Clustering:
K-Means and Mixtures of Gaussians

CS4780/5780 – Machine Learning
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Thorsten Joachims
Cornell University

Reading: Manning/Raghavan/Schuetze, Chapters 16 (not 16.3) and 17 (http://nlp.stanford.edu/IR-book/)

Outline

- Supervised vs. Unsupervised Learning
- Hierarchical Clustering
  - Hierarchical Agglomerative Clustering (HAC)
- Non-Hierarchical Clustering
  - K-means
  - Mixtures of Gaussians and EM-Algorithm

Non-Hierarchical Clustering

- K-means clustering ("hard")
- Mixtures of Gaussians and training via Expectation maximization Algorithm ("soft")

Clustering Criterion

- Evaluation function that assigns a (usually real-valued) value to a clustering
  - Clustering criterion typically function of
    - within-cluster similarity and
    - between-cluster dissimilarity
- Optimization
  - Find clustering that maximizes the criterion
    - Global optimization (often intractable)
    - Greedy search
    - Approximation algorithms

Centroid-Based Clustering

- Assumes instances are real-valued vectors.
- Clusters represented via ***centroids*** (i.e. average of points in a cluster) *c*:

$$\vec{\mu}(c) = \frac{1}{|c|}\sum_{\vec{x} \in c} \vec{x}$$

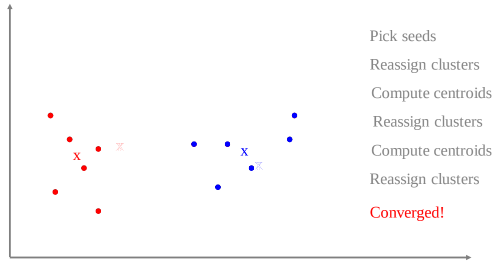
- Reassignment of instances to clusters is based on **distance** to the current cluster centroids.

K-Means Algorithm

- Input: k = number of clusters, distance measure d
- Select k random instances $\{s_1, s_2, \ldots s_k\}$ as seeds.
- Until clustering converges or other stopping criterion:
  - For each instance x_i:
    - Assign x_i to the cluster c_j such that $d(x_i, s_j)$ is min.
  - For each cluster c_j *//update the centroid of each cluster*
    - $s_j = \mu(c_j)$

K-means Example

(k=2)



Time Complexity

- Assume computing distance between two instances is O(*N*) where *N* is the dimensionality of the vectors.
- Reassigning clusters for *n* points: O(*kn*) distance computations, or O(*knN*).
- Computing centroids: Each instance gets added once to some centroid: O(*nN*).
- Assume these two steps are each done once for *i* iterations: O(*iknN*).
- Linear in all relevant factors, assuming a fixed number of iterations, more efficient than HAC.

Buckshot Algorithm

Problem

- Results can vary based on random seed selection, especially for high-dimensional data.
- Some seeds can result in poor convergence rate, or convergence to sub-optimal clusterings.

Idea: Combine HAC and K-means clustering.

- First randomly take a sample of instances of size
- Run group-average HAC on this sample $n^{1/2}$
- Use the results of HAC as initial seeds for K-means.
- Overall algorithm is efficient and avoids problems of bad seed selection.

Clustering as Prediction

- Setup
  - Learning Task: $P(X)$
  - Training Sample: $S = (\vec{x}_1, \dots, \vec{x}_n)$
  - Hypothesis Space: $H = \{h_1, \dots, h_{|H|}\}$ each describes $P(X|h_i)$ where h_i are parameters
  - Goal: learn which $P(X|h_i)$ produces the data
- What to predict?
  - Predict where new points are going to fall

Gaussian Mixtures and EM

- Gaussian Mixture Models
  - Assume

$$P(X = \vec{x}|h_i) = \sum_{j=1}^{k} P(X = \vec{x}|Y = j, h_i)P(Y = j)$$

  where $P(X = \vec{x}|Y = j, h) = N\left(X = \vec{x}\middle|\vec{\mu}_j, \Sigma_j\right)$ and $h = (\vec{\mu}_1, \dots, \vec{\mu}_k, \Sigma_1, \dots, \Sigma_k)$.
- EM Algorithm
  - Assume $P(Y)$ and k known and $\Sigma_i = 1$.
  - REPEAT
    - $\vec{\mu}_j = \frac{\sum_{i=1}^{n} P(Y=j|X=\vec{x}_i,\vec{\mu}_1,\dots,\vec{\mu}_k)\vec{x}_i}{\sum_{i=1}^{n} P(Y=j|X=\vec{x}_i,\vec{\mu}_1,\dots,\vec{\mu}_k)}$
    - $P(Y = j|X = \vec{x}_i, \vec{\mu}_1, \dots, \vec{\mu}_k) = \frac{P(X=\vec{x}_i|Y=j,\vec{\mu}_j)P(Y=j)}{\sum_{l=1}^{k} P(X=\vec{x}_i|Y=l,\vec{\mu}_l)P(Y=l)} = \frac{\mathrm{e}^{-0.5\left(\vec{x}_i-\vec{\mu}_j\right)^2} P(Y=j)}{\sum_{l=1}^{k} e^{-0.5\left(\vec{x}_i-\vec{\mu}_l\right)^2} P(Y=l)}$