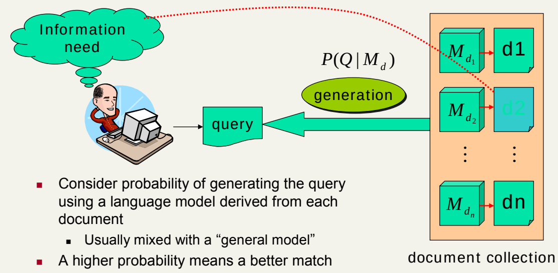
CS276A
Text Retrieval and Mining

Lecture 13

[Borrows slides from Ray Mooney and Soumen Chakrabarti]

Recap: The Language Model Approach to IR



- Consider probability of generating the query using a language model derived from each document
  - Usually mixed with a "general model"
- A higher probability means a better match
- Comparisons with vector space IR similarity

Today's Topic: Clustering 1

- Document clustering
  - Motivations
  - Document representations
  - Success criteria
- Clustering algorithms
  - K-means
  - Model-based clustering (EM clustering)

What is clustering?

- Clustering is the process of grouping a set of physical or abstract objects into classes of similar objects
  - It is the commonest form of unsupervised learning
    - Unsupervised learning = learning from raw data, as opposed to supervised data where the correct classification of examples is given
  - It is a common and important task that finds many applications in IR and other places

Why cluster documents?

- Whole corpus analysis/navigation
  - Better user interface
- For improving recall in search applications
  - Better search results
- For better navigation of search results
  - Effective "user recall" will be higher
- For speeding up vector space retrieval
  - Faster search

Navigating document collections

- Standard IR is like a book index
- Document clusters are like a table of contents
- People find having a table of contents useful

Index
Aardvark, 15
Blueberry, 200
Capricorn, 1, 45-55
Dog, 79-99
Egypt, 65
Falafel, 78-90
Giraffes, 45-59
…

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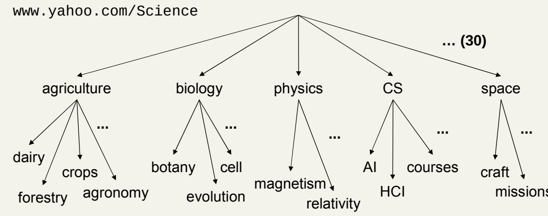
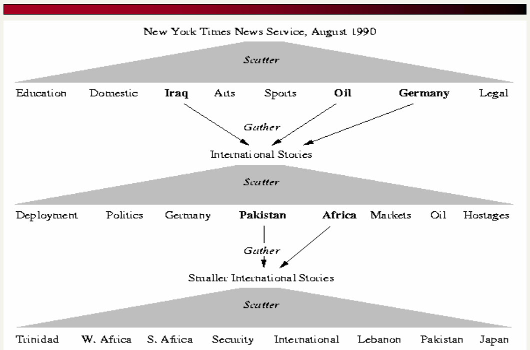
Corpus analysis/navigation

- Given a corpus, partition it into groups of related docs
  - Recursively, can induce a tree of topics
  - Allows user to browse through corpus to find information
  - Crucial need: meaningful labels for topic nodes.
- Yahoo!: manual hierarchy
  - Often not available for new document collection

Yahoo! Hierarchy

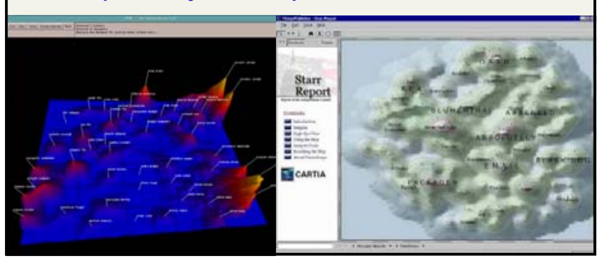


Scatter/Gather: Cutting, Karger, and Pedersen



For visualizing a document collection and its themes

- Wise et al, "Visualizing the non-visual" PNNL
- ThemeScapes, Cartia
  - [Mountain height = cluster size]



For improving search recall

- *Cluster hypothesis* - Documents with similar text are related
- Therefore, to improve search recall:
  - Cluster docs in corpus a priori
  - When a query matches a doc *D*, also return other docs in the cluster containing *D*
- Hope if we do this: The query "car" will also return docs containing *automobile*
  - Because clustering grouped together docs containing *car* with those containing *automobile.*

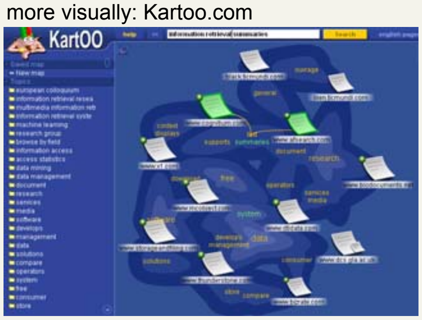
Why might this happen?

For better navigation of search results

- For grouping search results thematically
  - clusty.com / Vivisimo

For better navigation of search results

- And more visually: Kartoo.com



Navigating search results (2)

- One can also view grouping documents with the same sense of a word as clustering
- Given the results of a search (say Jaguar, or ***NLP***), partition into groups of related docs
- Can be viewed as a form of word sense disambiguation
- E.g., *jaguar* may have senses:
  - The car company
  - The animal
  - The football team
  - The video game
- Recall query reformulation/expansion discussion

For visualizing bookmarked pages

- Robertson, "Data Mountain" (Microsoft)

For speeding up vector space retrieval

- In vector space retrieval, we must find nearest doc vectors to query vector
- This entails finding the similarity of the query to every doc – slow (for some applications)
- By clustering docs in corpus a priori
  - find nearest docs in cluster(s) close to query
  - inexact but avoids exhaustive similarity computation

Exercise: Make up a simple example with points on a line in 2 clusters where this inexactness shows up.

Speeding up vector space retrieval

- Recall lecture 7 on leaders and followers
  - Effectively a fast simple clustering algorithm where documents are assigned to closest item in a set of randomly chosen leaders
- We could instead find natural clusters in the data
  - Cluster documents into *k* clusters
  - Retrieve closest cluster c_i to query
  - Rank documents in c_i and return to user

What Is A Good Clustering?

- Internal criterion: A good clustering will produce high quality clusters in which:
  - the intra-class (that is, intra-cluster) similarity is high
  - the inter-class similarity is low
  - The measured quality of a clustering depends on both the document representation and the similarity measure used
- External criterion: The quality of a clustering is also measured by its ability to discover some or all of the hidden patterns or latent classes
  - Assessable with gold standard data

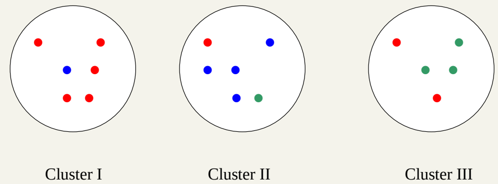
External Evaluation of Cluster Quality

- Assesses clustering with respect to ground truth
- Assume that there are C gold standard classes, while our clustering algorithms produce k clusters, $\pi_1, \pi_2, \ldots, \pi_k$ with n_i members.
- Simple measure: purity, the ratio between the dominant class in the cluster π_i and the size of cluster π_i

$$Purity(\pi_i) = \frac{1}{n_i} \max_j (n_{ij}) \quad j \in C$$

- Others are entropy of classes in clusters (or mutual information between classes and clusters)

Purity



Cluster I: Purity = 1/6 (max(5, 1, 0)) = 5/6

Cluster II: Purity = 1/6 (max(1, 4, 1)) = 4/6

Cluster III: Purity = 1/5 (max(2, 0, 3)) = 3/5

Issues for clustering

- Representation for clustering
  - Document representation
    - Vector space? Normalization?
  - Need a notion of similarity/distance
- How many clusters?
  - Fixed a priori?
  - Completely data driven?
    - Avoid “trivial” clusters - too large or small
      - In an application, if a cluster's too large, then for navigation purposes you've wasted an extra user click without whittling down the set of documents much.

What makes docs “related”?

- Ideal: semantic similarity.
- Practical: statistical similarity
  - We will use cosine similarity.
  - Docs as vectors.
  - For many algorithms, easier to think in terms of a *distance* (rather than similarity) between docs.
  - We will describe algorithms in terms of cosine similarity. Cosine similarity of normalized D_j, D_k:

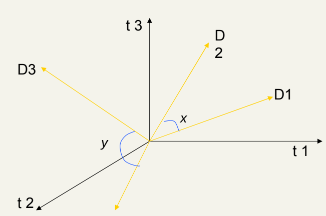
$$sim(D_j, D_k) = \sum_{i=1}^{m} w_{ij} \times w_{ik}$$

Aka normalized inner product.

Recall doc as vector

- Each doc j is a vector of *tf×idf* values, one component for each term.
- Can normalize to unit length.
- So we have a vector space
  - terms are axes - aka *features*
  - n docs live in this space
  - even with stemming, may have 20,000+ dimensions
  - do we really want to use all terms?
    - Different from using vector space for search. Why?

Intuition



Postulate: Documents that are “close together” in vector space talk about the same things.

Clustering Algorithms

- Partitioning "flat" algorithms
  - Usually start with a random (partial) partitioning
  - Refine it iteratively
    - *k* means/medoids clustering
    - Model based clustering
- Hierarchical algorithms
  - Bottom-up, agglomerative
  - Top-down, divisive

Partitioning Algorithms

- Partitioning method: Construct a partition of *n* documents into a set of *k* clusters
- Given: a set of documents and the number *k*
- Find: a partition of *k* clusters that optimizes the chosen partitioning criterion
  - Globally optimal: exhaustively enumerate all partitions
  - Effective heuristic methods: k-means and k-medoids algorithms

How hard is clustering?

- One idea is to consider all possible clusterings, and pick the one that has best inter and intra cluster distance properties
- Suppose we are given n points, and would like to cluster them into k-clusters
  - How many possible clusterings?

$$\frac{k^n}{k!}$$

- Too hard to do it brute force or optimally
- Solution: Iterative optimization algorithms
  - Start with a clustering, iteratively improve it (eg. K-means)

K-Means

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

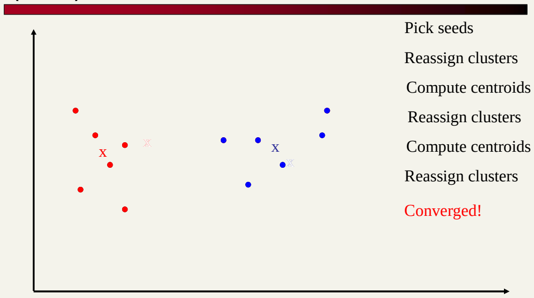
$$\vec{\mu}(c) = \frac{1}{|c|}\sum_{\vec{x} \in c} \vec{x}$$

- Reassignment of instances to clusters is based on distance to the current cluster centroids.
  - (Or one can equivalently phrase it in terms of similarities)

K-Means Algorithm

Let d be the distance measure between instances.
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 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)



Termination conditions

- Several possibilities, e.g.,
  - A fixed number of iterations.
  - Doc partition unchanged.
  - Centroid positions don't change.

Does this mean that the docs in a cluster are unchanged?

Convergence

- Why should the K-means algorithm ever reach a *fixed point*?
  - A state in which clusters don't change.
- K-means is a special case of a general procedure known as the *Expectation Maximization (EM) algorithm*.
  - EM is known to converge.
  - Number of iterations could be large.

Convergence of K-Means

- Define goodness measure of cluster k as sum of squared distances from cluster centroid:
  - $G_k = \Sigma_i (v_i - c_k)^2$ (sum all v_i in cluster k)
- $G = \Sigma_k G_k$
- Reassignment monotonically decreases G since each vector is assigned to the closest centroid.
- Recomputation monotonically decreases each G_k since: (m_k is number of members in cluster)
  - $\Sigma (v_{in} - a)^2$ reaches minimum for:
  - $\Sigma -2(v_{in} - a) = 0$

Convergence of K-Means

- $\Sigma -2(v_{in} - a) = 0$
- $\Sigma v_{in} = \Sigma a$
- $m_k a = \Sigma v_{in}$
- $a = (1/ m_k) \Sigma v_{in} = c_{kn}$

- K-means typically converges quite quickly

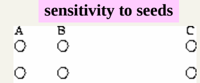
Time Complexity

- Assume computing distance between two instances is *O(m)* where *m* is the dimensionality of the vectors.
- Reassigning clusters: *O(kn)* distance computations, or *O(knm).*
- Computing centroids: Each instance vector gets added once to some centroid: *O(nm).*
- Assume these two steps are each done once for *i* iterations: *O(iknm).*
- Linear in all relevant factors, assuming a fixed number of iterations, more efficient than hierarchical agglomerative methods

Seed Choice

- Results can vary based on random seed selection.
- Some seeds can result in poor convergence rate, or convergence to sub-optimal clusterings.
  - Select good seeds using a heuristic (e.g., doc least similar to any existing mean)
  - Try out multiple starting points
  - Initialize with the results of another method.

Example showing sensitivity to seeds



**In the above, if you start with B and E as centroids you converge to {A,B,C} and {D,E,F}
If you start with D and F you converge to {A,B,D,E} {C,F}**

Exercise: find good approach for finding good starting points

How Many Clusters?

- Number of clusters k is given
  - Partition n docs into predetermined number of clusters
- Finding the "right" number of clusters is part of the problem
  - Given docs, partition into an "appropriate" number of subsets.
  - E.g., for query results - ideal value of k not known up front - though UI may impose limits.
- Can usually take an algorithm for one flavor and convert to the other.

k not specified in advance

- Say, the results of a query.
- Solve an optimization problem: penalize having lots of clusters
  - application dependent, e.g., compressed summary of search results list.
- Tradeoff between having more clusters (better focus within each cluster) and having too many clusters

k not specified in advance

- Given a clustering, define the Benefit for a doc to be the cosine similarity to its centroid
- Define the Total Benefit to be the sum of the individual doc Benefits.

Why is there always a clustering of Total Benefit n?

Penalize lots of clusters

- For each cluster, we have a Cost C.
- Thus for a clustering with k clusters, the Total Cost is kC.
- Define the Value of a clustering to be =

  Total Benefit - Total Cost.
- Find the clustering of highest value, over all choices of k.
  - Total benefit increases with increasing K. But can stop when it doesn't increase by "much". The Cost term enforces this.

K-means issues, variations, etc.

- Recomputing the centroid after every assignment (rather than after all points are re-assigned) can improve speed of convergence of K-means
- Assumes clusters are spherical in vector space
  - Sensitive to coordinate changes, weighting etc.
- Disjoint and exhaustive
  - Doesn't have a notion of "outliers"

Soft Clustering

- Clustering typically assumes that each instance is given a "hard" assignment to exactly one cluster.
- Does not allow uncertainty in class membership or for an instance to belong to more than one cluster.
- *Soft clustering* gives probabilities that an instance belongs to each of a set of clusters.
- Each instance is assigned a probability distribution across a set of discovered categories (probabilities of all categories must sum to 1).

Model based clustering

- Algorithm optimizes a probabilistic model criterion
- Clustering is usually done by the Expectation Maximization (EM) algorithm
  - Gives a soft variant of the K-means algorithm
  - Assume *k* clusters: $\{c_1, c_2, \ldots c_k\}$
  - Assume a probabilistic model of categories that allows computing $P(c_i \mid E)$ for each category, c_i, for a given example, E.
  - For text, typically assume a naïve Bayes category model.
  - Parameters $\theta = \{P(c_i), P(w_j \mid c_i): i \in \{1, \ldots k\}, j \in \{1, \ldots, |V|\}\}$

Expectation Maximization (EM) Algorithm

- Iterative method for learning probabilistic categorization model from unsupervised data.
- Initially assume random assignment of examples to categories.
- Learn an initial probabilistic model by estimating model parameters θ from this randomly labeled data.
- Iterate following two steps until convergence:
  - Expectation (E-step): Compute $P(c_i \mid E)$ for each example given the current model, and probabilistically re-label the examples based on these posterior probability estimates.
  - Maximization (M-step): Re-estimate the model parameters, θ, from the probabilistically re-labeled data.

EM Experiment [Soumen Chakrabarti]

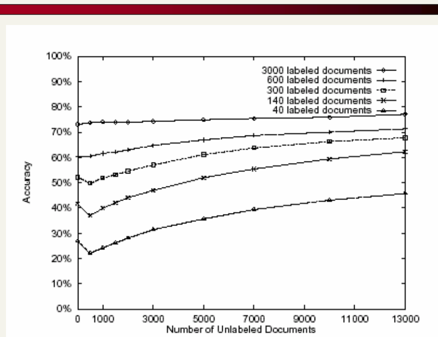
- Semi-supervised: some labeled and unlabeled data
- Take a completely labeled corpus D, and randomly select a subset as D_K.
- Also use the set $D^U \subseteq D$ of unlabeled documents in the EM procedure.
- Correct classification of a document
  => concealed class label = class with largest probability
- Accuracy with unlabeled documents > accuracy without unlabeled documents
  - Keeping labeled set of same size
- EM beats naïve Bayes with same size of labeled document set
  - Largest boost for small size of labeled set
  - Comparable or poorer performance of EM for large labeled sets

Belief in labeled documents

- Depending on one's faith in the initial labeling
  - Set before 1st iteration:
    - $\Pr(c_d \mid d) = 1 - \varepsilon$ and $\Pr(c' \mid d) = \varepsilon/(n-1)$ for all $c' \neq c_d$
  - With each iteration
    - Let the class probabilities of the labeled documents `smear' in reestimation process
- To limit 'drift' from initial labeled documents, one can add a damping factor in the E step to the contribution from unlabeled documents

Increasing D^U while holding D^K fixed also shows the advantage of using large unlabeled sets in the EM-like algorithm.

Purity



Summary

- Two types of clustering
  - Flat, partional clustering
  - Hierarchical, agglomerative clustering
- How many clusters?
- Key issues
  - Representation of data points
  - Similarity/distance measure
- K-means: the basic partitional algorithm
- Model-based clustering and EM estimation