Introduction to

Information Retrieval

Clustering

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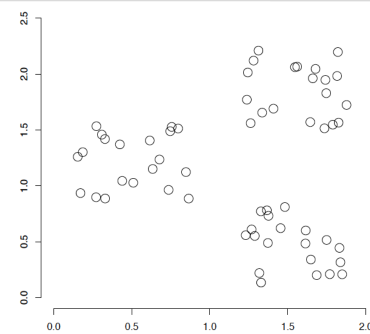
Today's Topic: Clustering

- Document clustering
  - Motivations
  - Document representations
  - Success criteria
- Clustering algorithms
  - Partitional
  - Hierarchical

What is clustering?

- Clustering: the process of grouping a set of objects into classes of similar objects
  - Documents within a cluster should be similar.
  - Documents from different clusters should be dissimilar.
- The commonest form of *unsupervised learning*
  - Unsupervised learning = learning from raw data, as opposed to supervised data where a classification of examples is given
  - A common and important task that finds many applications in IR and other places

A data set with clear cluster structure

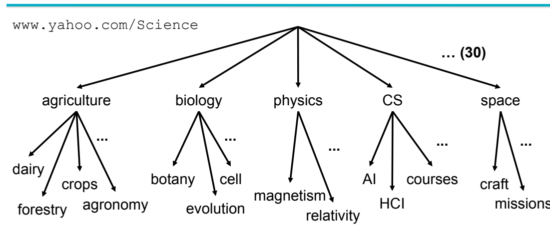


- How would you design an algorithm for finding the three clusters in this case?

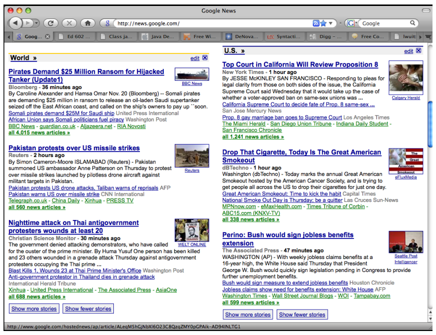
Applications of clustering in IR

- **Whole corpus analysis/navigation**
  - **Better user interface: search without typing**
- For improving recall in search applications
  - Better search results (like pseudo RF)
- For better navigation of search results
  - Effective "user recall" will be higher
- For speeding up vector space retrieval
  - Cluster-based retrieval gives faster search

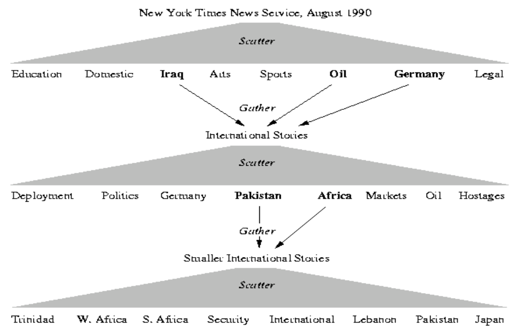
Yahoo! Hierarchy *isn't* clustering but *is* the kind of output you want from clustering



Google News: automatic clustering gives an effective news presentation metaphor



Scatter/Gather: Cutting, Karger, and Pedersen



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For improving search recall

- *Cluster hypothesis* - Documents in the same cluster behave similarly with respect to relevance to information needs
- 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?

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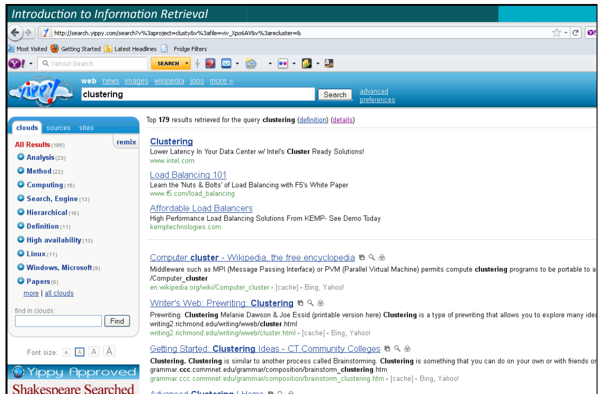

yippy.com – grouping search results 12

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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
      - 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.

Notion of similarity/distance

- Ideal: semantic similarity.
- Practical: term-statistical similarity (docs as vectors)
  - Cosine similarity
  - For many algorithms, easier to think in terms of a *distance* (rather than similarity) between docs.
  - We will mostly speak of Euclidean distance
    - But real implementations use cosine similarity

Hard vs. soft clustering

- Hard clustering: Each document belongs to exactly one cluster
  - More common and easier to do
- Soft clustering: A document can belong to more than one cluster.
  - Makes more sense for applications like creating browsable hierarchies
  - You may want to put a pair of sneakers in two clusters: (i) sports apparel and (ii) shoes
  - You can only do that with a soft clustering approach.
- We won't do soft clustering today. See IIR 16.5, 18

Clustering Algorithms

- Flat algorithms
  - Usually start with a random (partial) partitioning
  - Refine it iteratively
    - *K* means 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
    - Intractable for many objective functions
    - Ergo, exhaustively enumerate all partitions
  - Effective heuristic methods: *K*-means and *K*-medoids algorithms

See also Kleinberg NIPS 2002 – impossibility for natural clustering

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*:

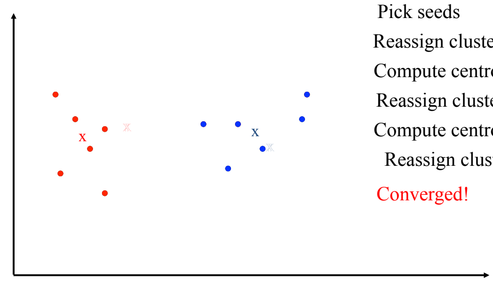
$$\vec{\mu}(c) = \frac{1}{|c|}\sum_{\vec{x} \in c} \vec{x}$$

- 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

Select *K* random docs $\{s_1, s_2, \dots s_K\}$ as seeds.
Until clustering *converges* (or other stopping criterion):
For each doc d_i:
Assign d_i to the cluster c_j such that $dist(x_i, s_j)$ is minimal.
(*Next, 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?

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.
    - But in practice usually isn't

Convergence of *K*-Means

- Residual Sum of Squares (RSS), a goodness measure of a cluster, is the sum of squared distances from the cluster centroid:
  - $RSS_j = \Sigma_i ||d_i - c_j||^2$ (sum over all d_i in cluster *j*)
- $RSS = \Sigma_j RSS_j$
- Reassignment monotonically decreases RSS since each vector is assigned to the closest centroid.
- Recomputation also monotonically decreases each RSS_j because …

Cluster recomputation in K-means

- $RSS_j = \Sigma_i \, || d_i - c_j ||^2 = \Sigma_i \Sigma_k \, (d_{ik} - c_{jk})^2$
  - i ranges over documents in cluster j
- RSS_j reaches minimum when:
- $\Sigma_i -2(d_{ik} - c_{jk}) = 0$ (for each c_{jk})
- $\Sigma_i \, c_{jk} = \Sigma_i \, d_{ik}$
- $m_j \, c_{jk} = \Sigma_i \, d_{ik}$ (m_j is # of docs in cluster j)
- $c_{jk} = (1/ m_j) \, \Sigma_i \, d_{ik}$
- *K*-means typically converges quickly

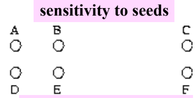
Time Complexity

- Computing distance between two docs is O(*M*) where *M* is the dimensionality of the vectors.
- Reassigning clusters: O(*KN*) distance computations, or O(*KNM*).
- Computing centroids: Each doc gets added once to some centroid: O(*NM*).
- Assume these two steps are each done once for *I* iterations: O(*IKNM*).

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}

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" by default
  - But can add outlier filtering

Dhillon et al. ICDM 2002 – variation to fix some issues with small document clusters

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.

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.

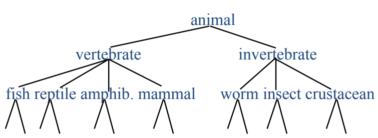
Why is there always a clustering of Total Benefit *n*?

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.

Hierarchical Clustering

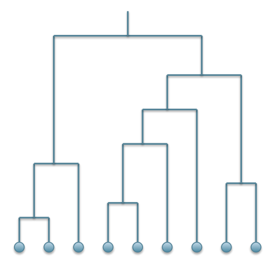
- Build a tree-based hierarchical taxonomy (*dendrogram*) from a set of documents.



- One approach: recursive application of a partitional clustering algorithm.

Dendrogram: Hierarchical Clustering

- Clustering obtained by cutting the dendrogram at a desired level: each connected component forms a cluster.



Hierarchical Agglomerative Clustering (HAC)

- Starts with each doc in a separate cluster
  - then repeatedly joins the *closest pair* of clusters, until there is only one cluster.
- The history of merging forms a binary tree or hierarchy.

Note: the resulting clusters are still "hard" and induce a partition

Closest pair of clusters

- Many variants to defining closest pair of clusters
- **Single-link**
  - Similarity of the *most* cosine-similar (single-link)
- **Complete-link**
  - Similarity of the "furthest" points, the *least* cosine-similar
- **Centroid**
  - Clusters whose centroids (centers of gravity) are the most cosine-similar
- **Group average**
  - Average cosine between all pairs of elements

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Single Link Agglomerative Clustering

- Use maximum similarity of pairs:

$$sim(c_i, c_j) = \max_{x \in c_i, y \in c_j} sim(x, y)$$

- Can result in "straggly" (long and thin) clusters due to chaining effect.
- After merging c_i and c_j, the similarity of the resulting cluster to another cluster, c_k, is:

$$sim((c_i \cup c_j), c_k) = \max(sim(c_i, c_k), sim(c_j, c_k))$$

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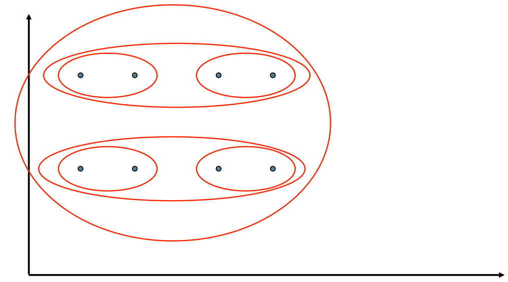
Single Link Example



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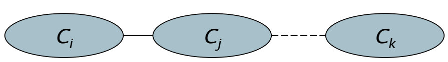
Complete Link

- Use minimum similarity of pairs:

$$sim(c_i, c_j) = \min_{x \in c_i, y \in c_j} sim(x, y)$$

- 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:

$$sim((c_i \cup c_j), c_k) = \min(sim(c_i, c_k), sim(c_j, c_k))$$



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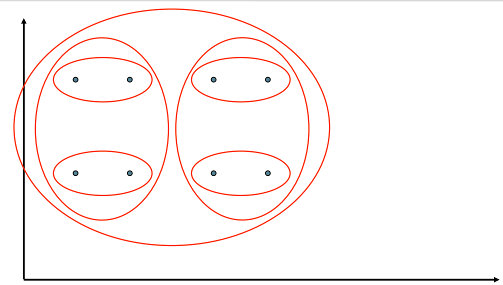
Complete Link Example



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General HAC algorithm and complexity

1. Compute similarity between all pairs of documents
   - O(N²) → $O(N^2)$
2. Do N – 1 times
   1. Find closest pair of documents/clusters to merge
      - Naïve: $O(N^2)$ Priority Queue: O(N) Single link: O(N)
   2. Update similarity of all documents/clusters to new cluster
      - Naïve: O(N) Priority Queue: O(N log N) Single link: O(N)

Best merge persistent!

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Group Average

- Similarity of two clusters = average similarity of all pairs within merged cluster.

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

- 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
- No clear difference in efficacy

Computing Group Average Similarity

- Always maintain sum of vectors in each cluster.

$$\vec{s}(c_j) = \sum_{\vec{x} \in c_j} \vec{x}$$

- Compute similarity of clusters in constant time:

$$sim(c_i, c_j) = \frac{(\vec{s}(c_i) + \vec{s}(c_j)) \bullet (\vec{s}(c_i) + \vec{s}(c_j)) - (|c_i| + |c_j|)}{(|c_i| + |c_j|)(|c_i| + |c_j| - 1)}$$

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 criteria for clustering quality

- Quality measured by its ability to discover some or all of the hidden patterns or latent classes in gold standard data
- Assesses a clustering with respect to ground truth … requires *labeled data*
- Assume documents with *C* gold standard classes, while our clustering algorithms produce *K* clusters, $\omega_1, \omega_2, \ldots, \omega_K$ with n_i members.

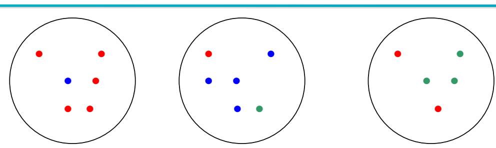
External Evaluation of Cluster Quality

- Simple measure: purity, the ratio between the dominant class in the cluster ω_i and the size of cluster ω_i

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

- Biased because having *n* clusters maximizes purity
- Others are entropy of classes in clusters (or mutual information between classes and clusters)

Purity example



Cluster I Cluster II Cluster III

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

Rand Index measures between pair decisions. Here RI = 0.68

Number of point pairs	Same Cluster in clustering	Different Clusters in clustering
Same class in ground truth	20	24
Different classes in ground truth	20	72

Rand index and Cluster F-measure

$$RI = \frac{A + D}{A + B + C + D}$$

Compare with standard Precision and Recall:

$$P = \frac{A}{A + B} \qquad R = \frac{A}{A + C}$$

People also define and use a cluster F-measure, which is probably a better measure.

Final word and resources

- In clustering, clusters are inferred from the data without human input (unsupervised learning)
- However, in practice, it's a bit less clear: there are many ways of influencing the outcome of clustering: number of clusters, similarity measure, representation of documents, . . .
- Resources
  - IIR 16 except 16.5
  - IIR 17.1–17.3