Clustering

- Partition unlabeled examples into disjoint subsets of *clusters*, such that:
 - Examples within a cluster are very similar
 - Examples in different clusters are very different
- Discover new categories in an *unsupervised* manner (no sample category labels provided).

Hierarchical Clustering

• Build a tree-based hierarchical taxonomy (*dendrogram*) from a set of unlabeled examples.



• Recursive application of a standard clustering algorithm can produce a hierarchical clustering.

Hierarchical Agglomerative Clustering (HAC)

- Assumes a *similarity function* for determining the similarity of two instances.
- Starts with all instances in a separate cluster and then repeatedly joins the two clusters that are most similar until there is only one cluster.
- The history of merging forms a binary tree or hierarchy.

HAC Algorithm

Start with all instances in their own cluster. Until there is only one cluster: Among the current clusters, determine the two clusters, c_i and c_j , that are most similar. Replace c_i and c_j with a single cluster $c_i \cup c_j$

Cluster Similarity

• Assume a similarity function that determines the similarity of two instances: *sim*(*x*,*y*).

- Cosine similarity of document vectors.

- How to compute similarity of two clusters each possibly containing multiple instances?
 - Single Link: Similarity of two most similar members.
 - Complete Link: Similarity of two least similar members.
 - Group Average: Average similarity between members.

Non-Hierarchical Clustering

- Typically must provide the number of desired clusters, *k*.
- Randomly choose *k* instances as *seeds*, one per cluster.
- Form initial clusters based on these seeds.
- Iterate, repeatedly reallocating instances to different clusters to improve the overall clustering.
- Stop when clustering converges or after a fixed number of iterations.

K-Means

- Assumes instances are real-valued vectors.
- Clusters based on *centroids*, *center of gravity*, or mean of points in a cluster, *c*:

$$\mathbf{r}_{\mu(c)} = \frac{1}{|c|} \sum_{x \in c} \mathbf{r}_{x}$$

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

Distance Metrics

• Euclidian distance (L₂ norm):

$$L_{2}(x, y) = \sqrt{\sum_{i=1}^{m} (x_{i} - y_{i})^{2}}$$

$$L_{1} \text{ norm:} \underset{L_{1}(x, y) = \sum_{i=1}^{m} |x_{i} - y_{i}|}{\sum_{i=1}^{m} |x_{i} - y_{i}|}$$

• Cosine Similarity (transform to a distance by subtracting from 1):

$$1 - \frac{x \cdot y}{|x| \cdot |y|}$$

K-Means Algorithm

Let *d* be the distance measure between instances. Select *k* random instances $\{s_1, s_2, \dots, s_k\}$ 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 minimal. (Update the seeds to the centroid of each cluster) For each cluster c_j

 $s_j = \mu(c_j)$

K Means Example (K=2)



Pick seeds Reassign clusters Compute centroids Reassign clusters Compute centroids Reassign clusters

Converged!

- Applications:
 - During retrieval, add other documents in the same cluster as the initial retrieved documents to improve recall.
 - Clustering of results of retrieval to present more organized results to the user
 - Automated production of hierarchical taxonomies of documents for browsing purposes (à la Yahoo or Seznam).

yes but we talk just about document clustering...

the problem of clustering rows in this matrix is that of clustering documents,

whereas that of clustering columns in this matrix is that of clustering words/tokens.

In reality, the two problems are closely related, as good clusters of words may be leveraged in order to find good clusters of documents and vice-versa.

- HAC and K-Means can be applied to text in a straightforward way but
- document-term matrix needs to be normalized to prevent from influence of outlying features, so that the L2-norm ||Xi|| of each document is one unit.
- Then there is no difference between the use of the Euclidean distance, cosine similarity, or the dot product similarity, after such a normalization has been performed.
- L2 norm is a standard method to compute the length of a vector in Euclidean space. Given x = [x1x2 ... xn]T, L2 norm of x is defined as the square root of the sum of the squares of the values in each dimension.

Tools

- scikit-learn contains several text clustering tools
- R : tm package can be used for preprocessing the documents
- R : stats package contains the kmeans and hclust functions by default
- Weka library also contains several Java implementations of clustering algorithms
- MATLAB has functions for k-means and hierarchical clustering. It also automatically computes the dendrogram from a data set.

Conclusions

- Unsupervised learning induces categories from unlabeled data.
- There are a variety of approaches, including: - HAC
 - k-means
 - -EM
- Semi-supervised learning uses both labeled and unlabeled data to improve results.