Clustering

- 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
- 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
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 (e.g., jaguar, 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 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

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 \( \pi_i \) and the size of cluster \( \pi_i \)

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

• 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.

Cosine similarity of normalized $D_j, D_k$:

\[ \text{sim}(D_j, D_k) = \frac{\sum_{i=1}^{m} w_{ij} \times w_{ik}}{\sum_{i=1}^{m} w_{ij}^2 \times \sum_{i=1}^{m} w_{ik}^2} \]

Aka normalized inner product.
Recall doc as vector

- Each doc $j$ is a vector of $tf\times idf$ values, one component for each term.
- Can normalize to unit length.
- So we have a vector space
  - terms are axis - 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 (e.g., 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:

\[ \bar{\mu}(c) = \frac{1}{|c|} \sum_{x \in c} x \]

• 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)

Pick seeds
Reassign clusters
Compute centroids
Reassign clusters
Compute centroids
Reassign clusters
Converged!
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?

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
Recap

• Why cluster documents?
  – For improving recall in search applications
  – For speeding up vector space retrieval
  – Navigation
  – Presentation of search results

• $k$-means basic iteration
  – At the start of the iteration, we have $k$ centroids.
  – Each doc assigned to the nearest centroid.
  – All docs assigned to the same centroid are averaged to compute a new centroid;
    • thus have $k$ new centroids.

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.
\textit{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

\textit{k} not specified in advance

- Given a clustering, define the \textbf{Benefit} for a doc to be the cosine similarity to its centroid
- Define the \textbf{Total Benefit} to be the sum of the individual doc \textbf{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 $\text{Value} = \text{Total Benefit} - \text{Total Cost}$.
- 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.

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:
  \[ G_k = \sum_i (v_i - c_k)^2 \] (sum all \( v_i \) in cluster k)
- \( G = \sum_k G_k \)
- Reassignment monotonically reduces \( G \) since each vector is assigned to the closest centroid.
- Recomputation monotonically decreases each \( G_k \) since:
  \[ \sum (v_{in} - a)^2 \text{ reaches minimum for:} \]
  \[ \sum -2(v_{in} - a) = 0 \]

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*,… *c_k*\}
  – Assume a probabilistic model of categories that allows computing \(P(c_i | E)\) for each category, \(c_i\), for a given example, \(E\).
  – For text, typically assume a naïve Bayes category model.
  – Parameters \(\theta = \{P(c_i), P(w_j | c_i): i\in\{1,...,k\}, j \in\{1,...,|V|}\}\)
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 $\theta$ from this randomly labeled data.
• Iterate following two steps until convergence:
  – Expectation (E-step): Compute $P(c_i | E)$ 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, $\theta$, 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:
    • \( \Pr(c \mid d) = 1 - \varepsilon \) 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.
“The Curse of Dimensionality”

- Why document clustering is difficult
  - While clustering looks intuitive in 2 dimensions, many of our applications involve 10,000 or more dimensions…
  - High-dimensional spaces look different: the probability of random points being close drops quickly as the dimensionality grows.
  - One way to look at it: in large-dimension spaces, random vectors are almost all almost perpendicular. Why?
- Solution: Dimensionality reduction … important for text

Hierarchical Clustering

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

```
animal
  vertebrate
    fish
    reptile
  invertebrate
    amphib. mammal
    worm
    insect
    crustacean
```

- One option to produce a hierarchical clustering is recursive application of a partitional clustering algorithm to 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.

A Dendogram: Hierarchical Clustering

- Dendrogram: Decomposes data objects into a several levels of nested partitioning (tree of clusters).
- Clustering of the data objects is obtained by cutting the dendrogram at the desired level, then each connected component forms a cluster.
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 $c_i \cup c_j$

Hierarchical Clustering algorithms

• **Agglomerative (bottom-up):**
  – Start with each document being a single cluster.
  – Eventually all documents belong to the same cluster.

• **Divisive (top-down):**
  – Start with all documents belong to the same cluster.
  – Eventually each node forms a cluster on its own.

• Does not require the number of clusters $k$ in advance
• Needs a termination/readout condition
  – The final mode in both Agglomerative and Divisive is of no use.
Dendrogram: Document Example

- As clusters *agglomerate*, docs likely to fall into a hierarchy of “topics” or concepts.

```
\begin{center}
\begin{tikzpicture}
\node[red, circle, fill=red] (d1) at (0,0) {d1};
\node[red, circle, fill=red] (d2) at (0,-1) {d2};
\node[red, circle, fill=red] (d3) at (1,0) {d3};
\node[red, circle, fill=red] (d4) at (1,-1) {d4};
\node[red, circle, fill=red] (d5) at (2,0) {d5};
\path (d1) -- (d2);
\path (d3) -- (d4);
\path (d3) -- (d5);
\end{tikzpicture}
\end{center}
```

“Closest pair” of clusters

- Many variants to defining closest pair of clusters
- “Center of gravity”
  - Clusters whose centroids (centers of gravity) are the most cosine-similar
- Average-link
  - Average cosine between pairs of elements
- Single-link
  - Similarity of the most cosine-similar (single-link)
- Complete-link
  - Similarity of the “furthest” points, the least cosine-similar
Hierarchical Clustering

• Key problem: as you build clusters, how do you represent the location of each cluster, to tell which pair of clusters is closest?

• Euclidean case: each cluster has a centroid = average of its points.
  – Measure intercluster distances by distances of centroids.

Single Link Agglomerative Clustering

• Use maximum similarity of pairs:

\[ \text{sim}(c_i, c_j) = \max_{x \in c_i, y \in c_j} \text{sim}(x, y) \]

• Can result in “straggly” (long and thin) clusters due to chaining effect.
  – Appropriate in some domains, such as clustering islands: “Hawaii clusters”

• After merging \( c_i \) and \( c_j \), the similarity of the resulting cluster to another cluster, \( c_k \), is:

\[ \text{sim}((c_i \cup c_j), c_k) = \max(\text{sim}(c_i, c_k), \text{sim}(c_j, c_k)) \]
Single Link Example

Complete Link Agglomerative Clustering

- Use minimum similarity of pairs:
  \[ \text{sim}(c_i, c_j) = \min_{x \in c_i, y \in c_j} \text{sim}(x, y) \]

- Makes “tighter,” spherical clusters that are typically preferable.

- After merging \( c_i \) and \( c_j \), the similarity of the resulting cluster to another cluster, \( c_k \), is:
  \[ \text{sim}((c_i \cup c_j), c_k) = \min(\text{sim}(c_i, c_k), \text{sim}(c_j, c_k)) \]
• In the first iteration, all HAC methods need to compute similarity of all pairs of \( n \) individual instances which is \( O(n^2) \).

• In each of the subsequent \( n-2 \) merging iterations, it must compute the distance between the most recently created cluster and all other existing clusters.
  
  – Since we can just store unchanged similarities

• In order to maintain an overall \( O(n^2) \) performance, computing similarity to each other cluster must be done in constant time.
  
  – Else \( O(n^2 \log n) \) or \( O(n^3) \) if done naively
Key notion: cluster representative

- We want a notion of a representative point in a cluster.
- Representative should be some sort of “typical” or central point in the cluster, e.g.,
  - point inducing smallest radii to docs in cluster
  - smallest squared distances, etc.
  - point that is the “average” of all docs in the cluster
    - Centroid or center of gravity

Example: $n=6$, $k=3$, closest pair of centroids
Outliers in centroid computation

- Can ignore outliers when computing centroid.

- What is an outlier?
  - Lots of statistical definitions, e.g.
    - moment of point to centroid > $M \times$ some cluster moment.

Group Average Agglomerative Clustering

- Use average similarity across all pairs within the merged cluster to measure the similarity of two clusters.

$$sim(c_i, c_j) = \frac{1}{|c_i \cup c_j|(|c_i \cup c_j| - 1)} \sum_{\bar{x} \in (c_i \cup c_j)} \sum_{\bar{y} \in (c_i \cup c_j)} \sum_{\bar{x} \neq \bar{y}} sim(\bar{x}, \bar{y})$$

- Compromise between single and complete link.
- Two options:
  - Averaged across all ordered pairs in the merged cluster
  - Averaged over all pairs between the two original clusters
- Some previous work has used one of these options; some the other. No clear difference in efficacy
Computing Group Average Similarity

- Assume cosine similarity and normalized vectors with unit length.
- Always maintain sum of vectors in each cluster.
  \[ \overline{s}(c_j) = \sum_{\bar{x} \in c_j} \bar{x} \]
- Compute similarity of clusters in constant time:
  \[ \text{sim}(c_i, c_j) = \frac{(\overline{s}(c_i) + \overline{s}(c_j)) \cdot (\overline{s}(c_i) + \overline{s}(c_j)) - (|c_i| + |c_j|)}{(|c_i| + |c_j|)(|c_i| + |c_j| - 1)} \]

Efficiency: Medoid As Cluster Representative

- The centroid does not have to be a document.
- Medoid: A cluster representative that is one of the documents
- For example: the document closest to the centroid
- One reason this is useful
  - Consider the representative of a large cluster (>1000 documents)
  - The centroid of this cluster will be a dense vector
  - The medoid of this cluster will be a sparse vector
- Compare: mean/centroid vs. median/medoid
Exercise

• Consider agglomerative clustering on $n$ points on a line. Explain how you could avoid $n^3$ distance computations - how many will your scheme use?

Efficiency: “Using approximations”

• In standard algorithm, must find closest pair of centroids at each step
• Approximation: instead, find nearly closest pair
  – use some data structure that makes this approximation easier to maintain
  – simplistic example: maintain closest pair based on distances in projection on a random line
Term vs. document space

• So far, we clustered docs based on their similarities in term space.
• For some applications, e.g., topic analysis for inducing navigation structures, can “dualize”:
  – use docs as axes
  – represent (some) terms as vectors
  – proximity based on co-occurrence of terms in docs
  – now clustering terms, not docs

Term vs. document space

• Cosine computation
  – Constant for docs in term space
  – Grows linearly with corpus size for terms in doc space
• Cluster labeling
  – clusters have clean descriptions in terms of noun phrase co-occurrence
  – Easier labeling?
• Application of term clusters
  – Sometimes we want term clusters (example?)
  – If we need doc clusters, left with problem of binding docs to these clusters

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Multi-lingual docs

- E.g., Canadian government docs.
- Every doc in English and equivalent French.
  - Must cluster by concepts rather than language
- Simplest: pad docs in one language with dictionary equivalents in the other
  - thus each doc has a representation in both languages
- Axes are terms in both languages

Feature selection

- Which terms to use as axes for vector space?
- Large body of (ongoing) research
- IDF is a form of feature selection
  - Can exaggerate noise e.g., mis-spellings
- Better is to use highest weight mid-frequency words – the most discriminating terms
- Pseudo-linguistic heuristics, e.g.,
  - drop stop-words
  - stemming/lemmatization
  - use only nouns/noun phrases
- Good clustering should “figure out” some of these
Major issue - labeling

• After clustering algorithm finds clusters - how can they be useful to the end user?
• Need pithy label for each cluster
  – In search results, say “Animal” or “Car” in the jaguar example.
  – In topic trees (Yahoo), need navigational cues.
    • Often done by hand, a posteriori.

How to Label Clusters

• Show titles of typical documents
  – Titles are easy to scan
  – Authors create them for quick scanning!
  – But you can only show a few titles which may not fully represent cluster
• Show words/phrases prominent in cluster
  – More likely to fully represent cluster
  – Use distinguishing words/phrases
    • Differential labeling
  – But harder to scan
Labeling

• Common heuristics - list 5-10 most frequent terms in the centroid vector.
  – Drop stop-words; stem.
• Differential labeling by frequent terms
  – Within a collection “Computers”, clusters all have the word computer as frequent term.
  – Discriminant analysis of centroids.

• Perhaps better: distinctive noun phrase
Evaluation of clustering

- Perhaps the most substantive issue in data mining in general:
  - how do you measure goodness?
- Most measures focus on computational efficiency
  - Time and space
- For application of clustering to search:
  - Measure retrieval effectiveness

Approaches to evaluating

- Anecdotal
- User inspection
- Ground “truth” comparison
  - Cluster retrieval
- Purely quantitative measures
  - Probability of generating clusters found
  - Average distance between cluster members
- Microeconomic / utility
Anecdotal evaluation

• Probably the commonest (and surely the easiest)
  – “I wrote this clustering algorithm and look what it found!”
• No benchmarks, no comparison possible
• Any clustering algorithm will pick up the easy stuff like partition by languages
• Generally, unclear scientific value.

User inspection

• Induce a set of clusters or a navigation tree
• Have subject matter experts evaluate the results and score them
  – some degree of subjectivity
• Often combined with search results clustering
• Not clear how reproducible across tests.
• Expensive / time-consuming
Ground “truth” comparison

• Take a union of docs from a taxonomy & cluster
  – Yahoo!, ODP, newspaper sections …
• Compare clustering results to baseline
  – e.g., 80% of the clusters found map “cleanly” to
    taxonomy nodes
  – How would we measure this?
• But is it the “right” answer?
  – There can be several equally right answers
• For the docs given, the static prior taxonomy may
  be incomplete/wrong in places
  – the clustering algorithm may have gotten right things
    not in the static taxonomy

Ground truth comparison

• Divergent goals
• Static taxonomy designed to be the “right”
  navigation structure
  – somewhat independent of corpus at hand
• Clusters found have to do with vagaries of
  corpus
• Also, docs put in a taxonomy node may not
  be the most representative ones for that topic
  – cf Yahoo!
Microeconomic viewpoint

- Anything - including clustering - is only as good as the economic utility it provides
- For clustering: net economic gain produced by an approach (vs. another approach)
- Strive for a concrete optimization problem
- Examples
  - recommendation systems
  - clock time for interactive search
    - expensive

Evaluation example: Cluster retrieval

- Ad-hoc retrieval
- Cluster docs in returned set
- Identify best cluster & only retrieve docs from it
- How do various clustering methods affect the quality of what’s retrieved?
- Concrete measure of quality:
  - Precision as measured by user judgements for these queries
- Done with TREC queries
Evaluation

• Compare two IR algorithms
  – 1. send query, present ranked results
  – 2. send query, cluster results, present clusters
• Experiment was simulated (no users)
  – Results were clustered into 5 clusters
  – Clusters were ranked according to percentage relevant documents
  – Documents within clusters were ranked according to similarity to query

Sim-Ranked vs. Cluster-Ranked

<table>
<thead>
<tr>
<th>CutOff</th>
<th>Sim-Ranked</th>
<th>Cluster-Ranked</th>
<th>% Increase</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>.342</td>
<td>.428</td>
<td>.252</td>
</tr>
<tr>
<td>10</td>
<td>.314</td>
<td>.401</td>
<td>.277</td>
</tr>
<tr>
<td>20</td>
<td>.276</td>
<td>.363</td>
<td>.312</td>
</tr>
</tbody>
</table>

Table 4: Precision at small document cutoff levels for the one-step algorithm.
Relevance Density of Clusters

Buckshot Algorithm

- Another way to an efficient implementation:
  - Cluster a sample, then assign the entire set
- First randomly take a sample of instances of size $\sqrt{n}$
- Run group-average HAC on this sample, which takes only $O(n)$ time.
- Use the results of HAC as initial seeds for K-means.
- Overall algorithm is $O(n)$ and avoids problems of bad seed selection.

Uses HAC to bootstrap K-means
Bisecting K-means

- Divisive hierarchical clustering method using K-means
- For \( I=1 \) to \( k-1 \) do {
  - Pick a leaf cluster \( C \) to split
  - For \( J=1 \) to \( \text{ITER} \) do {
    - Use K-means to split \( C \) into two sub-clusters, \( C_1 \) and \( C_2 \)
    - Choose the best of the above splits and make it permanent
  }\}

- Steinbach et al. suggest HAC is better than k-means but Bisecting K-means is better than HAC for their text experiments

Resources

  - Cutting/Karger/Pedersen/Tukey
  - [http://citeseer.ist.psu.edu/cutting92scattergather.html](http://citeseer.ist.psu.edu/cutting92scattergather.html)

- Data Clustering: A Review (1999)
  - Jain/Murty/Flynn
  - [http://citeseer.ist.psu.edu/jain99data.html](http://citeseer.ist.psu.edu/jain99data.html)

- A Comparison of Document Clustering Techniques
Latent Semantic Analysis

- **Latent semantic space**: illustrative example

    ![Illustrative example](courtesy of Susan Dumais)

Performing the maps

- Each row and column of $A$ gets mapped into the $k$-dimensional LSI space, by the SVD.
- Claim – this is not only the mapping with the best (Frobenius error) approximation to $A$, but in fact *improves* retrieval.
- A query $q$ is also mapped into this space, by

  $$q_k = q^T U_k \Sigma_k^{-1}$$

  - Query NOT a sparse vector.
Empirical evidence

- Experiments on TREC 1/2/3 – Dumais
- Lanczos SVD code (available on netlib) due to Berry used in these expts
  - Running times of ~ one day on tens of thousands of docs
- Dimensions – various values 250-350 reported
  - (Under 200 reported unsatisfactory)
- Generally expect recall to improve – what about precision?

Empirical evidence

- Precision at or above median TREC precision
  - Top scorer on almost 20% of TREC topics
- Slightly better on average than straight vector spaces
- Effect of dimensionality:

<table>
<thead>
<tr>
<th>Dimensions</th>
<th>Precision</th>
</tr>
</thead>
<tbody>
<tr>
<td>250</td>
<td>0.367</td>
</tr>
<tr>
<td>300</td>
<td>0.371</td>
</tr>
<tr>
<td>346</td>
<td>0.374</td>
</tr>
</tbody>
</table>
Failure modes

- Negated phrases
  - TREC topics sometimes negate certain query/terms phrases – automatic conversion of topics to

- Boolean queries
  - As usual, freetext/vector space syntax of LSI queries precludes (say) “Find any doc having to do with the following 5 companies”

- See Dumais for more.

But why is this clustering?

- We’ve talked about docs, queries, retrieval and precision here.
- What does this have to do with clustering?
- Intuition: Dimension reduction through LSI brings together “related” axes in the vector space.
Intuition from block matrices

$n$ documents

Vocabulary partitioned into $k$ topics (clusters); each doc discusses only one topic.
Intuition from block matrices

$n$ documents

$m$ terms

Block 1

Block 2

\[ \ldots \]

Block $k$

What's the best rank-$k$ approximation to this matrix?

0's

0's

= non-zero entries.

Likely there's a good rank-$k$ approximation to this matrix.

wiper
tire
V6

Block 1

Block 2

\[ \ldots \]

Block $k$

Few nonzero entries

Few nonzero entries

car 1 0
automobile 0 1

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The "dimensionality" of a corpus is the number of distinct topics represented in it.

More mathematical wild extrapolation:
- if $A$ has a rank $k$ approximation of low Frobenius error, then there are no more than $k$ distinct topics in the corpus.
LSI has many other applications

• In many settings in pattern recognition and retrieval, we have a feature-object matrix.
  – For text, the terms are features and the docs are objects.
  – Could be opinions and users … more in 276B.
• This matrix may be redundant in dimensionality.
  – Can work with low-rank approximation.
  – If entries are missing (e.g., users’ opinions), can recover if dimensionality is low.
• Powerful general analytical technique
  – Close, principled analog to clustering methods.

Resources

• http://www.cs.utk.edu/~berry/lsi++/
• http://lsi.argreenhouse.com/lsi/LSIpapers.html