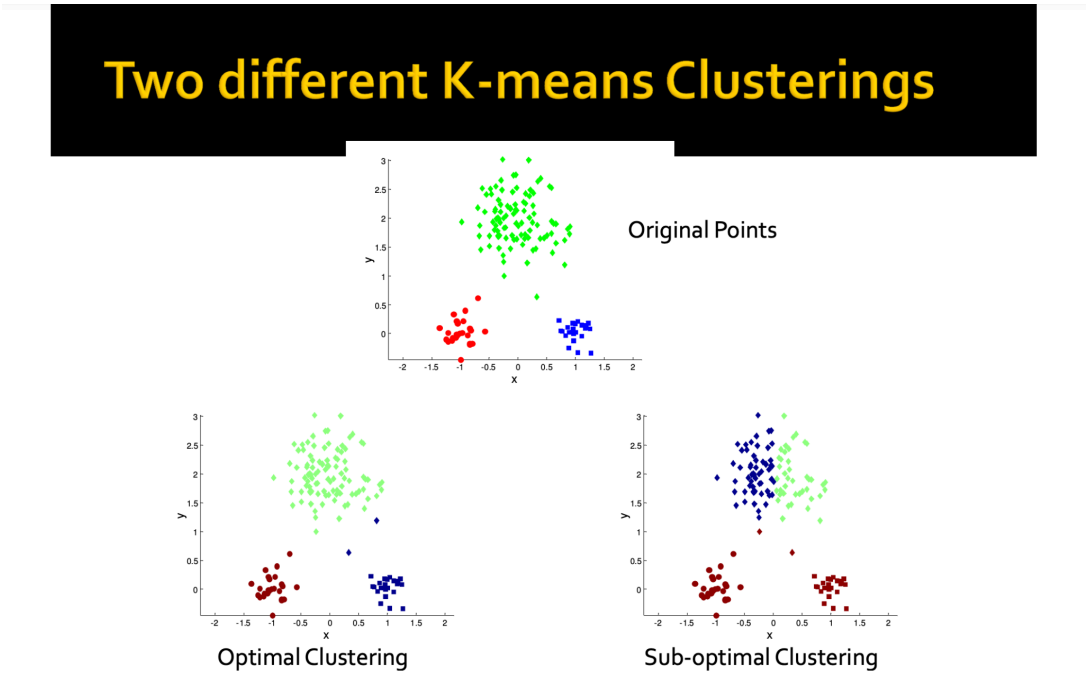
02 - K-Means++

While the K-Means algorithm is the simplest model for clustering, there are some drawbacks that come with it.

Drawbacks of K-Means

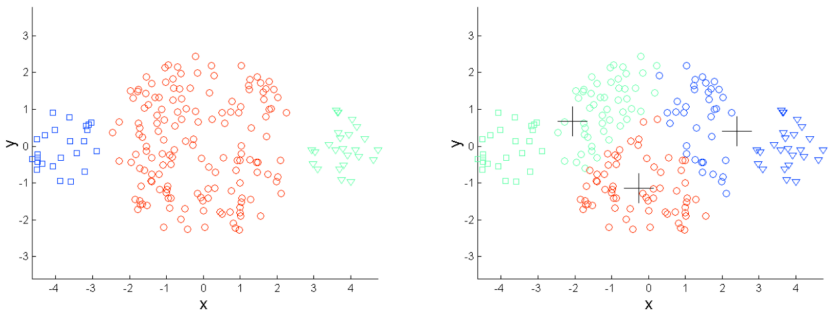
1. K-means is initialization dependent. This means, that the same data, with different initialization, will get different results (different clusters).
   For example;



   Use this visualization tool to see this problem and try it out by yourself!

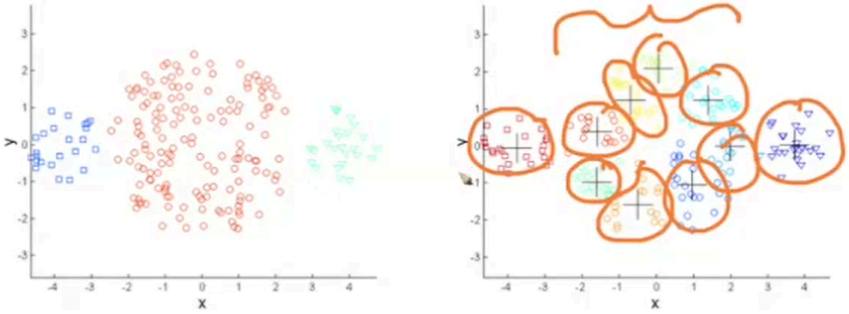
2. The k-means algorithm may not give the best results for data where the clusters are of varying size or density.

Limitations of K-means: Differing Sizes



Original Points K-means (3 Clusters)

- One way of solving this problem would be to increase the value of K.
- Once clusters are formed, similar clusters can be grouped together to form a mega cluster.

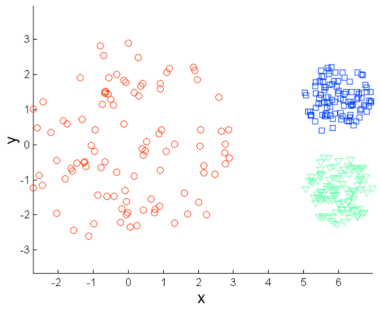


Original Points K-means Clusters

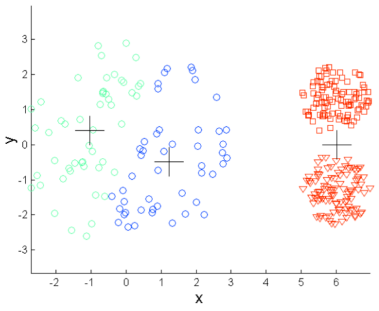
One solution is to use many clusters.
Find parts of clusters, but need to put together.

- The problem with this approach is the grouping of similar clusters is not easy

Limitations of K-means: Differing Density



Original Points

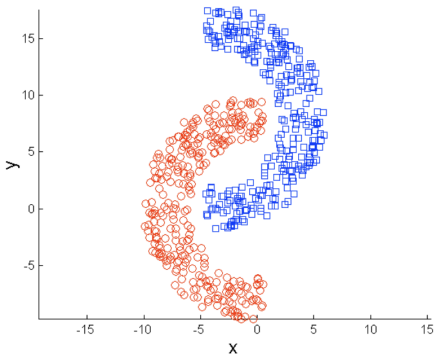


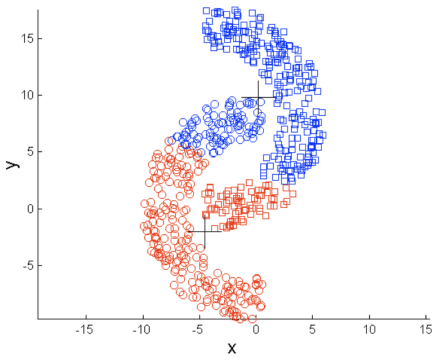
K-means (3 Clusters)

3. The number of clusters (k) needs to be defined prior to clustering.

4. It does not work well with non-globular clusters.

Limitations of K-means: Non-globular Shapes





K-Means++

- To overcome the drawback due to the random initialization of centroids in K-means clustering, we use K-means++. It is smarter to initialize the centroids in order to improve the clustering algorithm.

- Consider data where we want to initialize 3 centroids.
    - We pick the first centroid at random
    - Now, to pick the second centroid, we want to pick a point that is as far away as possible
- If you think about it, we would want to pick a point that is far away, because if two centroids are closer to each other, two clusters for that region of data points will be formed

- Most of the time data points belonging to the same region will share similar characteristics and they should ideally belong to one cluster, instead of two.
- So, what we do is compute the distance from the centroid C1 of all the data points present in our dataset D such as: $D - \{C_1\}$
- But there's a little risk with this. If we select a datapoint as a second centroid with the farthest distance, then an outlier might be picked as a centroid, and we might have a cluster with the centroid C_2 only.

- So, what we do is pick a centroid probabilistically, instead of picking it deterministically.
- It is done in such a way that the probability of picking a centroid is proportional to the distance from the first centroid C_1.

- The steps involved in the initialization of centroids are:
    - ➔ Select the first centroid randomly from the data points.
    - ➔ Choose the next center as the farthest point from the first center.
    - ➔ The next center would be a data point farthest from both the first and second centers.

- Repeat steps 2 and 3 until **k** centroids have been sampled.

- If there are **outliers** in our data, then instead of choosing them as centroid, we can choose the farthest point as the centroid with a **probability proportional to the distance.** This is the implementation that sklearn follows by default..