Machine Learning

Clustering

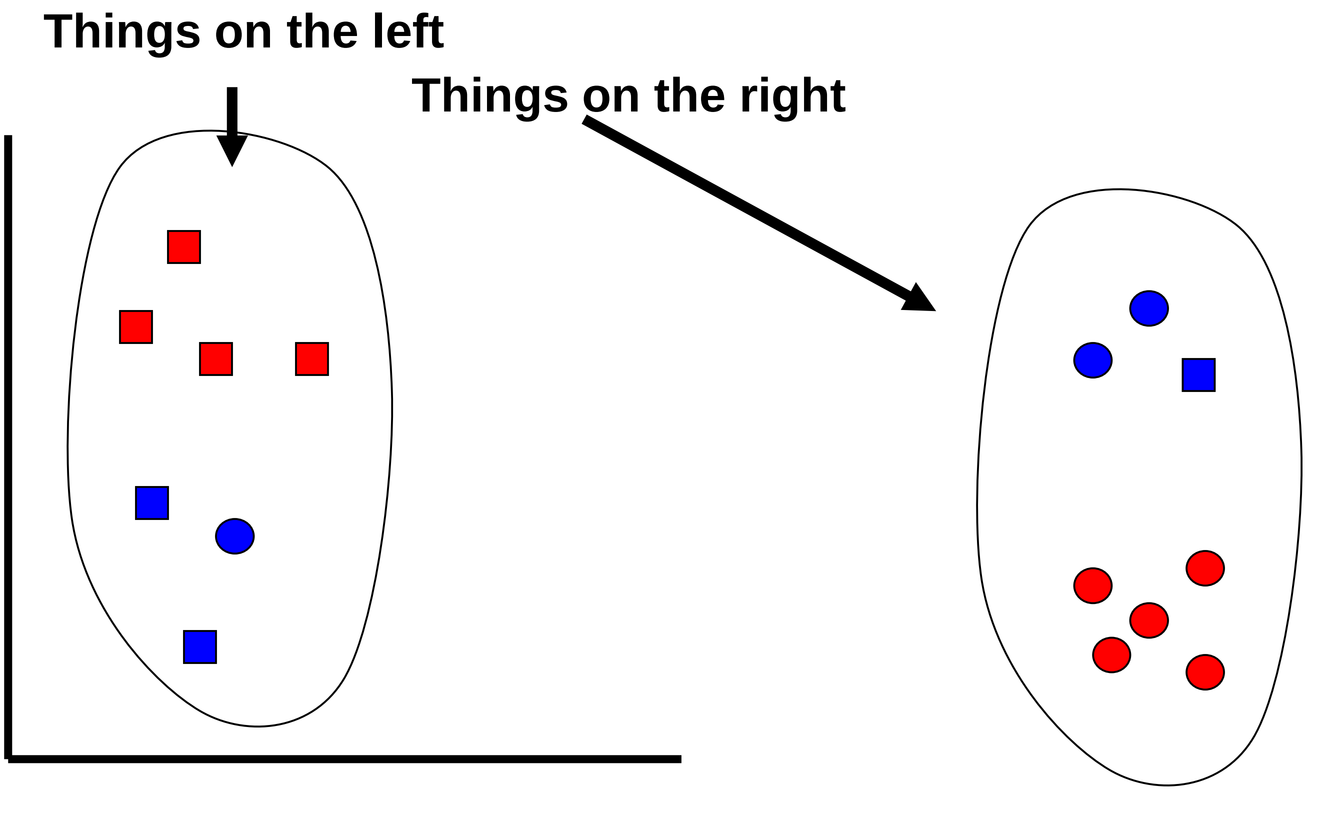
Some slides from B. Pardo, P. Domingos

First, some epistemology

- There are known knowns. These are things we know that we know.
  - Databases!
- There are known unknowns. That is to say, there are things that we know we don't know.
  - Supervised Machine Learning
- But there are also unknown unknowns. There are things we don't know we don't know
  - Unsupervised Machine Learning (Clustering)

Clustering

- Grouping data into (hopefully useful) sets.



Clustering

- Unsupervised Learning
  - No labels
- Why do clustering?
  - Hypothesis Generation/Data Understanding
    - Clusters might suggest natural groups.
  - Visualization
  - Data pre-processing, e.g.:
    - Converting continuous attributes to nominal
    - For *efficiency*

Some definitions

- Let X be the dataset:

$$X = \{x_1, x_2, x_3, \ldots x_n\}$$

- An ***m-clustering*** of X is a partition of X into m sets (clusters) $C_1, \ldots C_m$ such that:

1. Clusters are non-empty: $\quad C_i \neq \{\}, 1 \leq i \leq m$
2. Clusters cover all of X: $\quad \bigcup_{i=1}^{m} C_i = X$
3. Clusters do not overlap: $\quad C_i \cap C_j = \{\}, \text{ if } j \neq i$

How many possible clusterings?
(Stirling numbers)

Size of dataset

$$S(n,m) = \frac{1}{m!}\sum_{i=0}^{m}(-1)^{m-i}\binom{m}{i} i^n$$

Number of clusterings

$$S(15,3) = 2,375,101$$

$$S(20,4) = 45,232,115,901$$

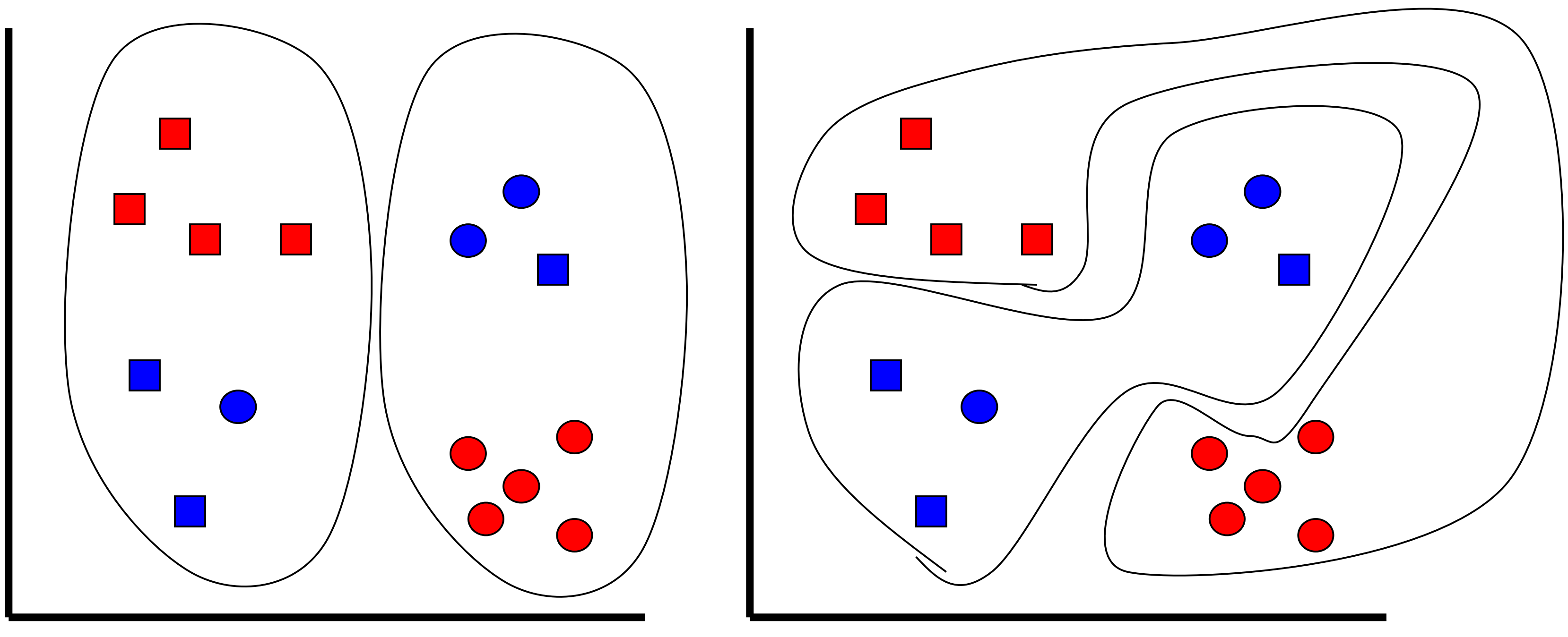
$$S(100,5) \approx 10^{68}$$

What does this mean?

- We can’t try all possible clusterings.
- Clustering algorithms look at a small fraction of all partitions of the data.
- The exact partitions tried depend on the kind of clustering used.

Who is right?

- Different techniques cluster the same data set DIFFERENTLY.
- Who is right? Is there a “right” clustering?



Steps in Clustering

- Select Features
- Define a Proximity Measure
- Choose a Clustering Algorithm
- Validate the Results
- Interpret the Results

Kinds of Clustering

- Sequential
  - Fast
  - Results depend on data order
- Cost Optimization
  - Fixed number of clusters (typically)
  - Probabilistic models
- Hierarchical
  - Start with many clusters
  - join clusters at each step

A Sequential Clustering Method

- Basic Sequential Algorithmic Scheme (BSAS)
  - S. Theodoridis and K. Koutroumbas, Pattern Recognition, Academic Press, London England, 1999
- Assumption: The number of clusters is not known in advance.
- Let:

d(x,C)	be the *distance* between feature vector x and cluster C.
Θ	be the *threshold of dissimilarity*
q	be the *maximum number of clusters*

BSAS Pseudo Code

$m = 1$

$C_1 = \{x_1\}$

For $i = 2$ to n

    Find $C_k : d(x_i, C_k) = \min_{\forall j} d(x_i, C_j)$

    If $(d(x_i, C_k) > \Theta)$ and $(m < q)$

        $m = m + 1$

        $C_m = \{x_i\}$

    Else

        $C_k = C_k \cup \{x_i\}$

    End

End

Where is the cluster, exactly?

$d(x, C)$ = distance from x to C

How to compute?

BSAS Characteristics

Advantages

- Fast! Only examine each data point once (takes O(nq))
- Number of clusters tuned from data

Disadvantages

- Must set q, Θ
- Sensitive to initial conditions

Kinds of Clustering

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  - Often probabilistic models
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A Cost-optimization method

- K-means clustering
  - J. B. MacQueen (1967): "Some Methods for classification and Analysis of Multivariate Observations, *Proceedings of 5-th Berkeley Symposium on Mathematical Statistics and Probability*", Berkeley, University of California Press, 1:281-297
- A greedy algorithm
- Partitions *n* samples into *k* clusters
- minimizes the sum of the squared distances to the cluster centers

The K-means algorithm

- Place K points into the space represented by the objects that are being clustered. These points represent initial group centroids (means).
- Assign each object to the group that has the closest centroid (mean).
- When all objects have been assigned, recalculate the positions of the K centroids (means).
- Repeat Steps 2 and 3 until the centroids no longer move.

K-means clustering

- The way to initialize the mean values is not specified.
  - Randomly choose k samples?
- Results depend on the initial means
  - Try multiple starting points?
- Assumes K is known.
  - How do we choose this?
- Demo:
  - http://shabal.in/visuals/kmeans/1.html

Mixture Models

$$P(x) = \sum_{i=1}^{n_c} P(c_i) P(x|c_i)$$

Objective function: Log likelihood of data

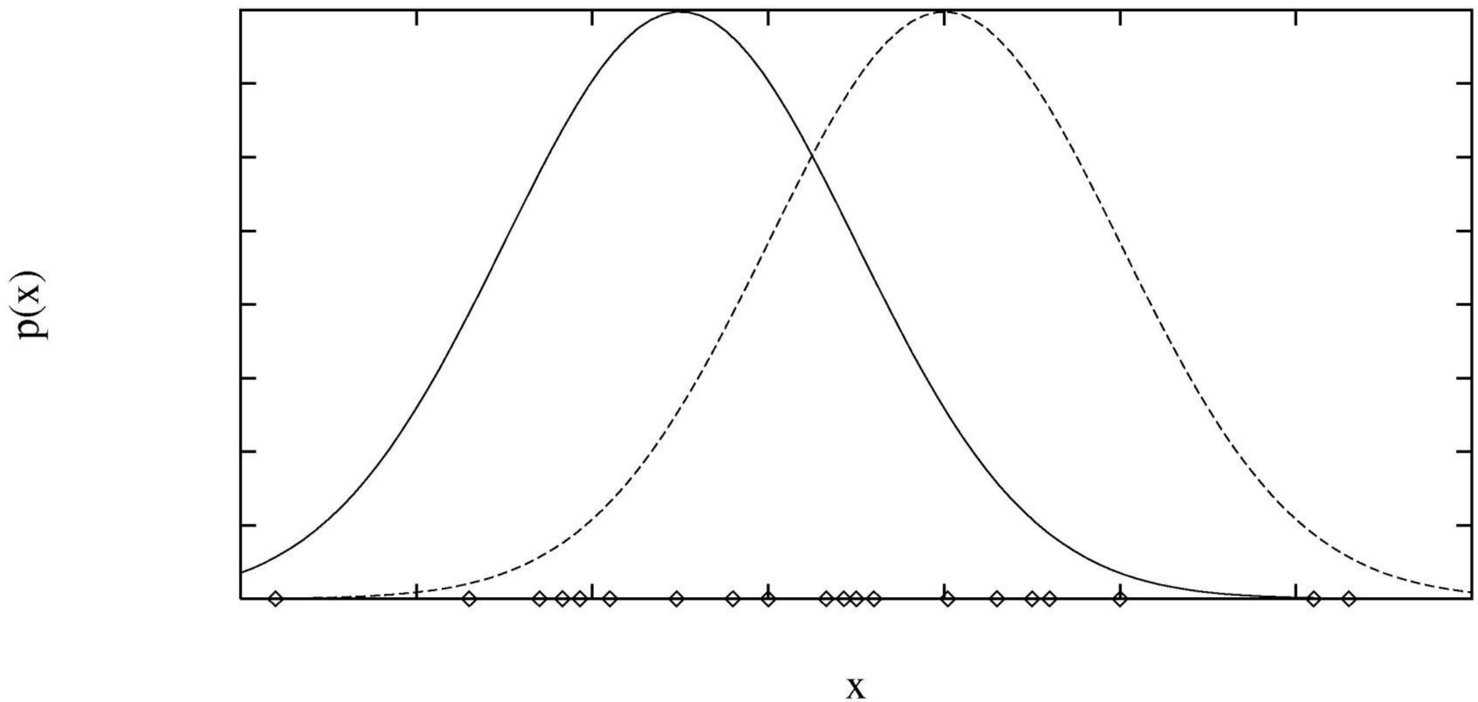
Naive Bayes: $P(x|c_i) = \prod_{j=1}^{n_d} P(x_j|c_i)$

AutoClass: Naive Bayes with various x_j models

Mixture of Gaussians: $P(x|c_i) =$ Multivariate Gaussian

In general: $P(x|c_i)$ can be any distribution

Mixtures of Gaussians



$$P(x|\mu_i) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{1}{2}\left(\frac{x-\mu_i}{\sigma}\right)^2\right]$$

The EM Algorithm

Initialize parameters ignoring missing information

Repeat until convergence:

E step: Compute expected values of unobserved variables, assuming current parameter values

M step: Compute new parameter values to maximize probability of data (observed & estimated)

(Also: Initialize expected values ignoring missing info)

EM for Mixtures of Gaussians

Initialization: Choose means at random, etc.

E step: For all examples x_k:

$$P(\mu_i|x_k) = \frac{P(\mu_i)P(x_k|\mu_i)}{P(x_k)} = \frac{P(\mu_i)P(x_k|\mu_i)}{\sum_{i'} P(\mu_{i'})P(x_k|\mu_{i'})}$$

M step: For all components c_i:

$$\begin{aligned}
P(c_i) &= \frac{1}{n_e}\sum_{k=1}^{n_e} P(\mu_i|x_k) \\
\mu_i &= \frac{\sum_{k=1}^{n_e} x_k \, P(\mu_i|x_k)}{\sum_{k=1}^{n_e} P(\mu_i|x_k)} \\
\sigma_i^2 &= \frac{\sum_{k=1}^{n_e} (x_k - \mu_i)^2 \, P(\mu_i|x_k)}{\sum_{k=1}^{n_e} P(\mu_i|x_k)}
\end{aligned}$$

Mixtures of Gaussians (cont.)

- K-means clustering $\prec$ EM for mixtures of Gaussians
- Mixtures of Gaussians $\prec$ Bayes nets
- Also good for estimating joint distribution of continuous variables

Mixture Models for Documents

- Learn simultaneously P(w | topic), P(topic | doc)

“Arts”	“Budgets”	“Children”	“Education”
NEW	MILLION	CHILDREN	SCHOOL
FILM	TAX	WOMEN	STUDENTS
SHOW	PROGRAM	PEOPLE	SCHOOLS
MUSIC	BUDGET	CHILD	EDUCATION
MOVIE	BILLION	YEARS	TEACHERS
PLAY	FEDERAL	FAMILIES	HIGH
MUSICAL	YEAR	WORK	PUBLIC
BEST	SPENDING	PARENTS	TEACHER
ACTOR	NEW	SAYS	BENNETT
FIRST	STATE	FAMILY	MANIGAT
YORK	PLAN	WELFARE	NAMPHY
OPERA	MONEY	MEN	STATE
THEATER	PROGRAMS	PERCENT	PRESIDENT
ACTRESS	GOVERNMENT	CARE	ELEMENTARY
LOVE	CONGRESS	LIFE	HAITI

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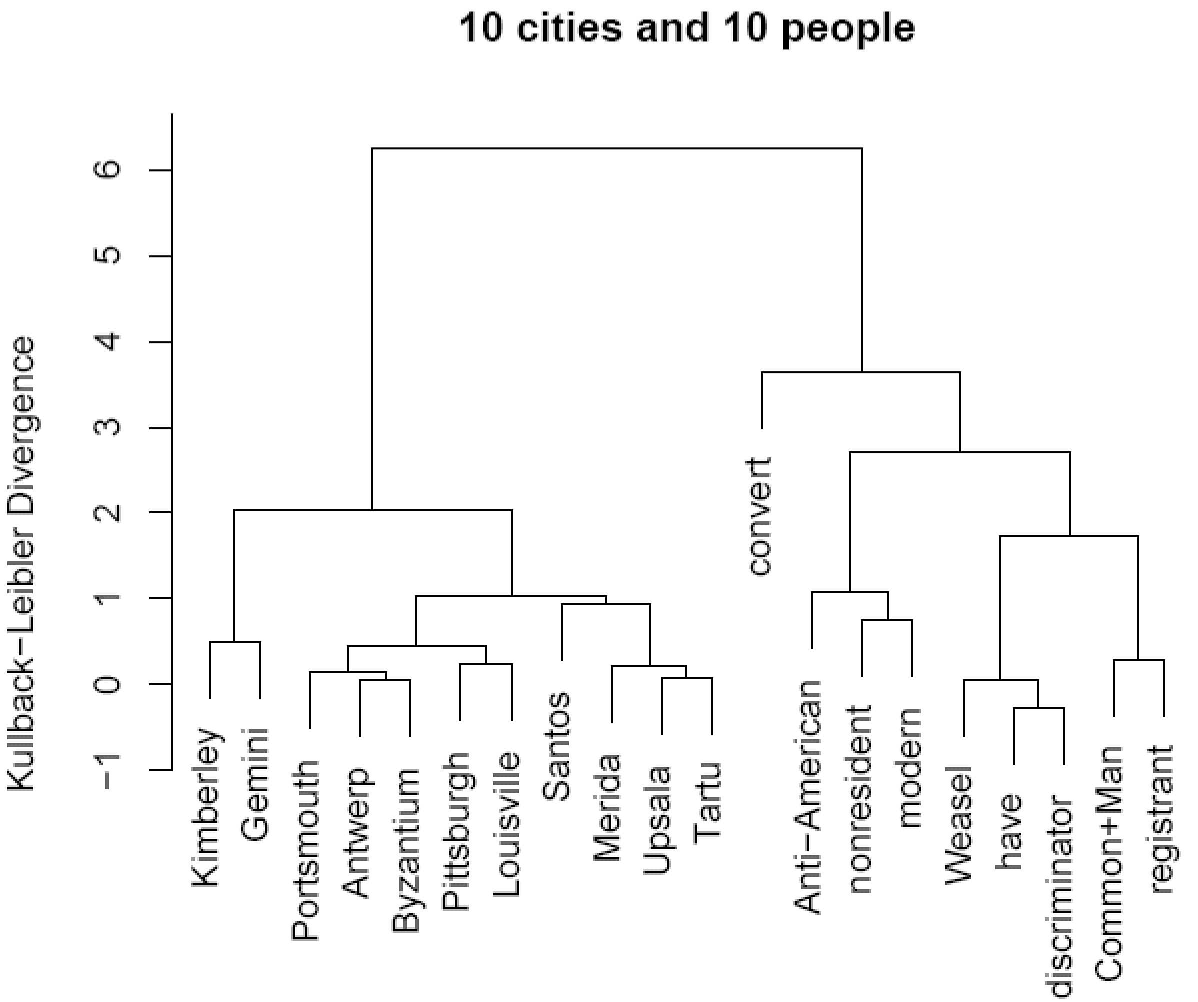
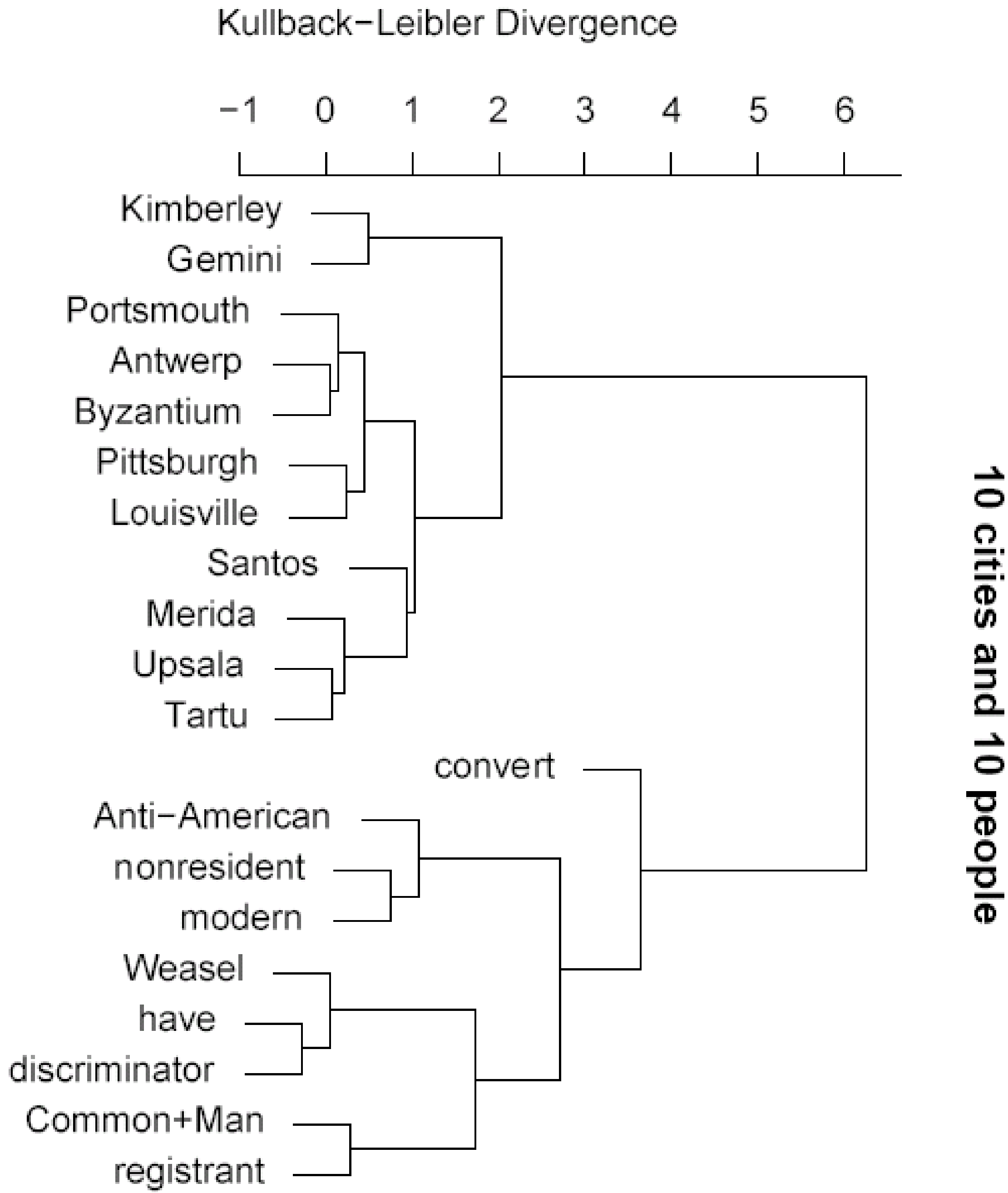
Greedy Hierarchical Clustering

- Initialize one cluster for each data point
- Until *done*
  - Merge the two *nearest* clusters

Hierarchical Clustering on Strings

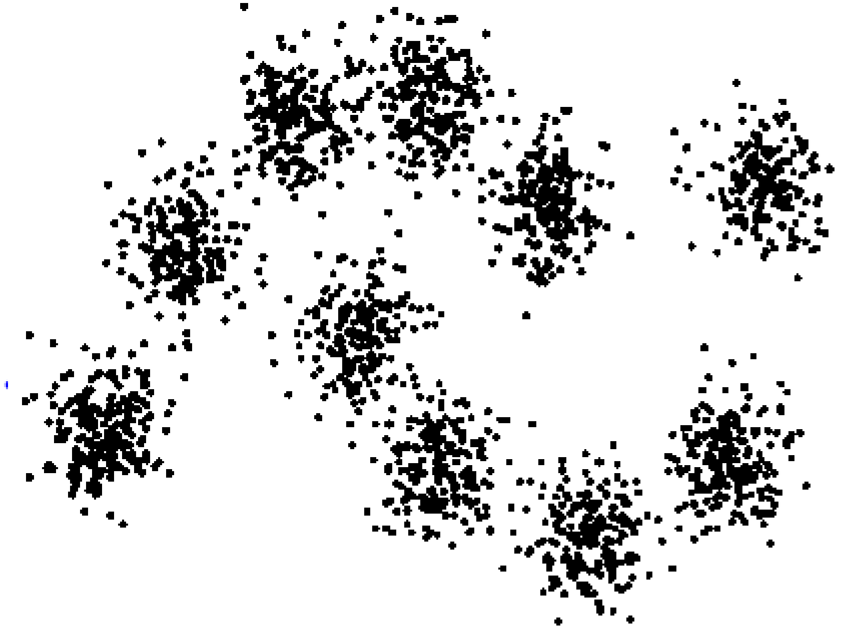
- Features = *contexts* in which strings appear





Kullback−Leibler Divergence
−1 0 1 2 3 4 5 6
Kimberley
Gemini
Portsmouth
Antwerp
Byzantium
Pittsburgh
Louisville
Santos
Merida
Upsala
Tartu
convert
Anti−American
nonresident
modern
Weasel
have
discriminator
Common+Man
registrant
10 cities and 10 people

Classic Example: Half Moons



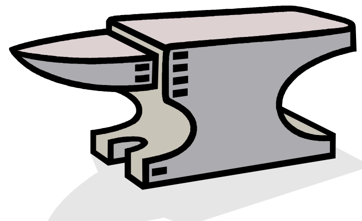
From Batra et al., http://www.cs.cmu.edu/~rahuls/pub/bmvc2008-clustering-rahuls.pdf

Summary

- Algorithms:
  - Sequential clustering
    - Requires key distance threshold, sensitive to data order
  - K-means clustering
    - Requires # of clusters, sensitive to initial conditions
    - Special case of mixture modeling
  - Greedy agglomerative clustering
    - Naively takes O(n^3) runtime
    - Hard to tell when you’re “done”

Optional Reading

- Elements of Statistical Learning
  - Ch 6.8, 8.5, 14
  - http://statweb.stanford.edu/~tibs/ElemStatLearn/



Throw(person, *x*)

?

Weight(x) < 50lbs ^
Max_dim(x) < 20ft ^ … ^
=>Throw(person, x)

Weight(baseball) = 5oz ^…. =>
Throw(person, baseball)

"throwable objects such as"

Web Images Maps Shopping Books More Search tools

About 5,050 results (0.19 seconds)

[Patent US5984812 - Grippable surface for throwable object - Google ...]

www.google.com/patents/US5984812

This invention relates to a grippable surface for **throwable objects such as** a football, baseball, etc. which enhances the ease with which the object may be ...

[PDF] [Name Juggle.pdf - GOAL Consulting]

www.goalconsulting.org/page3/files/Name%20Juggle.pdf

Materials: Many soft **throwable objects such as** fleece balls, wadded up pieces of paper, Nerf™ balls. Level: Grades K and higher. Suggested Procedure. 1.

`Cities such as X`

`Y, mayor of X`

- The Web makes hard AI problems easier
- …but
- Link to word vector demo: tp://radimrehurek.com/2014/02/word2vec-tutorial/#app