

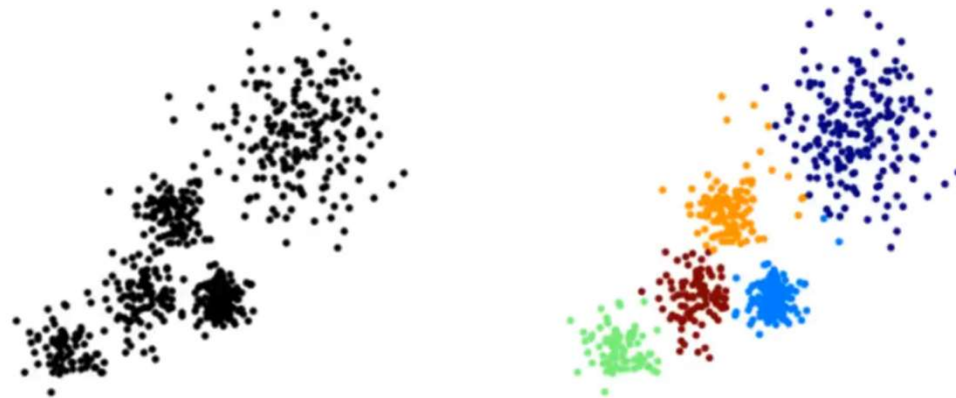


K – Means Clustering

- K Means Clustering is an unsupervised learning algorithm that will attempt to group similar clusters together in the data
- What does a typical clustering problem look like?
 - Cluster similar documents
 - Cluster customers based on features
 - Market Segmentation
 - Identify similar physical groups

K – Means Clustering

- The overall goal is to divide data into distinct groups such that observations within each group are similar



K –Means Clustering

- The K – Means Algorithm
 - Choose a number of clusters “k”
 - Randomly assign each point to a cluster
 - Until clusters stop changing, repeat the following:
 - For each cluster, compute the cluster centroid by taking the mean vector of the points in the cluster
 - Assign each data point to the cluster for which the centroid is the closest

K - Means

Step 1: Select the number of clusters you want to identify in your data. This is the “K” in “K-means clustering”.

In this case, we’ll select $K=3$. That is to say, we want to identify 3 clusters.



There is a fancier way to select a value for “K”, but we’ll talk about that later.

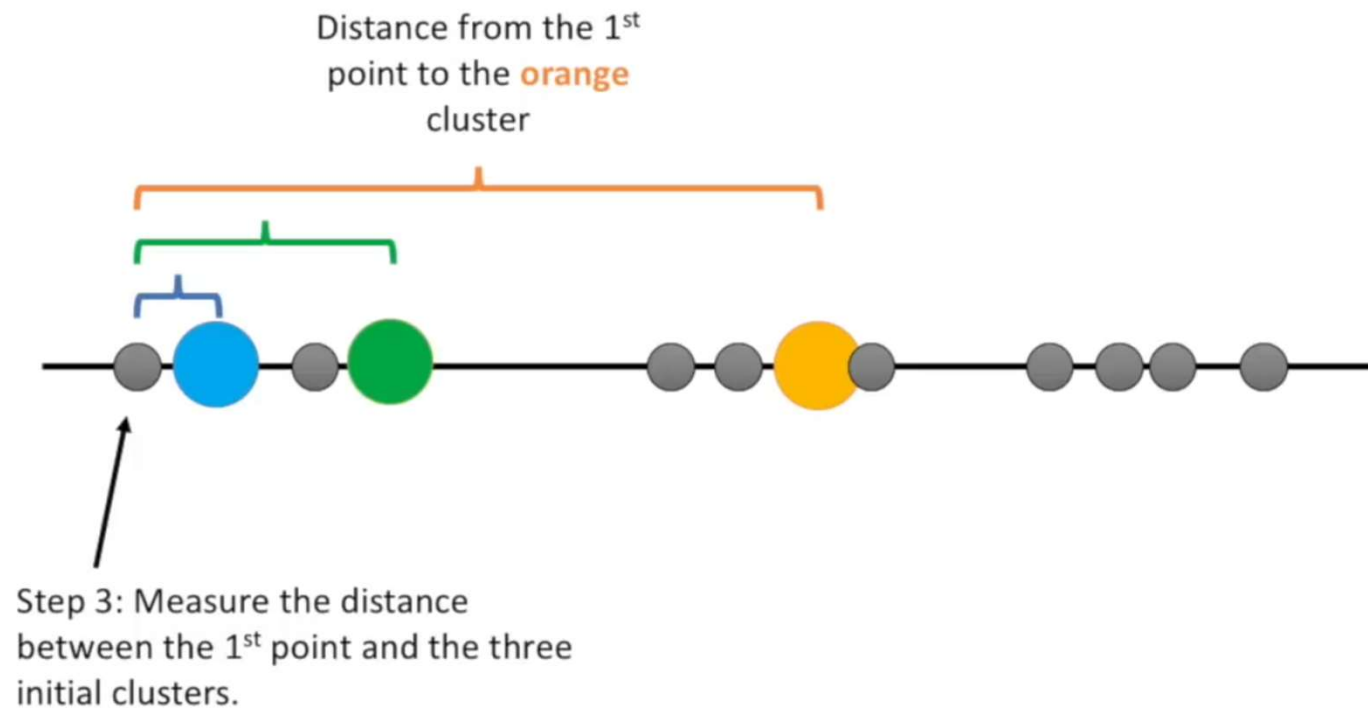


K - Means

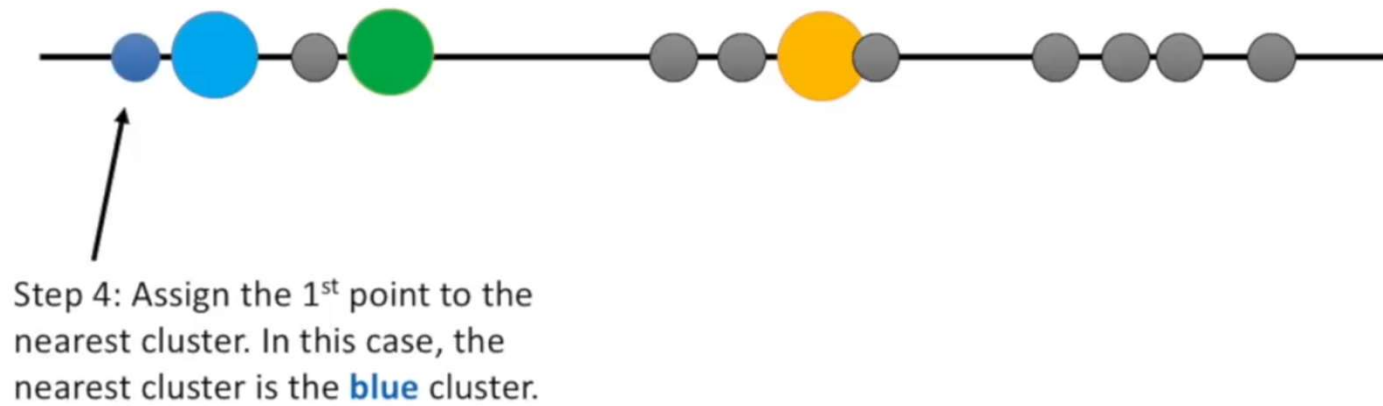
Step 2: Randomly select 3 distinct data points.



K - Means

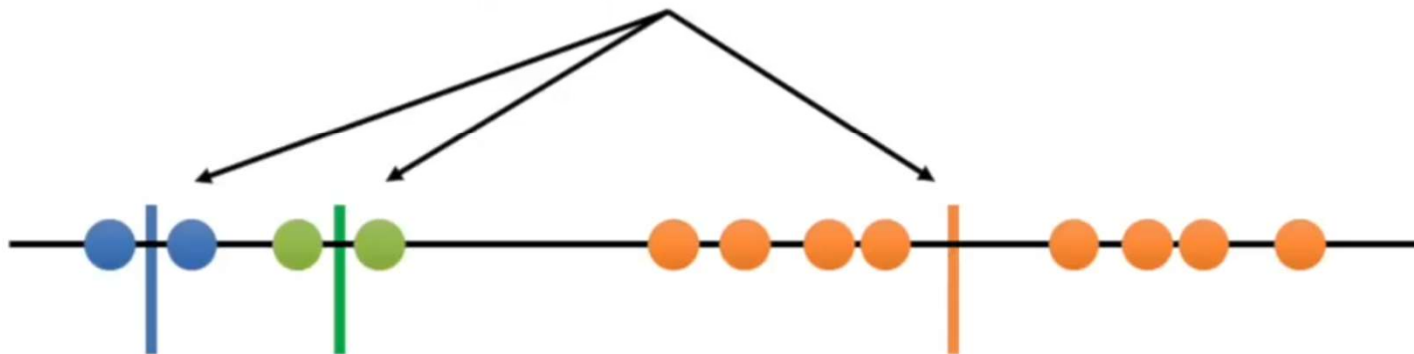


K - Means

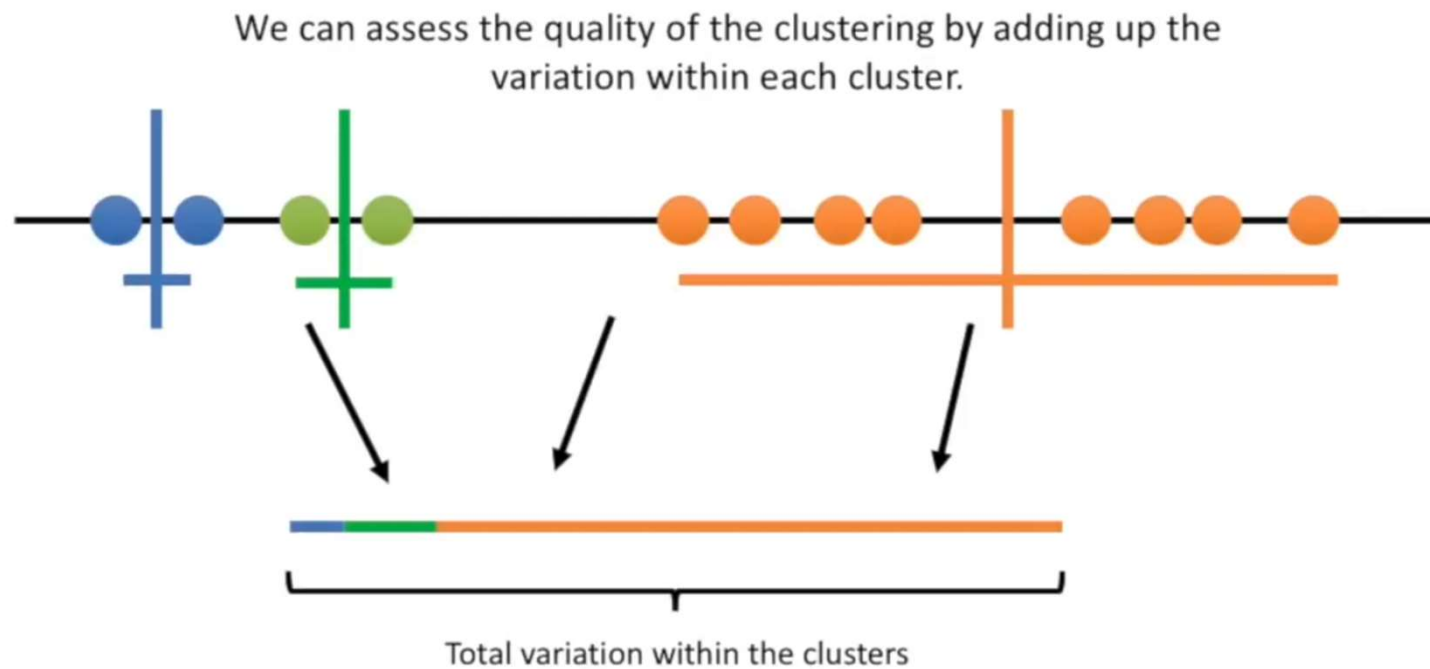


Repeat the steps for the next point

Step 5: calculate the mean of each cluster.

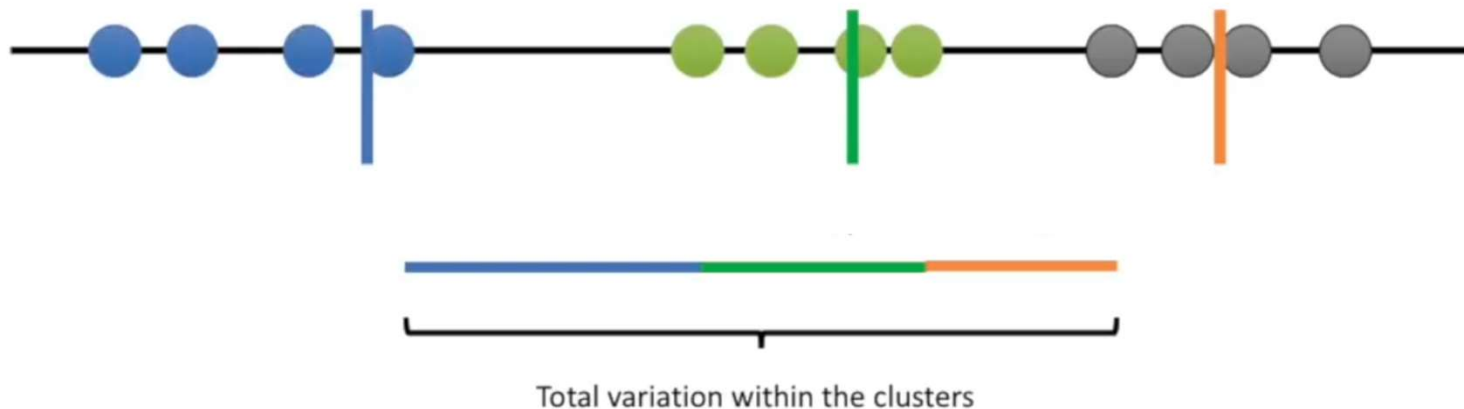


K - Means



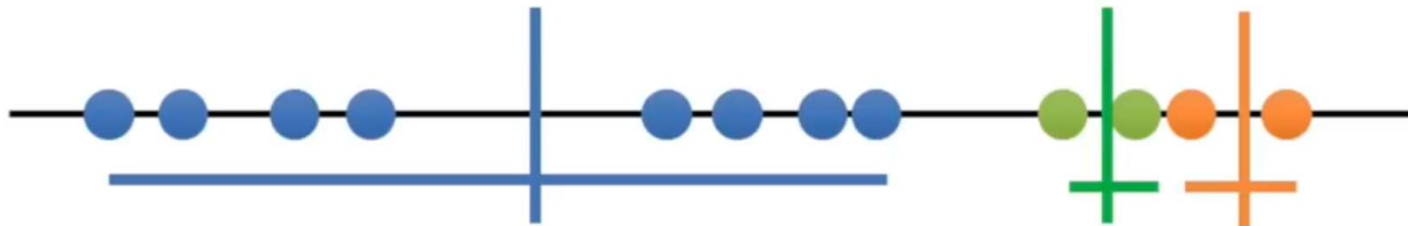
K - Means

...and then clusters all the remaining points, calculates the mean of each cluster and then reclusters based on the new means. It repeats until the clusters no longer change.



K - Means

At this point, K-means clustering knows that *the 2nd clustering is the best clustering so far*. But it doesn't know if it's *the best overall*, so it will do a few more clusters (it does as many as you tell it to do) and then come back and return that one if it is still the best.



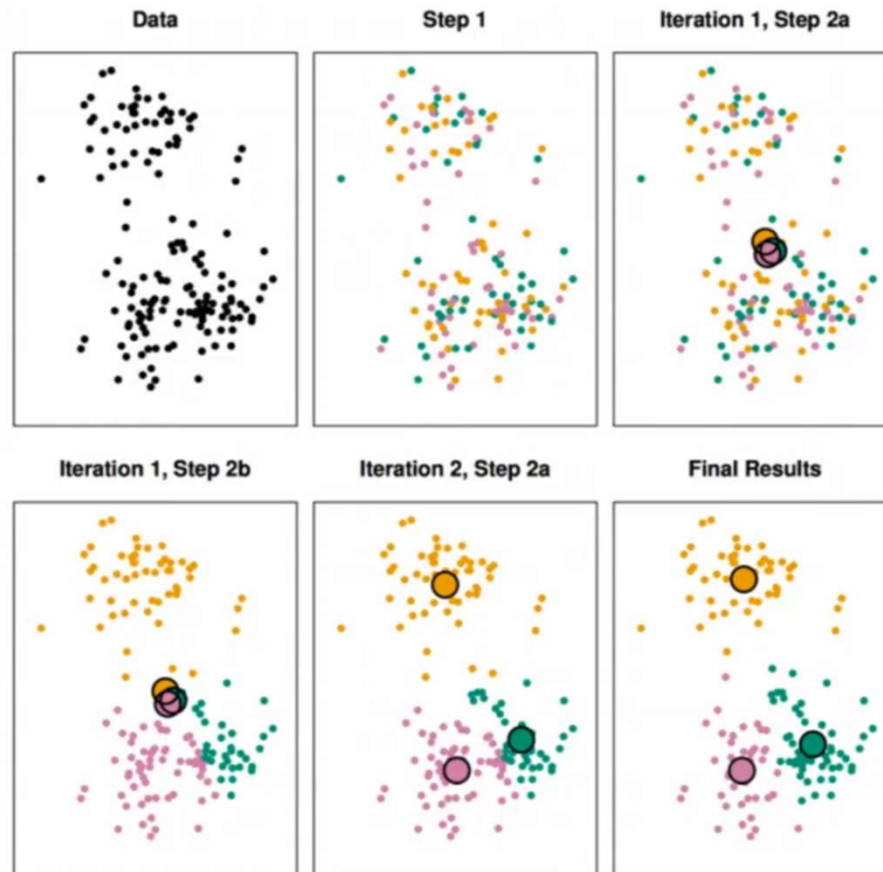
1st cluster attempt:

2nd cluster attempt:

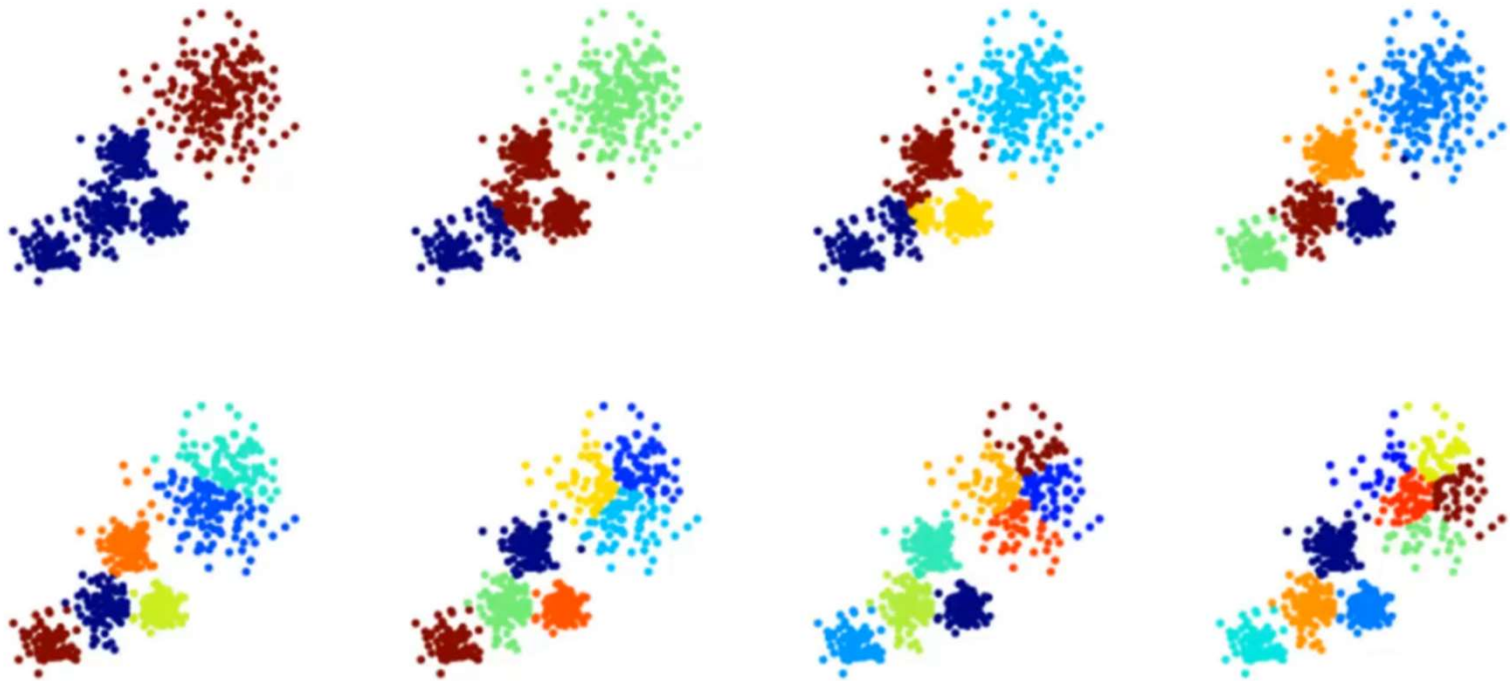
The winner!!

3rd cluster attempt:

K – Means Clustering



Choosing a K Value

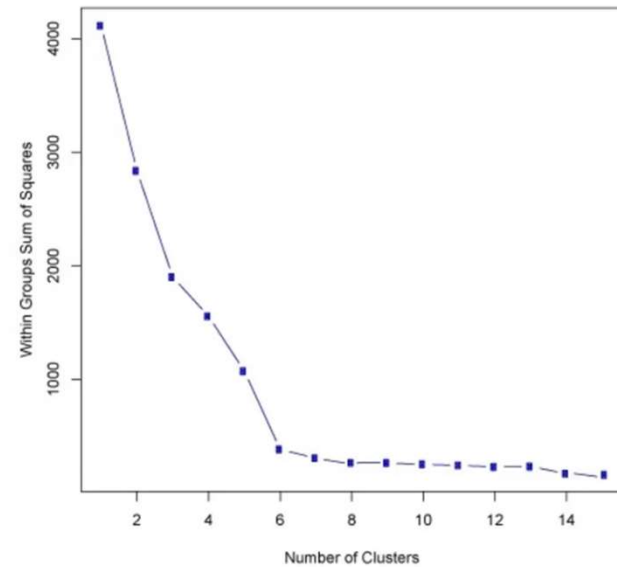


Choosing a K Value

- There is no easy answer for choosing the best K value
- One way is called as the Elbow Method
- First, compute the sum of squared error (SSE) for some values of K (for example: 2, 4, 6, 8...)
- The SSE is defined as the SS distance between each member of the cluster and its centroid
- If you plot k against SSE, you will see error decreases as k gets larger, this is because when the number of cluster increases, they should be smaller, so distortion is also smaller

Choosing K Value

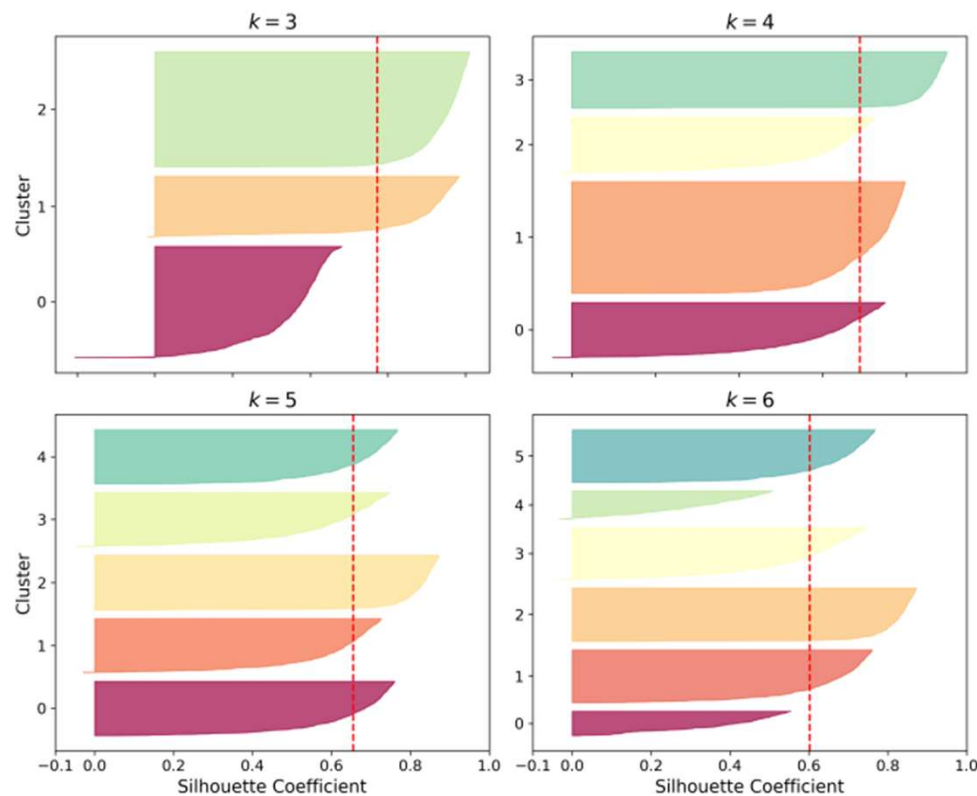
- The idea of the elbow method is to choose the k at which the SSE decreases abruptly
- This produces an elbow effect as shown in the graph:



Silhouette score

- Silhouette score, which is the mean silhouette coefficient over all the instances.
- An instance's silhouette coefficient is equal to $(b - a) / \max(a, b)$ where a is the mean distance to the other instances in the same cluster (it is the mean intra-cluster distance), and b is the mean nearest-cluster distance, that is the mean distance to the instances of the next closest cluster (defined as the one that minimizes b , excluding the instance's own cluster).
- The silhouette coefficient can vary between -1 and +1: a coefficient close to +1 means that the instance is well inside its own cluster and far from other clusters, while a coefficient close to 0 means that it is close to a cluster boundary, and finally a coefficient close to -1 means that the instance may have been assigned to the wrong cluster.

Silhouette Score



We can see that when $k=3$ and when $k=6$, we get bad clusters. But when $k=4$ or $k=5$, the clusters look pretty good – most instances extend beyond the dashed line, to the right and closer to 1.0.