# Machine Learning in Python: Clustering

Dr. Ilkay Altintas

- Articulate the goal of cluster analysis
- Discuss whether cluster analysis is supervised or unsupervised
- List some ways that cluster results can be applied

## Cluster Analysis Overview

Goal: Organize similar items into groups

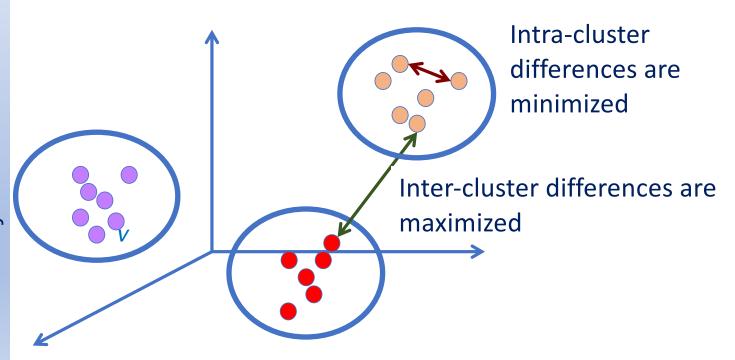


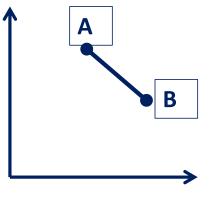
#### Cluster Analysis Examples

- Segment customer base into groups
- Characterize different weather patterns for a region
- Group news articles into topics
- Discover crime hot spots

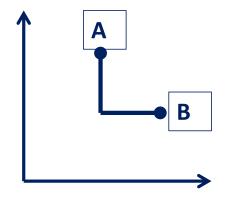
### Cluster Analysis

- Divides data into clusters
- Similar items are placed in same cluster

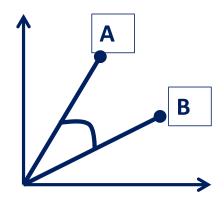




**Euclidean Distance** 



Manhattan Distance

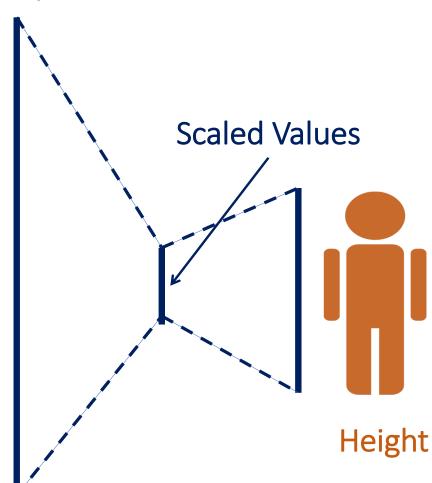


**Cosine Similarity** 

#### Normalizing Input Variables



Weight



#### Cluster Analysis Notes

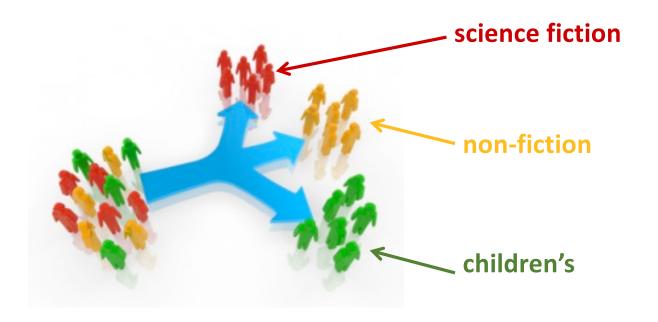
Unsupervised

There is no 'correct' clustering

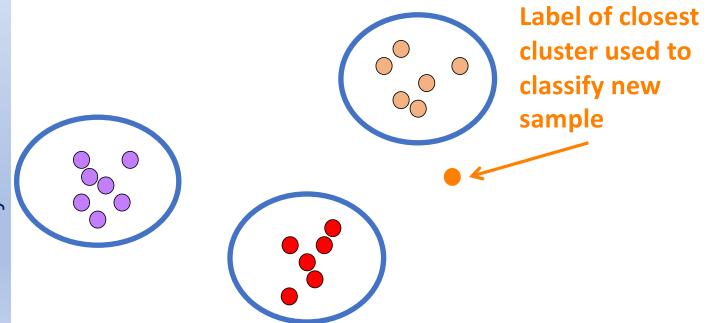
Clusters don't come with labels

Interpretation and analysis required to make sense of clustering results!

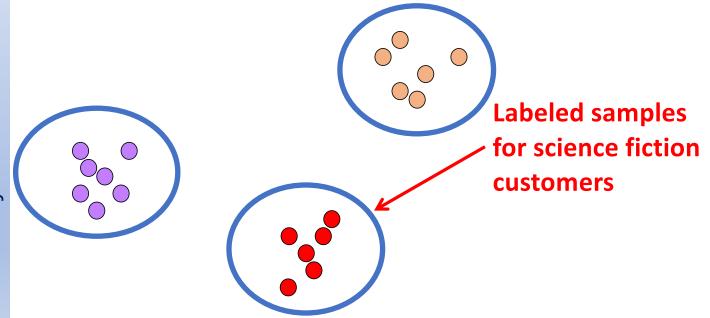
- Data segmentation
  - Analysis of each segment can provide insights



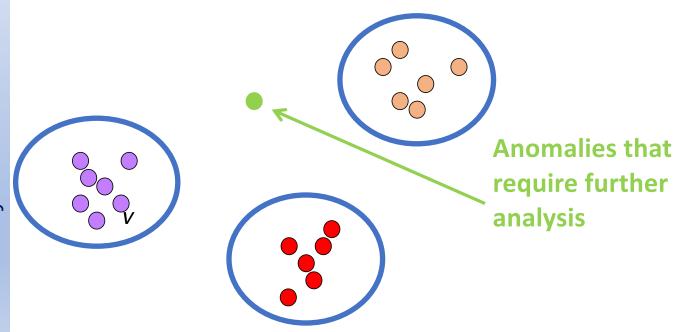
- Categories for classifying new data
  - New sample assigned to closest cluster



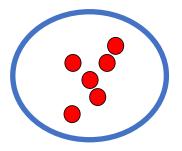
- Labeled data for classification
  - Cluster samples used as labeled data



- Basis for anomaly detection
  - Cluster outliers are anomalies



- Organize similar items into groups
- Analyzing clusters often leads to useful insights about data
- Clusters require analysis and interpretation

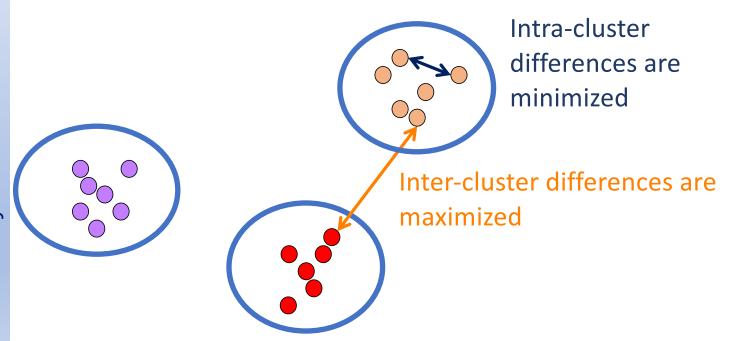


# Machine Learning in Python: k-Means Clustering

- Describe the steps in the k-means algorithm
- Explain what the 'k' stands for in k-means
- Define cluster centroid

# Cluster Analysis

- Divides data into clusters
- Similar items are in same cluster



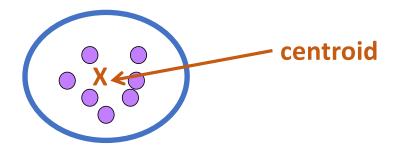
#### k-Means Algorithm

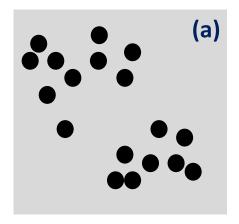
Select k initial centroids (cluster centers) Repeat

Assign each sample to closest centroid

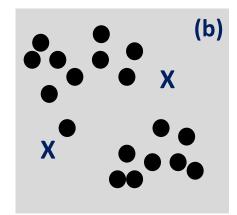
Calculate mean of cluster to determine new centroid

Until some stopping criterion is reached

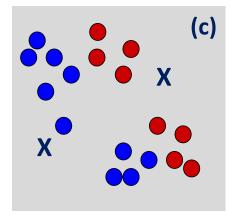




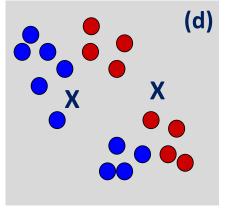
Original samples



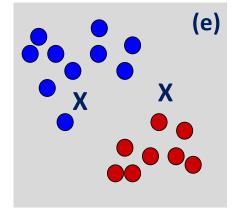
Initial centroids



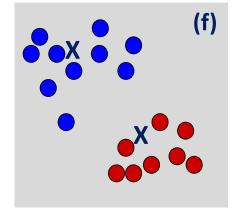
Assign samples



Re-calculate centroids



Assign samples



Re-calculate centroids

### Choosing Initial Centroids

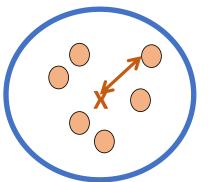
#### Issue:

Final clusters are sensitive to initial centroids

#### **Solution:**

Run k-means multiple times with different random initial centroids, and choose best results

# **Evaluating Cluster Results**



error = distance between sample & centroid

squared error = error<sup>2</sup>

Sum of squared errors between all samples & centroid

Sum over all clusters



**WSSE** 

Within-Cluster Sum of Squared Error

#### Using WSSE

WSSE<sub>1</sub> < WSSE<sub>2</sub>



WSSE1 is better numerically

#### Caveats:

- Does not mean that cluster set 1 is more 'correct' than cluster set 2
- Larger values for k will always reduce **WSSE**

# Choosing Value for k

• Approaches:

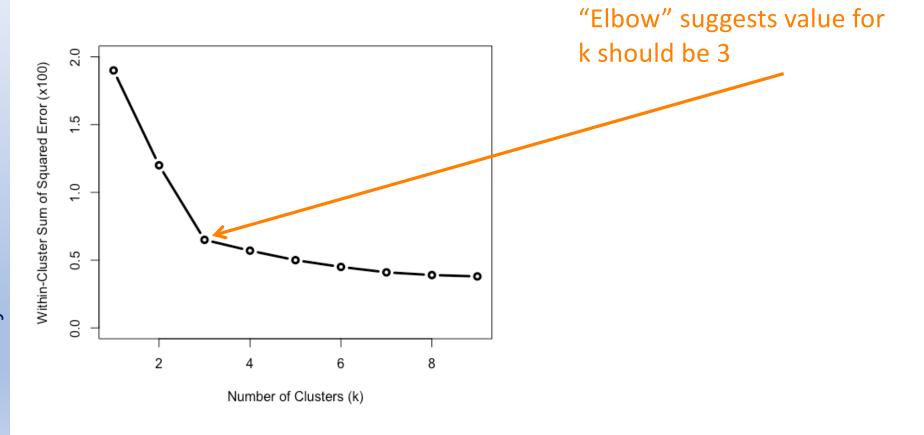


Visualization

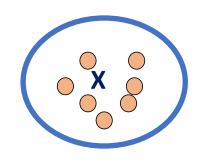
Application-Dependent

• Data-Driven

# Elbow Method for Choosing k



## **Stopping Criteria**

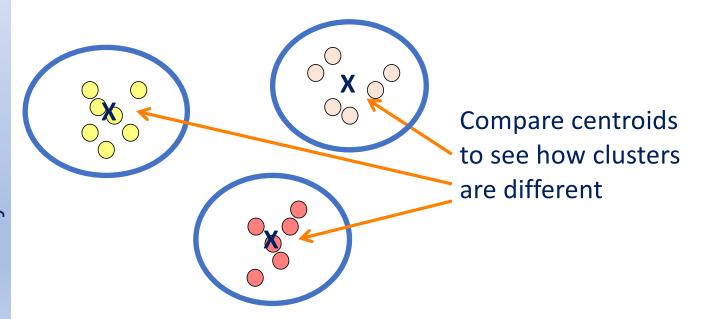


#### When to stop iterating?

- No changes to centroids
- Number of samples changing clusters is below threshold

## Interpreting Results

- Examine cluster centroids
  - How are clusters different?



### K-Means Summary

- Classic algorithm for cluster analysis
- Simple to understand and implement and is efficient
- Value of k must be specified
- Final clusters are sensitive to initial centroids

