## INTRO TO DATA SCIENCE CLUSTER ANALYSIS

AGENDA 2

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

## I. CLUSTER ANALYSIS

	continuous	categorical
supervised	???	???
unsupervised	???	???
•	???	???

#### **LOGISTIC REGRESSION**

# supervised<br/>unsupervisedregression<br/>dimension reductionclassification<br/>clustering

Q: What is a cluster?

Q: What is a cluster?

A: A group of similar data points.

#### **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.

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?

CLUSTER ANALYSIS 11

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.

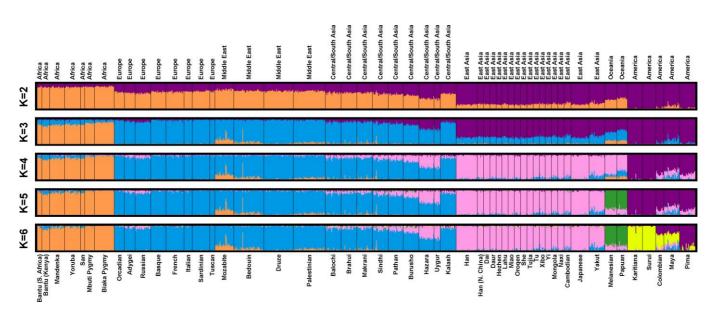
Clustering provides a layer of abstraction from individual data points.

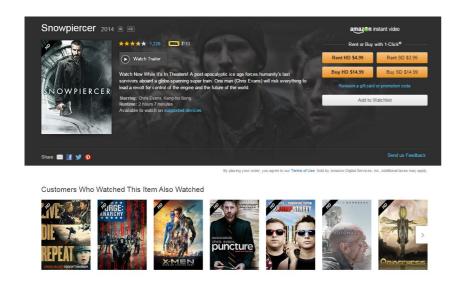
Q: What is the purpose of cluster analysis?

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





Google		→ Q +Josiah III 🗘 🛨 🕻	
News	U.S. edition • Modern •	*	
Top Stories	Top Stories	»  Get Google News on the go.	×
San Francisco Giants Tim Cook International Space Station LeBron James Ukraine	FBI Most-Wanted Fugitive Eric Frein Captured / ABC News -21 minutes ago	Try the free app for your phone or tablet.  It it is, was  GET IT ON  GOOGLE Play  App Store	
Thomas Menino Facebook	reatime coverage  In Depth: Áccused Pa. cop killer Eric Frein captured USATODAY Related Pennsylvania State Police » Police » Pennsylvania »	Personalize Google News	
Halloween Taylor Swift	ABC7 News - SF Bay Area	World	
Burkina Faso	ABC/ News - Sr Bay Area 4 hours ago - Google+	U.S.	+
Arlington, Virginia	CAPTURED! Pennsylvania State Police have captured a man accus ambushing two troopers. Jeaving one dead and another seriously inju-		+
Vorld	Frein was on the run for 48 days. READ MORE ABOUT THE A	Technology -	+
J.S.		Entertainment	
Business		> Sports -	+
echnology	CAIN CAIN CAIN East Vale S	Science -	+
ntertainment	Attacks on Islamic State may help Assad admits Chu	Daniel Daniel	+
Sports	Hagel	Add any news topic +	
Science	PENTAGON Chief Chuck Hagel has acknowledged that US-led air s against the Islamic State group could help President Bashar al-Assad		
Health	Trending on Google+: Foreign jihadists flocking to Irag and Syria on	Adjust Sources	
Spotlight see realtime coverage	restrine 'unprecedented scale' - UN The Guardian	Adjust the frequency of any news source	
	Opinion: Hagel Worried About Syria Plan Daily Beast In Depth: Few Arrests of Americans Who Fought In Syria or Iraq, as on Small ARC Mease	s Feds Focus New York Times	+

CLUSTER ANALYSIS 17



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

There are many kinds of classification 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

#### **K-MEANS CLUSTERING**

Q: How does the algorithm work?

- 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

#### STEP 1 — CHOOSING INITIAL CENTROIDS

Q: How do you choose the initial centroid positions?

#### STEP 1 — CHOOSING INITIAL CENTROIDS

Q: How do you choose the initial centroid positions?

A: There are several options:

#### STEP 1 — CHOOSING INITIAL CENTROIDS

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)

#### STEP 2 – ASSESS SIMILARITY

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**:

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

#### STEP 3 — RECOMPUTING THE CENTER

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)

#### **STEP 4 – CONVERGENCE**

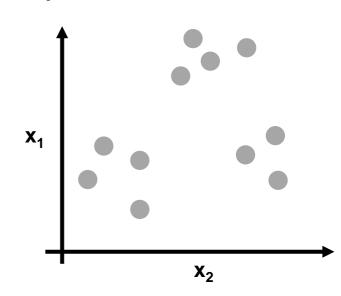
We iterate until some stopping criteria are met; in general, suitable convergence is achieved in a small number of steps.

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  $\varepsilon$ ) or on the points (eg, if no more than x% change clusters between iterations).

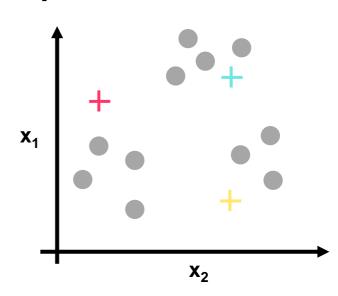
- 2) for each point:
  - find distance to each centroid
  - assign point to nearest centroid

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



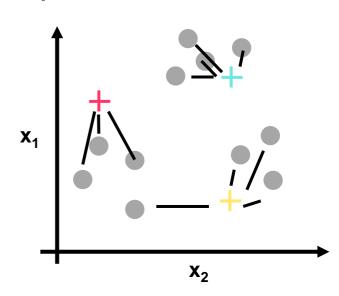
- 2) for each point:
  - find distance to each centroid
  - assign point to nearest centroid

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



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

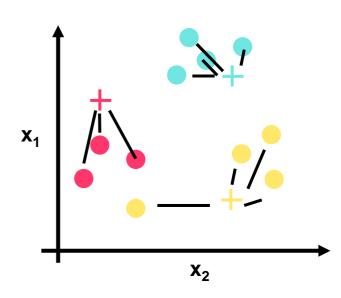
- 3) recalculate centroid positions
- 4) repeat steps 2-3 until stopping criteria met



## 2) for each point:

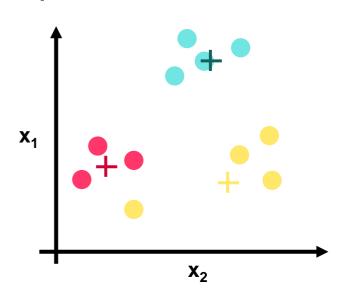
- find distance to each centroid
- assign point to nearest centroid

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



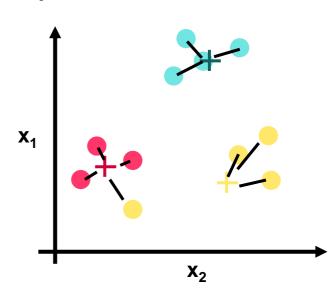
- 2) for each point:
  - find distance to each centroid
  - assign point to nearest centroid

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



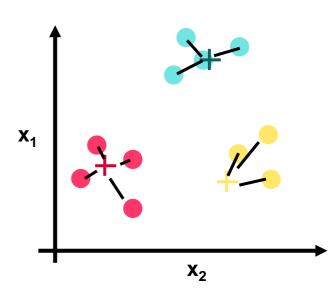
- 2) for each point:
  - find distance to each centroid
  - assign point to nearest centroid

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



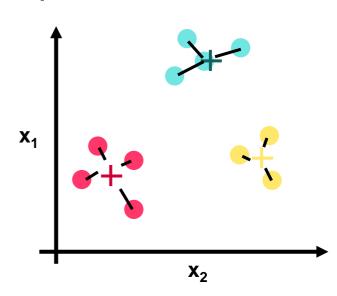
- 2) for each point:
  - find distance to each centroid
  - assign point to nearest centroid

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



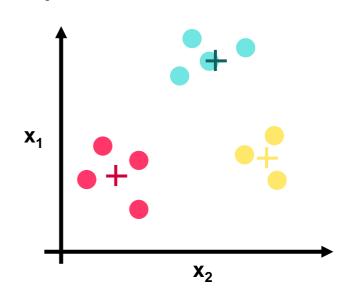
- 2) for each point:
  - find distance to each centroid
  - assign point to nearest centroid

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



- 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.

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

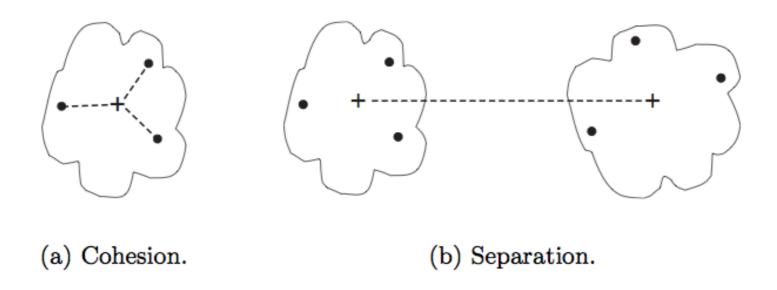


Figure 8.28. Prototype-based view of cluster cohesion and separation.

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

$$SC_i = \frac{b_i - a_i}{max(a_i, b_i)}$$

such that:

 $a_i$  = average in-cluster distance to  $x_i$   $b_{ij}$  = average between-cluster distance to  $x_i$  $b_i$  =  $min_i(b_{ij})$  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 the cluster  $C_i$  is given by the average silhouette coefficient across all points in  $C_i$ :

$$SC(C_i) = \frac{1}{m_i} \sum_{x \in C_i} SC_i$$

The silhouette coefficient for the cluster  $C_i$  is given by the average silhouette coefficient across all points in  $C_i$ :

$$SC(C_i) = \frac{1}{m_i} \sum_{x \in C_i} SC_i$$

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

$$SC_{total} = \frac{1}{k} \sum_{i=1}^{k} SC(C_i)$$

The silhouette coefficient for the cluster  $C_i$  is given by the average silhouette coefficient across all points in  $C_i$ :

$$SC(C_i) = \frac{1}{m_i} \sum_{x \in C_i} SC_i$$

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

$$SC_{total} = \frac{1}{k} \sum_{1}^{k} SC(C_i)$$

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 SSE or SC for different values of k.

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 is not suitable for data with widely varying shapes and densities.

# EX: K-MEANS CLUSTERING