Machine Learning, STOR 565

Clustering: Overview and Basic Methods

Andrew Nobel

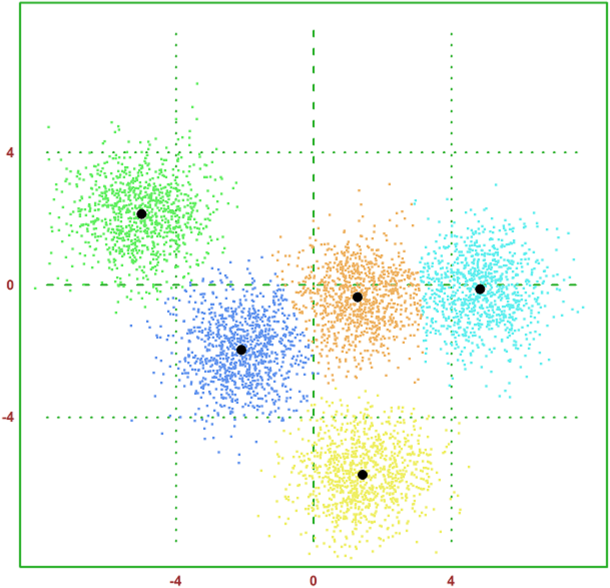
January, 2020

Overview of Clustering

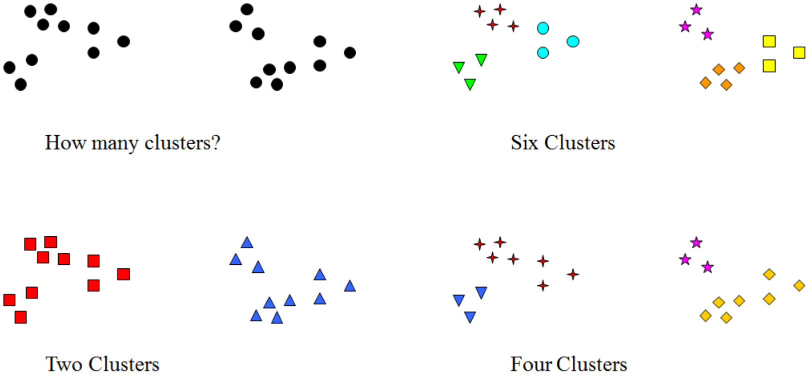
a. The basic problem

b. Some clustering schemes

Example (http://rosettacode.org)



Example (https://apandre.files.wordpress.com)



How many clusters?

Six Clusters

Two Clusters

Four Clusters

General Setting

Given

- Objects $x_1, \dots, x_n$ in feature space $\mathcal{X}$
- Dissimilarity/distance $d(x_i, x_j)$ between objects

Goal: Find division $\pi = \{C_1, \dots, C_k\}$ of objects into a small number of disjoint groups, called *clusters*, such that

- Objects in same cluster are close together
- Objects in different clusters are far apart

Terminology: π is *complete* if it partitions $\mathcal{X}$ and *incomplete* if it partitions only $x_1, \dots, x_n$.

Clustering identifies group structure in unlabeled objects. Special case of

- exploratory data analysis
- unsupervised learning

Note: In *supervised learning* we have samples $(X_1, Y_1), \ldots (X_n, Y_n)$, with $X \in \mathcal{X}$ and $Y_i \in \{-1, +1\}$ or $\mathbb{R}$ and the goal is to predict Y from X.

- classification
- regression

Clustering: Areas of Application

Genomics, Biology

Data Compression

Psychology

Computer Science

Social and Political Science

Feature Vectors

Objects $\mathbf{x} \in \mathcal{X}$ typically represented by a *feature vector*

$$\mathbf{x} = (x_1, \ldots, x_p)$$

where x_i is a numerical/categorical measurement of interest:

- $x_i \in \mathbb{R}$ numerical feature
- $x_i \in \{a, b, \ldots\}$ categorical feature

Examples

Medicine

- Object $=$ patient
- Feature $x_i =$ outcome of a diagnostic test on patient

Microarrays (Genomics)

- Object $=$ tissue sample
- Feature $x_i =$ measured expression level of gene i in that sample

Data Mining

- Object $=$ consumer
- Features $x_i =$ type, location, or amount of recent purchases

Dissimilarities/Distances Between Feature Vectors

Euclidean $d(\mathbf{u}, \mathbf{v}) = \sqrt{\sum_i (u_i - v_i)^2}$

Manhattan $d(\mathbf{u}, \mathbf{v}) = \sum_i |u_i - v_i|$

Correlation $d(\mathbf{u}, \mathbf{v}) = 1 - \text{corr}(u, v)$

Hamming $d(\mathbf{u}, \mathbf{v}) = \sum_i I\{u_i \neq v_i\}$

Mixtures of these

Basic Steps in Clustering

Acquisition of Objects $\mathbf{x}_1, \dots, \mathbf{x}_n$

$$\Downarrow$$

Selection and Extraction of Features

$$\Downarrow$$

Dissimilarity matrix $D = \{d(\mathbf{x}_i, \mathbf{x}_j) : 1 \leq i, j \leq n\}$

$$\Downarrow$$

Clustering Algorithm

$$\Downarrow$$

Partition $\pi = \{C_1, \dots, C_k\}$ of $\mathbf{x}_1, \dots, \mathbf{x}_n$.

Some Clustering Methods

Hierarchical: Candidate divisions of data described by a binary tree

- Agglomerative (bottom-up)
- Divisive (top-down)

Iterative: Search for local minimum of simple cost function

- k-means and variants
- partitioning around medioids, self organizing maps

Model-based: Fit feature vectors with a finite mixture model

Spectral: Threshold eigenvectors of Laplacian of Dissimilarity Matrix

Centroids

Definition: The centroid of vectors $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^p$ is their average

$$\mathbf{c} \;=\; \frac{1}{n}\sum_{i=1}^{n} \mathbf{x}_i$$

The centroid $\mathbf{c}$ is the center of mass of the point configuration $\mathbf{x}_1, \ldots, \mathbf{x}_n$, and is an optimal representative for the configuration in the sense that

$$\sum_{i=1}^{n} ||\mathbf{x}_i - \mathbf{c}||^2 \;\leq\; \sum_{i=1}^{n} ||\mathbf{x}_i - \mathbf{v}||^2$$

for every vector $\mathbf{v} \in \mathbb{R}^p$.

Nearest Neighbor Partitions

Definition: The Voronoi (nearest neighbor) partition of points $\mathbf{c}_1, \ldots, \mathbf{c}_k \in \mathbb{R}^p$ is a collection $\pi = \{A_1, \ldots, A_k\}$ where the cell

$$A_j = \{\mathbf{x} : ||\mathbf{x} - \mathbf{c}_j|| \leq ||\mathbf{x} - \mathbf{c}_s|| \text{ all } s \neq j\}$$

contains vectors that are as close or closer to $\mathbf{c}_j$ than any other $\mathbf{c}_s$.

Structure of Cells: Note that

$$A_j = \bigcap_{s \neq j} \{\mathbf{x} : ||\mathbf{x} - \mathbf{c}_j|| \leq ||\mathbf{x} - \mathbf{c}_s||\}$$

is an intersection of half-spaces. Thus it is a *polytope* in $\mathbb{R}^p$ with at most $n - 1$ faces.

The k-Means Algorithm

Clustering Problem: Divide $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^p$ into k clusters.

Optimization: Find centers $\mathbf{c}_1, \ldots, \mathbf{c}_k$ to minimize sum of squares (SoS) cost function

$$\text{Cost}(\mathbf{c}_1, \ldots, \mathbf{c}_k) \ = \ \sum_{i=1}^{n} \min_{1 \leq j \leq k} ||\mathbf{x}_i - \mathbf{c}_j||^2$$

i.e., sum of squared distances from each point to its nearest center. Then the clusters are the Voronoi partition of $\mathbf{x}_1, \ldots, \mathbf{x}_n$ with centers $\mathbf{c}_1, \ldots, \mathbf{c}_k$

Problem: Solution of optimization problem is not computationally feasible. Resort to iterative methods that find local optima of SoS cost.

The k-Means Algorithm

Fix in advance

- Number of clusters k
- Initial centers $\mathcal{C}_0 = \{\mathbf{c}_1, \ldots, \mathbf{c}_k\}$

Iterate: For $m = 1, 2, \ldots$ do:

- Let π_m be the nearest neighbor (Voronoi) partition of the centers $\mathcal{C}_{m-1}$.
- Let $\mathcal{C}_m$ be the centroids (averages) of the vectors in each cell of π_m

Stop: When Cost$(\mathcal{C}_m)$ is close to Cost$(\mathcal{C}_{m+1})$

The k-Means Algorithm

Recall: Sum of Squares (SoS) cost function

$$\text{Cost}(\mathbf{c}_1, \ldots, \mathbf{c}_k) \; = \; \sum_{i=1}^{n} \min_{1 \leq j \leq k} ||\mathbf{x}_i - \mathbf{c}_j||^2$$

Note: Cost function decreases at each stage of the k-means algorithm.

In practice

- Choose multiple initial sets of representative vectors $\mathcal{C}_0 = \{c_1, \ldots, c_k\}$
- Run the iterative k-means procedure
- Choose the partition associated with the smallest final cost

Example: `http://www.onmyphd.com/?p=k-means.clustering`.

Features of Clusters

If clusters are present, their features can affect performance of different clustering procedures.

- Spherical or elliptical in shape
- Similar in overall variance/spread
- Similar in size (number of points)

K-Means tends to perform best when clusters are spherical, similar in variance and size

Binary Trees

1. Distinguished node called the **root** with zero or two children but no parent

2. Every other node has one parent and zero or two children

   - Nodes with no children are called **leaves**

   - Nodes with two children are called **internal**

Note: Tree usually drawn upside-down, with root node at the top

Agglomerative Clustering

Stage 0: Assign each object x_i to its own cluster

Stage k:

- Find the two *closest* clusters at stage $k-1$
- Combine them into a single cluster

Stop: When all objects x_i belong to a single cluster

Output: Binary tree T called a *dendrogram*

Note: Closeness of clusters C, C' can be measured in different ways

Distances Between Clusters

Single Linkage

$$d_s(C, C') \;=\; \min_{x_i \in C,\; x_j \in C'} d(x_i, x_j)$$

Average Linkage

$$d_a(C, C') \;=\; \frac{1}{|C|\,|C'|} \sum_{x_i \in C,\; x_j \in C'} d(x_i, x_j)$$

Total Linkage

$$d_t(C, C') \;=\; \max_{x_i \in C,\; x_j \in C'} d(x_i, x_j)$$

Dendrogram

Binary tree associated with the agglomerative clustering procedure: it is a graphical record of the clustering process

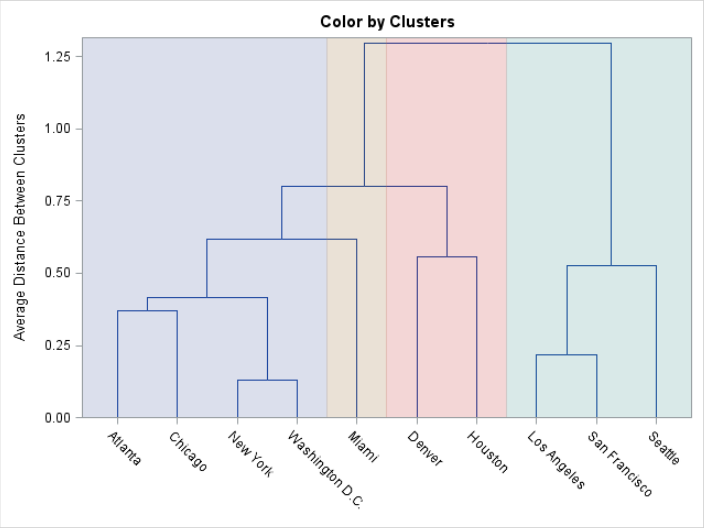
Initialize: Each singleton cluster $\{x_i\}$ corresponds to a node at height 0

Update: If two clusters C, C' are combined, their respective nodes are joined to a parent node at height $d(C, C')$

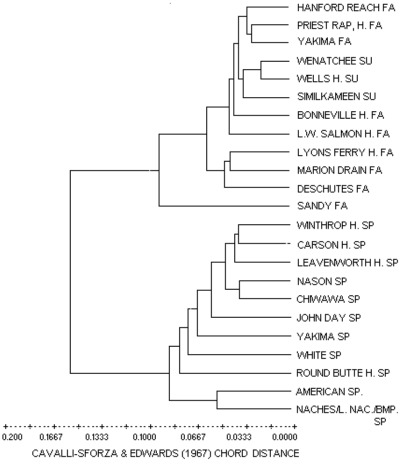
Each node of dendrogram corresponds to a set of objects. Objects associated with two nodes are merged when forming their parent.

- Leaves correspond to individual objects
- The root corresponds to all objects

Cities by Distance (blogs.sas.com)



Salmon by Genetic Similarity



Dendrogram, cont.

Note: Dendrogram T represents many possible clusterings, one for each (rooted) subtree.

Methods for selecting a clustering/subtree

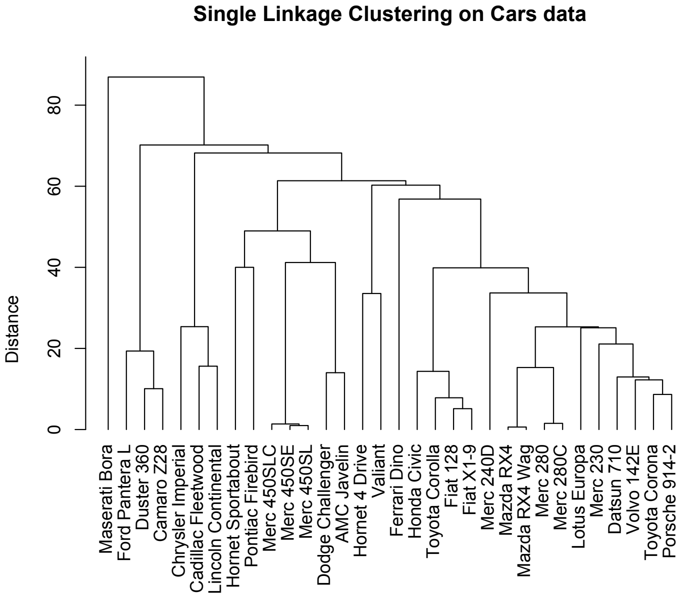
- Ad hoc selection (by eye)
- “Cutting” dendrogram at fixed level
- Penalized pruning

Visualization of clustering structure

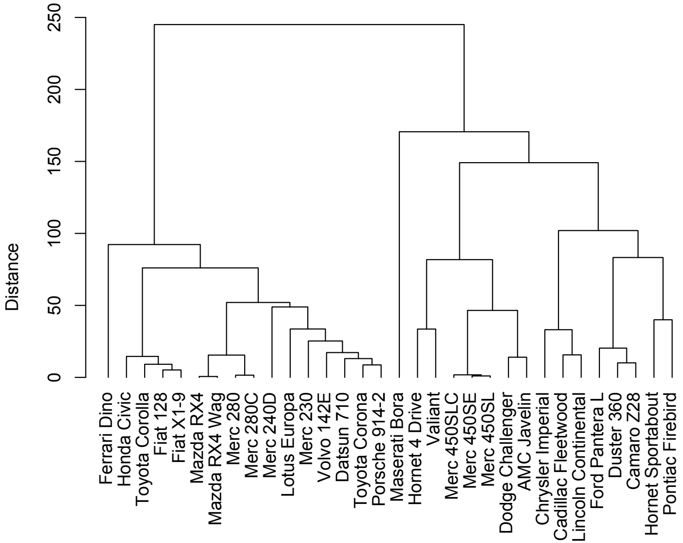
- Order objects in the same way as the leaves of the dendrogram
- Caveat: many orderings possible

Cars Data

- **Samples**: 32 unique cars
- **Variables**: 11 descriptive variables, including gas mileage, horsepower, number of cylinders, etc.
- Freely available in **R**: *data(mtcars)*


Single Linkage Clustering on Cars data
Distance
0
20
40
60
80
Maserati Bora
Ford Pantera L
Duster 360
Camaro Z28
Chrysler Imperial
Cadillac Fleetwood
Lincoln Continental
Hornet Sportabout
Pontiac Firebird
Merc 450SLC
Merc 450SE
Merc 450SL
Dodge Challenger
AMC Javelin
Hornet 4 Drive
Valiant
Ferrari Dino
Honda Civic
Toyota Corolla
Fiat 128
Fiat X1-9
Merc 240D
Mazda RX4
Mazda RX4 Wag
Merc 280
Merc 280C
Lotus Europa
Merc 230
Datsun 710
Volvo 142E
Toyota Corona
Porsche 914-2

Average Linkage Clustering on Cars data

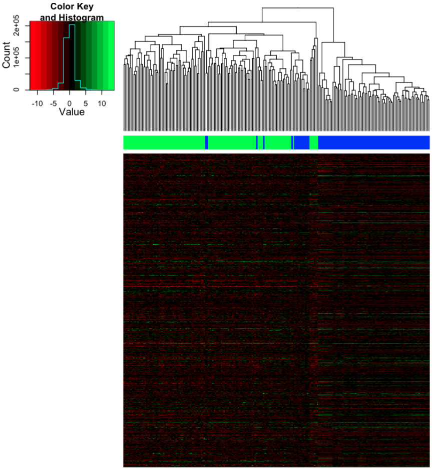


TCGA Data

Gene expression data from The Cancer Genome Atlas (TCGA)

- **Samples**
  - 95 Luminal A breast tumors
  - 122 Basal breast tumors
- **Variables**: 2000 randomly selected genes

TCGA Data



- Clustered samples (breast tumor subtype)
- Colors: Luminal A and Basal

Important Questions

- What is the right number of clusters?
- What is right measure of distance?
- What is the best clustering method for the data?
- How robust is an observed clustering to small perturbations of the data?
- What significance can be assigned to the clusters?