GENERAL ASSEMBLY

INTRO TO DATA SCIENCE

CLUSTER ANALYSIS

I. CLUSTER ANALYSIS
II. THE K-MEANS ALGORITHM
III. CHOOSING K
IV. EXAMPLE

I. CLUSTER ANALYSIS

	continuous	*categorical*
supervised	???	???
unsupervised	???	???

	continuous	categorical
supervised	regression	classification
unsupervised	dimension reduction	clustering

Q: What is a cluster?

Q: What is a cluster?

A: A group of **similar** *data points.*

Q: What is a cluster?

A: A group of **similar** *data points.*

The concept of similarity is central to the definition of a cluster, and therefore to cluster analysis.

Q: What is a cluster?

A: A group of **similar** *data points.*

The concept of similarity is central to the definition of a cluster, and therefore to cluster analysis.

In general, greater similarity between points leads to better clustering.

Q: What is the purpose of cluster analysis?

Q: What is the purpose of cluster analysis?

A: To enhance our understanding of a dataset by dividing the data into groups.

Q: What is the purpose of cluster analysis?

A: To enhance our understanding of a dataset by dividing the data into groups.

Clustering provides a layer of abstraction from individual data points.

Q: What is the purpose of cluster analysis?

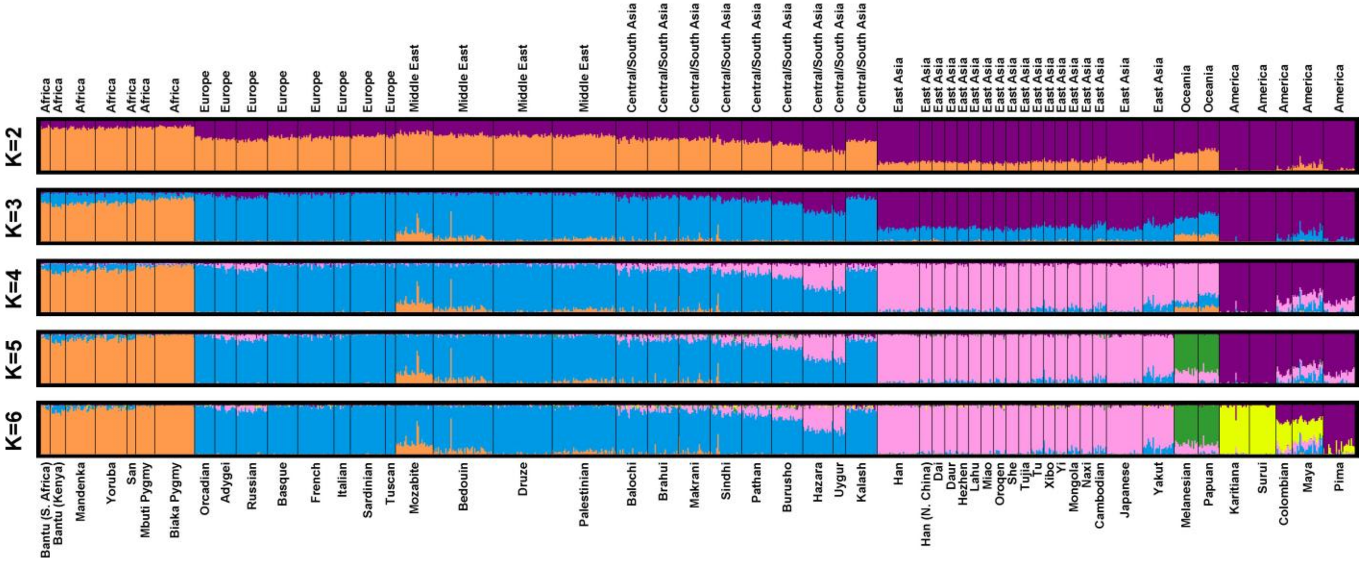
A: To enhance our understanding of a dataset by dividing the data into groups.

Clustering provides a layer of abstraction from individual data points.

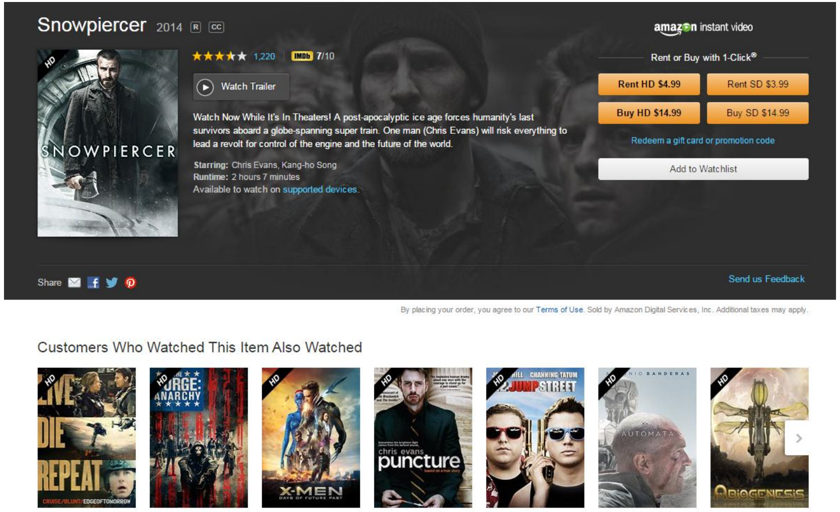
The goal is to extract and enhance the natural structure of the data

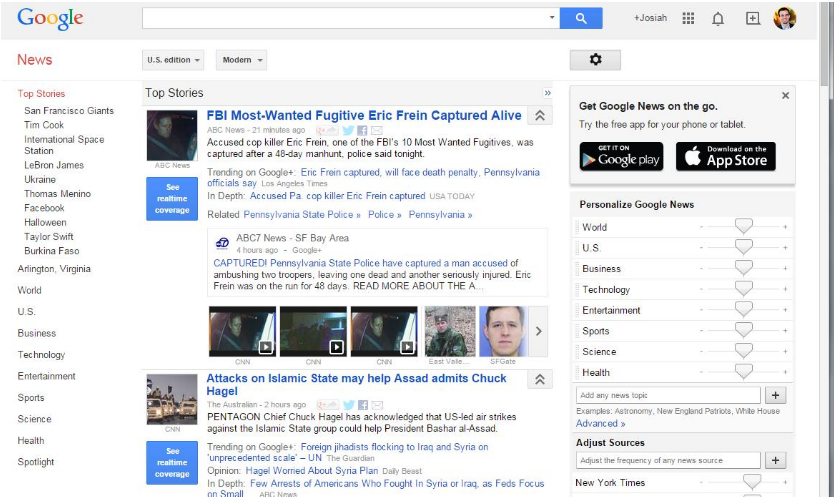
Clustering can be useful in a wide variety of domains, including genetics, consumer internet and business.

Clustering can be useful in a wide variety of domains, including ***genetics****, consumer internet and business.*



*Clustering can be useful in a wide variety of domains, including genetics, **consumer internet** and business.*





*Clustering can be useful in a wide variety of domains, including genetics, consumer internet and **business**.*

http://i.huffpost.com/gen/1563531/thumbs/o-GROCERY-STORE-facebook.jpg

There are many kinds of clustering procedures. For our class, we will be focusing on K-means clustering, which is one of the most popular clustering algorithms.

K-means is an iterative method that partitions a data set into k clusters.

II. K-MEANS CLUSTERING

Q: How does the algorithm work?

1) *choose k initial centroids (note that k is an input)*

2) *for each point:*
   - *find distance to each centroid*
   - *assign point to nearest centroid*

3) *recalculate centroid positions*
4) *repeat steps 2-3 until stopping criteria met*

Q: How do you choose the initial centroid positions?

Q: How do you choose the initial centroid positions?

A: There are several options:

Q: How do you choose the initial centroid positions?

A: There are several options:

- randomly (but may yield divergent behavior)

Q: How do you choose the initial centroid positions?

A: There are several options:

- randomly (but may yield divergent behavior)

- perform alternative clustering task, use resulting centroids as initial k-means centroids

Q: How do you choose the initial centroid positions?

A: There are several options:

- randomly (but may yield divergent behavior)

- perform alternative clustering task, use resulting centroids as initial k-means centroids

- start with global centroid, choose point at max distance, repeat (but might select outlier)

Q: How do you determine which centroid a given point is most similar to?

Q: How do you determine which centroid a given point is most similar to?

The similarity criterion is determined by the measure we choose.

Q: How do you determine which centroid a given point is most similar to?

The similarity criterion is determined by the measure we choose.

In the case of k-means clustering, the similarity metric is the ***Euclidian distance:***

Q: How do you determine which centroid a given point is most similar to?

The similarity criterion is determined by the measure we choose.

In the case of k-means clustering, the similarity metric is the ***Euclidian distance:***

$$d(x_1, x_2) = \sqrt{\sum_{i=1}^{N} (x_{1i} - x_{2i})^2}$$

Q: How do we recompute the positions of the centers at each iteration of the algorithm?

A: By calculating the centroid (i.e., the geometric center)

We iterate until some stopping criteria are met; in general, suitable convergence is achieved in a small number of steps.

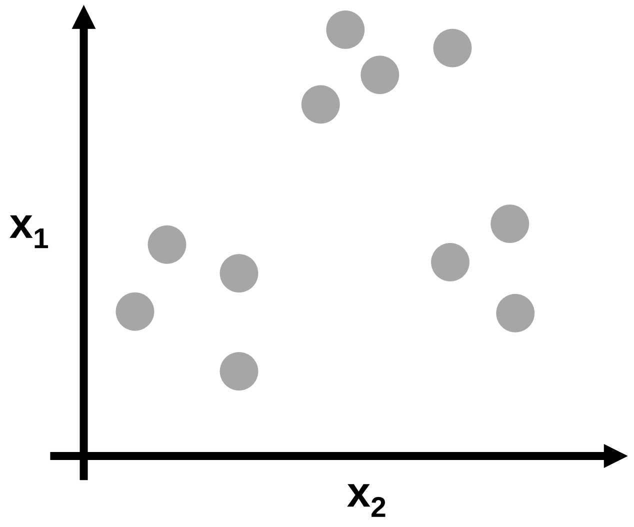
We iterate until some stopping criteria are met; in general, suitable convergence is achieved in a small number of steps.

Stopping criteria can be based on the centroids (eg, if positions change by no more than ε) or on the points (eg, if no more than x% change clusters between iterations).

1) *choose k initial centroids (note that k is an input)*

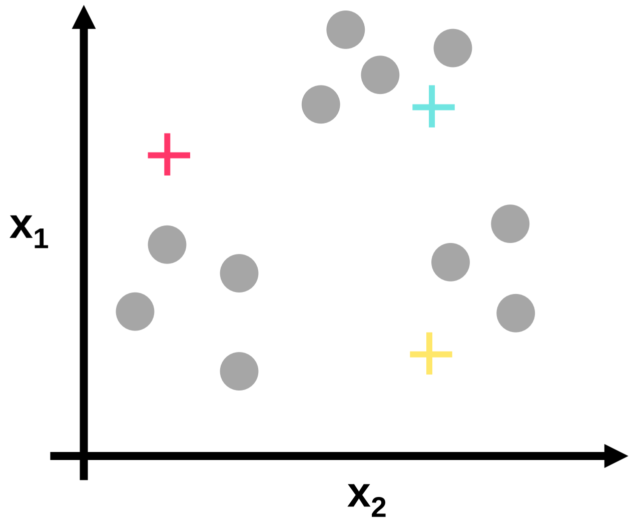
2) *for each point:*
   - *find distance to each centroid*
   - *assign point to nearest centroid*

3) *recalculate centroid positions*
4) *repeat steps 2-3 until stopping criteria met*



1) *choose k initial centroids (note that k is an input)*

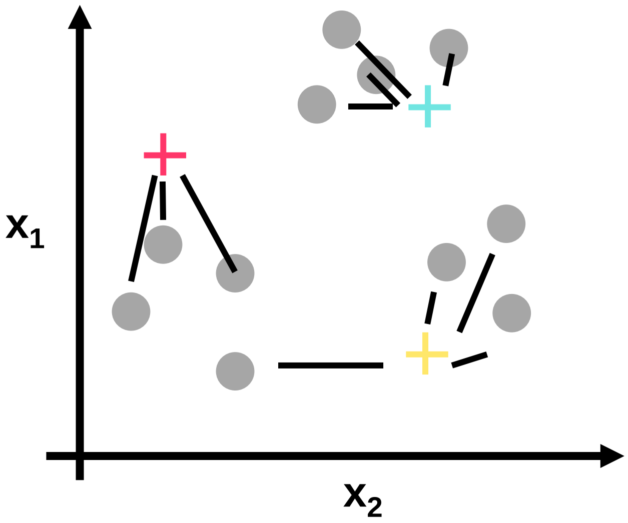
2) *for each point:*
   - *find distance to each centroid*
   - *assign point to nearest centroid*



3) *recalculate centroid positions*
4) *repeat steps 2-3 until stopping criteria met*

1) *choose k initial centroids (note that k is an input)*

2) ***for each point:***
   - ***find distance to each centroid***
   - *assign point to nearest centroid*



3) *recalculate centroid positions*

4) *repeat steps 2-3 until stopping criteria met*

1) choose k initial centroids (note that k is an input)

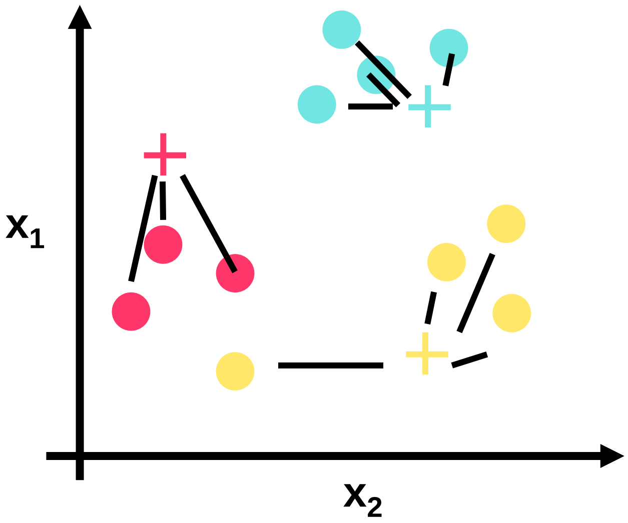
2) for each point:

- find distance to each centroid

- assign point to nearest centroid

3) recalculate centroid positions

4) repeat steps 2-3 until stopping criteria met

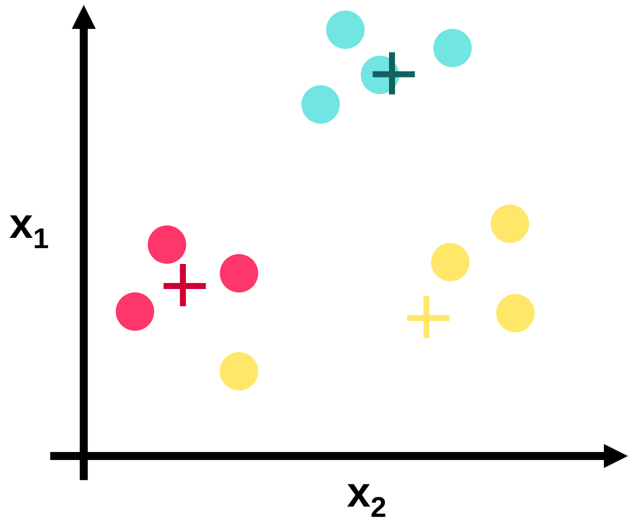


1) *choose k initial centroids (note that k is an input)*

2) *for each point:*
   - *find distance to each centroid*
   - *assign point to nearest centroid*

3) ***recalculate centroid positions***

4) *repeat steps 2-3 until stopping criteria met*

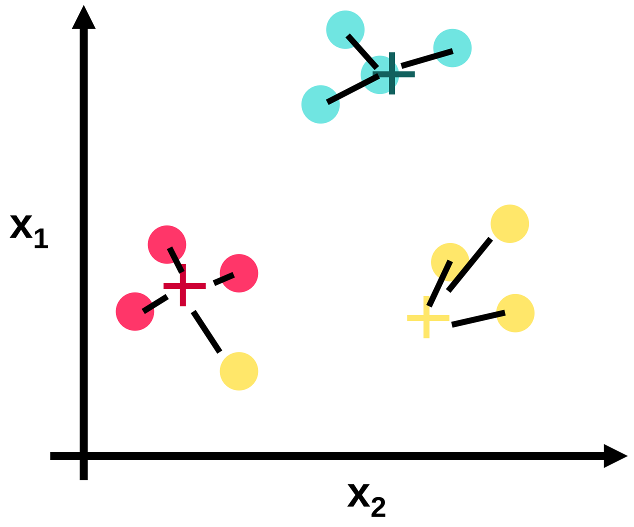


1) choose k initial centroids (note that k is an input)

2) for each point:

- find distance to each centroid

- assign point to nearest centroid

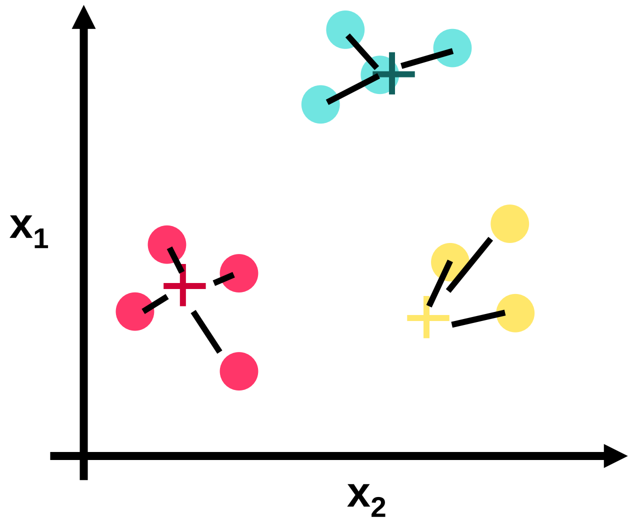


3) recalculate centroid positions

4) repeat steps 2–3 until stopping criteria met

1) *choose k initial centroids (note that k is an input)*

2) *for each point:*
   - *find distance to each centroid*
   - *assign point to nearest centroid*

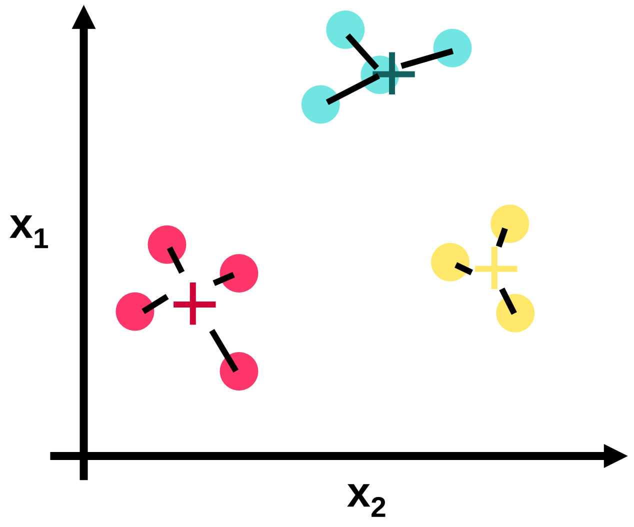


3) *recalculate centroid positions*

4) ***repeat steps 2–3 until stopping criteria met***

1) choose k initial centroids (note that k is an input)

2) for each point:
- find distance to each centroid
- assign point to nearest centroid



3) recalculate centroid positions

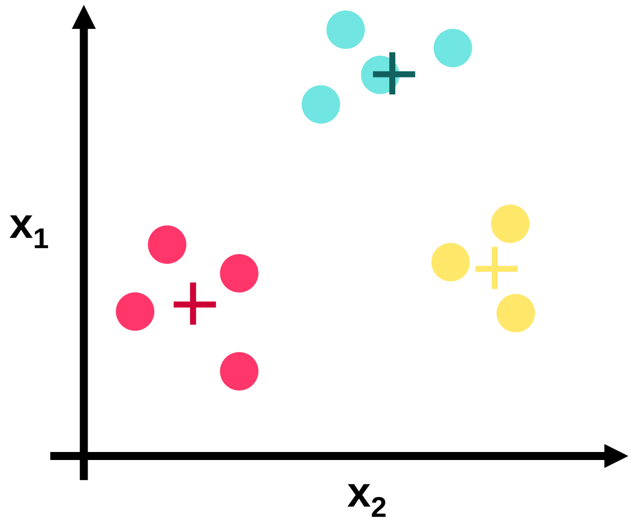
4) repeat steps 2-3 until stopping criteria met

1) *choose k initial centroids (note that k is an input)*

2) *for each point:*
   - *find distance to each centroid*
   - *assign point to nearest centroid*

3) *recalculate centroid positions*

4) ***repeat steps 2-3 until stopping criteria met***



III. CLUSTER VALIDATION

In general, k-means will converge to a solution and return a partition of k clusters, even if no natural clusters exist in the data.

In general, k-means will converge to a solution and return a partition of k clusters, even if no natural clusters exist in the data.

We will look at two validation metrics useful for partitional clustering, **cohesion** *and* **separation***.*

Cohesion *measures clustering effectiveness within a cluster.*

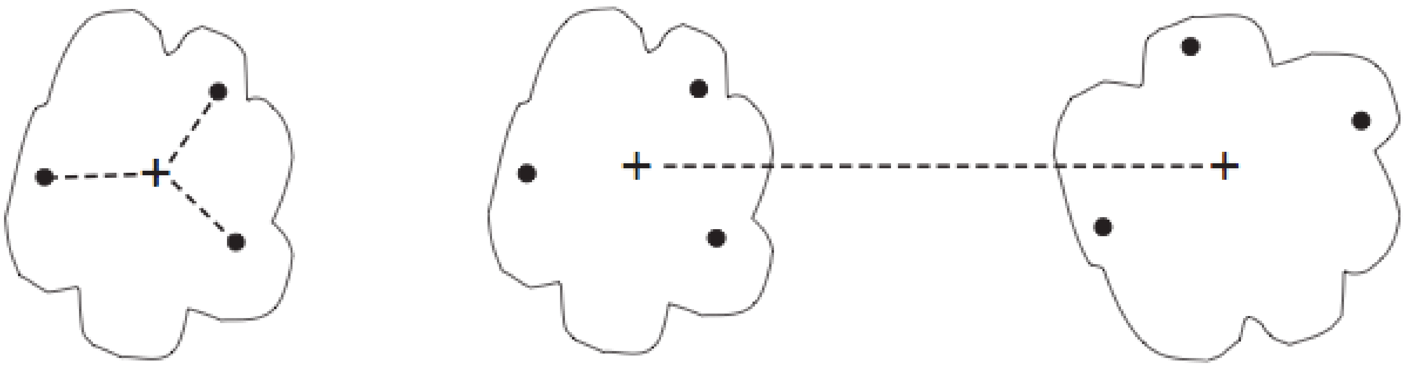
$$\hat{C}(C_i) = \sum_{x \in C_i} d(x, c_i)$$

Cohesion *measures clustering effectiveness within a cluster.*

$$\hat{C}(C_i) = \sum_{x \in C_i} d(x, c_i)$$

Separation *measures clustering effectiveness between clusters.*

$$\hat{S}(C_i, C_j) = d(c_i, c_j)$$



(a) Cohesion. (b) Separation.

Figure 8.28. Prototype-based view of cluster cohesion and separation.

source: http://www-users.cs.umn.edu/~kumar/dmbook/ch8.pdf

One useful measure than combines the ideas of cohesion and separation is the **silhouette coefficient**. *For a single point, this is given by:*

$$SC = \frac{b - a}{\max(a, b)}$$

a = The mean distance between a sample and all other points in the same class.

Source: scikit learn

One useful measure than combines the ideas of cohesion and separation is the **silhouette coefficient***. For a single point, this is given by:*

$$SC = \frac{b - a}{\max(a, b)}$$

b = The mean distance between a sample and all other points in the next nearest cluster.

Source: scikit learn

Generally, this formula simplifies to the following:

$$SC = 1 - \frac{a}{b}$$

This is because generally b > a:

The silhouette coefficient can take values between -1 and 1.

In general, we want separation to be high and cohesion to be low. This corresponds to a value of SC close to +1.

A negative silhouette coefficient means the cluster radius is larger than the space between clusters, and thus clusters overlap.

The silhouette coefficient for a cluster is given by the average silhouette coefficient across all points in that cluster:

The silhouette coefficient for a cluster is given by the average silhouette coefficient across all points in that cluster:

The overall silhouette coefficient is given by the average silhouette coefficient across all points:

$$SC_{total} = \frac{1}{N}\sum_{1}^{N} SC_i$$

The silhouette coefficient for a cluster is given by the average silhouette coefficient across all points in that cluster:

The overall silhouette coefficient is given by the average silhouette coefficient across all points:

$$SC_{total} = \frac{1}{N}\sum_{1}^{N} SC_i$$

NOTE

This gives a summary measure of the overall clustering quality.

One useful application of cluster validation is to determine the best number of clusters for your dataset.

One useful application of cluster validation is to determine the best number of clusters for your dataset.

Q: How would you do this?

One useful application of cluster validation is to determine the best number of clusters for your dataset.

Q: How would you do this?

A: By computing the SC for different values of k.

A: Another commonly used metric is the within sum of squared errors

Ultimately, cluster validation and clustering in general are suggestive techniques that rely on human interpretation to be meaningful.

Strengths:

K-means is a popular algorithm because of its computational efficiency and simple and intuitive nature.

Strengths:

K-means is a popular algorithm because of its computational efficiency and simple and intuitive nature.

Weaknesses:

However, K-means is highly scale dependent, and may produce misleading results for data with widely varying shapes and densities.

EX: K-MEANS CLUSTERING