Machine Learning - Clustering

CS102 Spring 2020

Data Tools and Techniques

- Basic Data Manipulation and Analysis
 Performing well-defined computations or asking well-defined questions ("queries")
- Data Mining
 Looking for patterns in data
- Machine Learning
 Using data to build models and make predictions
- Data Visualization
 Graphical depiction of data
- Data Collection and Preparation

Machine Learning

Using data to build models and make predictions

Supervised machine learning

- Set of labeled examples to learn from: training data
- Develop model from training data
- Use model to make predictions about new data

Unsupervised machine learning

 Unlabeled data, look for patterns or structure (similar to data mining)

Like classification, data items consist of values for a set of features (numeric or categorical)

Medical patients
 Feature values: age, gender, symptom1-severity, symptom2-severity, test-result1, test-result2

Web pages
 Feature values: URL domain, length, #images, heading₁, heading₂, ..., heading_n

Products
 Feature values: category, name, size, weight, price

Like classification, data items consist of values for a set of features (numeric or categorical)

- Medical patients
 Feature values: age, g
 symptom2-severity, test-result; test-resultz
 Unlike classification,
 there is no label
 result; test-resultz
- Web pages
 Feature values: URL domain, length, #images, heading₁, heading₂, ..., heading_n
- Products
 Feature values: category, name, size, weight, price

Like K-nearest neighbors, for any pair of data items i_1 and i_2 , from their feature values can compute distance function: $distance(i_1,i_2)$

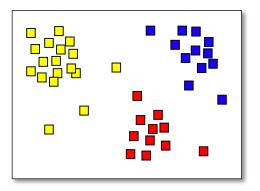
Example:

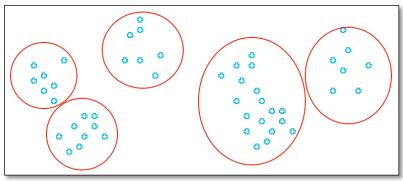
```
Features - gender, profession, age, income, postal-code
person<sub>1</sub> = (male, teacher, 47, $25K, 94305)
person<sub>2</sub> = (female, teacher, 43, $28K, 94309)
distance(person<sub>1</sub>, person<sub>2</sub>)
```

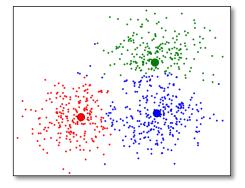
distance() can be defined as inverse of similarity()

GOAL: Given a set of data items, partition them into groups (= clusters) so that items within groups are close to each other based on distance function

- Sometimes number of clusters is pre-specified
- > Typically clusters need not be same size

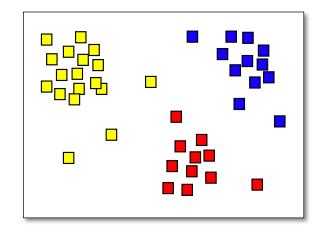






Some Uses for Clustering

- Classification!
 - Assign labels to clusters
 - Now have labeled training data for future classification



- Identify similar items
 - For substitutes or recommendations
 - For de-duplication
- Anomaly (outlier) detection
 - Items that are far from any cluster

K-Means Clustering

Reminder: for any pair of data items i_1 and i_2 have $distance(i_1,i_2)$

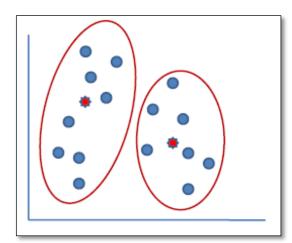
For a group of items, the mean value (centroid) of the group is the item *i* (in the group or not) that minimizes the sum of *distance(i,i')* for all *i'* in the group

K-Means Clustering

For a group of items, the mean value (centroid) of the group is the item *i* (in the group or not) that minimizes the sum of *distance(i,i')* for all *i'* in the group

- Error for each item: distance d from the mean for its group; squared error is d²
- Error for the entire clustering: sum of squared errors (SSE)

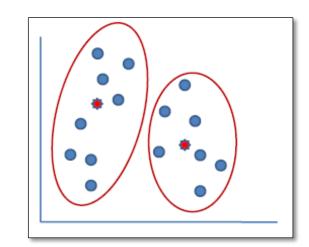
Remind you of anything?



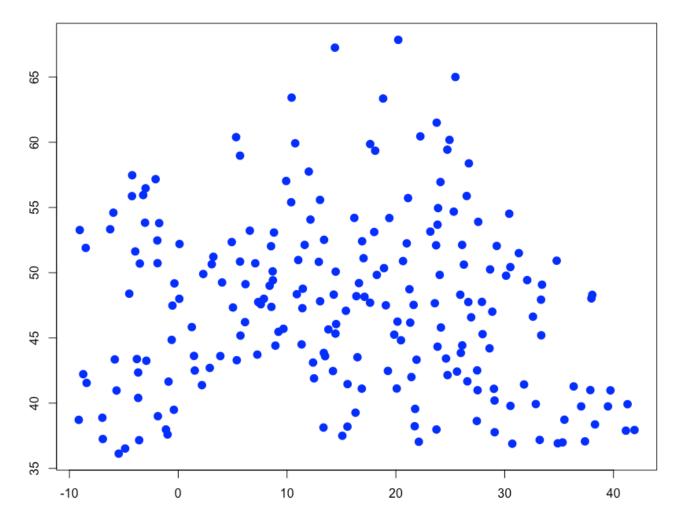
K-Means Clustering

Given set of data items and desired number of clusters k, K-means groups the items into k clusters minimizing the SSE

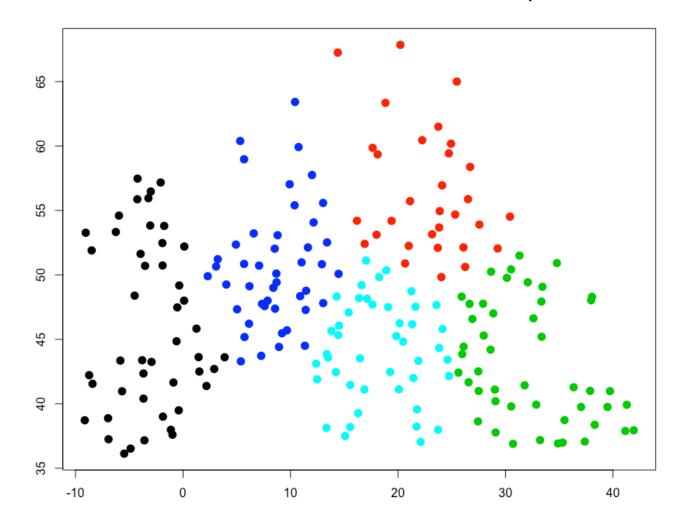
- Extremely difficult to compute efficiently
 - ➤ In fact, impossible
- Most algorithms compute an approximate solution (might not be absolute lowest SSE)



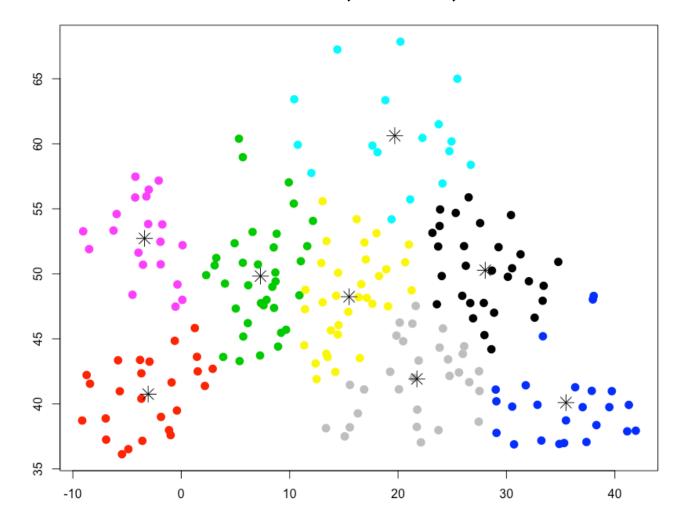
By geographic distance, then by temperature



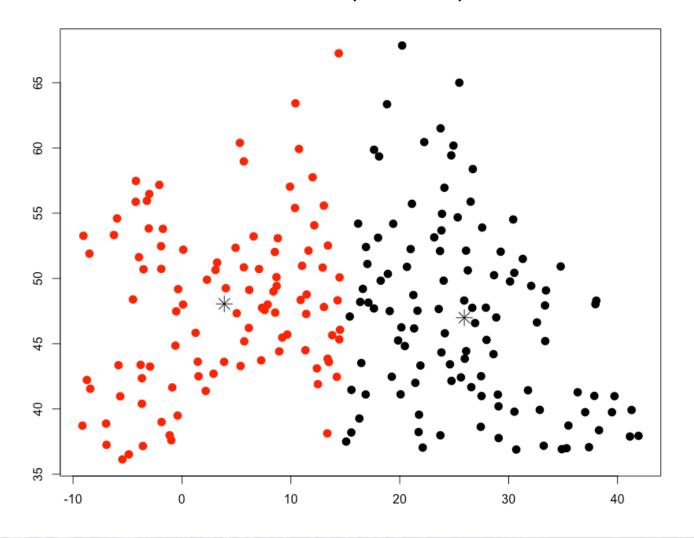
Distance = actual distance, k = 5



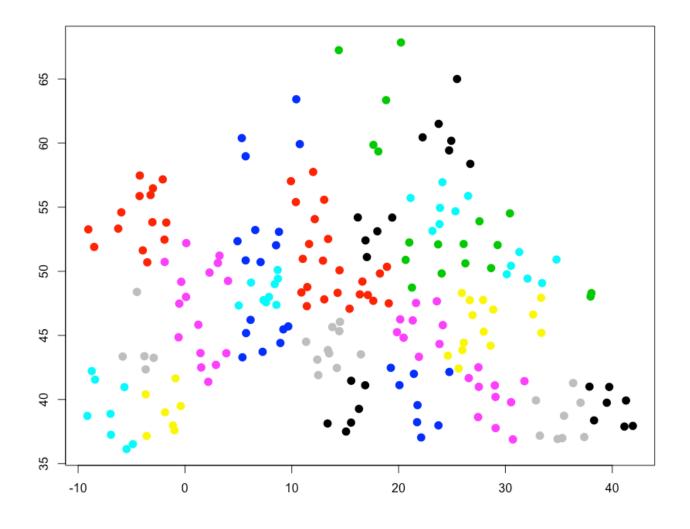
Distance = actual distance, k = 8, with cluster means



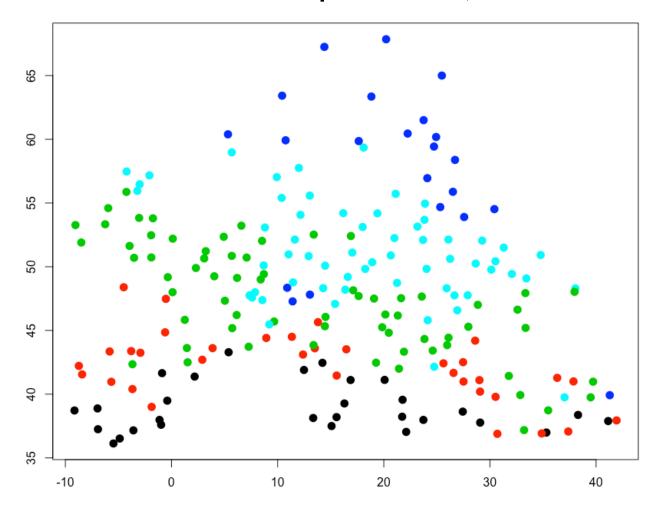
Distance = actual distance, k = 2, with cluster means



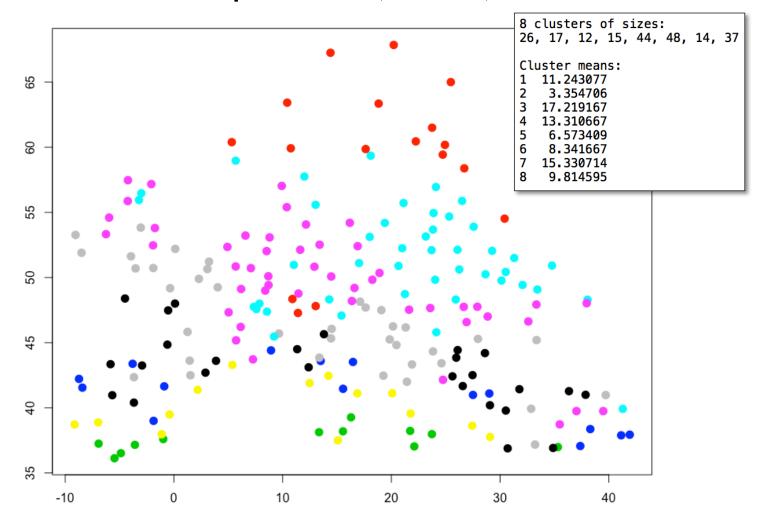
Distance = actual distance, k = 30



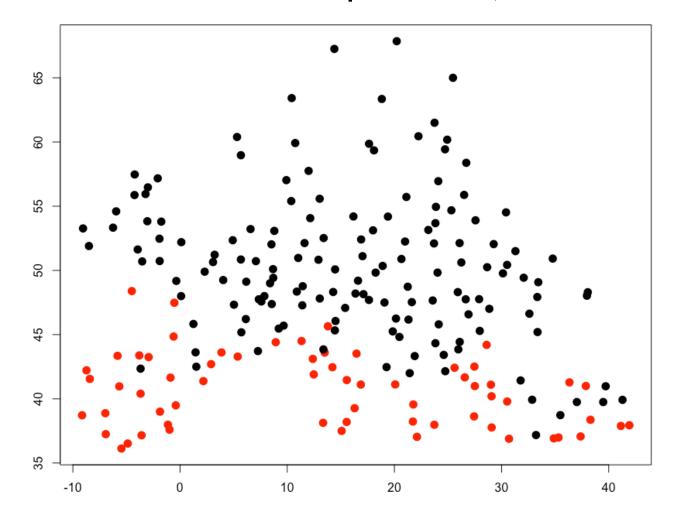
Distance = temperature, k = 5



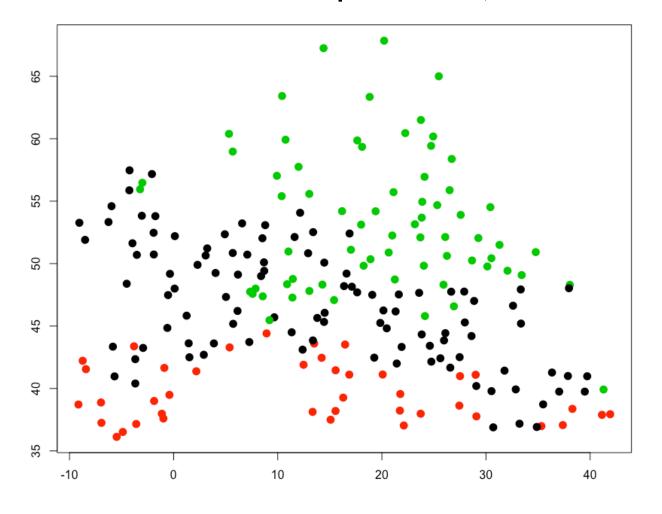
Distance = temperature, k = 8, with means



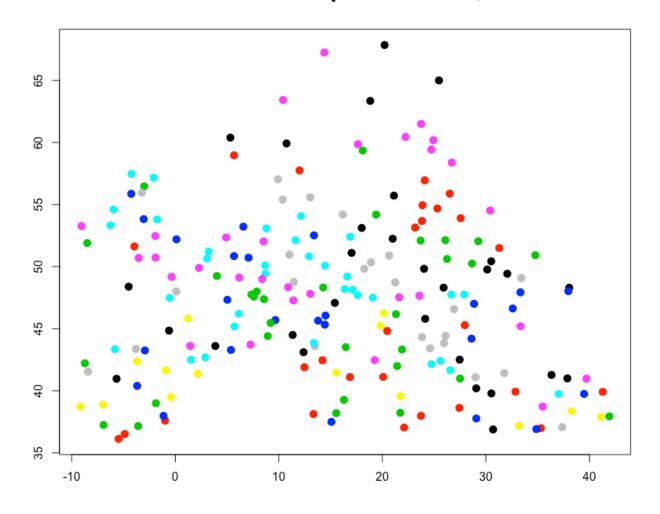
Distance = temperature, k = 2



Distance = temperature, k = 3



Distance = temperature, k = 30



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