Introduction to Information Retrieval
http://informationretrieval.org

IIR 16: Flat Clustering

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Overview

1. Recap
2. Introduction
3. Clustering in IR
4. K-means
5. Evaluation
6. How many clusters?

Outline

1. Recap
2. Introduction
3. Clustering in IR
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MI example for *poultry*/EXPORT in Reuters

	$e_c = e_{poultry} = 1$	$e_c = e_{poultry} = 0$
$e_t = e_{\text{EXPORT}} = 1$	$N_{11} = 49$	$N_{10} = 27{,}652$
$e_t = e_{\text{EXPORT}} = 0$	$N_{01} = 141$	$N_{00} = 774{,}106$

Plug these values into formula:

$$
\begin{aligned}
I(U;C) &= \frac{49}{801{,}948}\log_2\frac{801{,}948\cdot 49}{(49+27{,}652)(49+141)} \\
&\quad+\frac{141}{801{,}948}\log_2\frac{801{,}948\cdot 141}{(141+774{,}106)(49+141)} \\
&\quad+\frac{27{,}652}{801{,}948}\log_2\frac{801{,}948\cdot 27{,}652}{(49+27{,}652)(27{,}652+774{,}106)} \\
&\quad+\frac{774{,}106}{801{,}948}\log_2\frac{801{,}948\cdot 774{,}106}{(141+774{,}106)(27{,}652+774{,}106)} \\
&\approx 0.000105
\end{aligned}
$$

Linear classifiers

- Linear classifiers compute a linear combination or weighted sum $\sum_i w_i x_i$ of the feature values.
- Classification decision: $\sum_i w_i x_i > \theta$?
- Geometrically, the equation $\sum_i w_i x_i = \theta$ defines a line (2D), a plane (3D) or a hyperplane (higher dimensionalities).
- Assumption: The classes are linearly separable.
- Methods for finding a linear separator: Perceptron, Rocchio, Naive Bayes, many others

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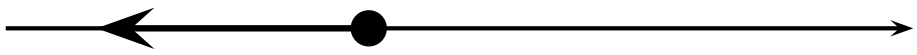

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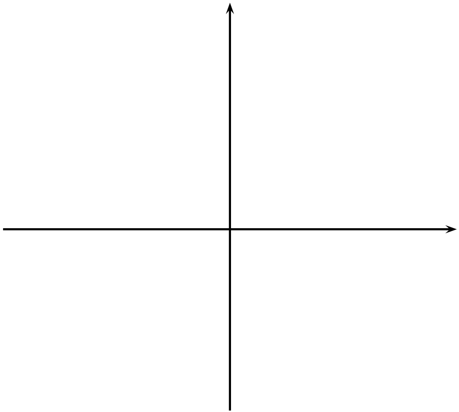
A linear classifier in 2D



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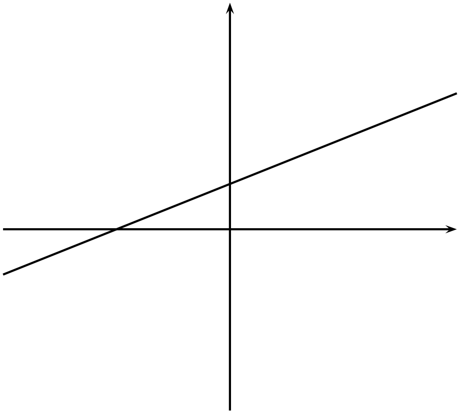

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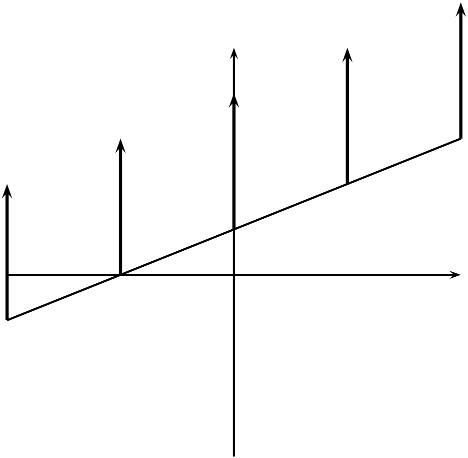

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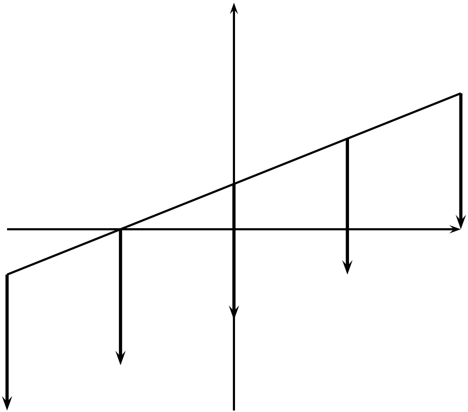

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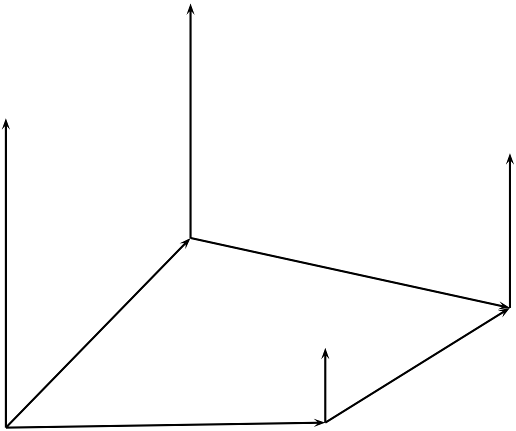

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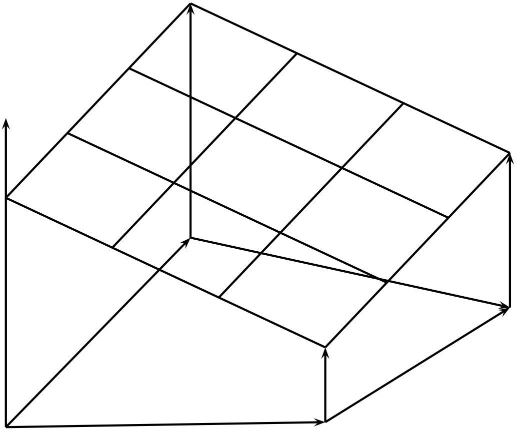

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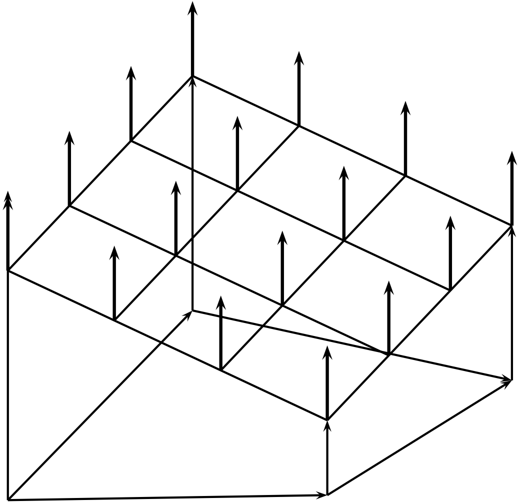

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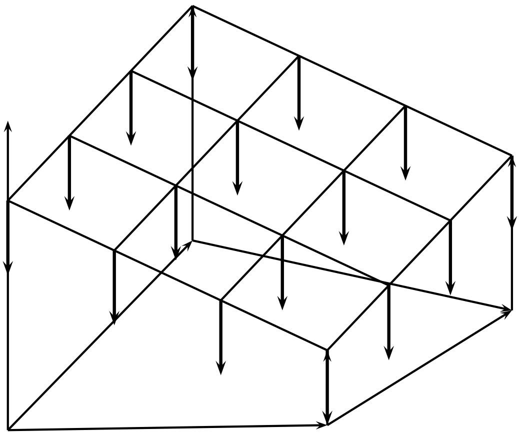

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Rocchio as a linear classifier

- Rocchio is a linear separator defined by:

$$\sum_{i=1}^{M} w_i d_i = \vec{w}\vec{d} = \theta$$

where the normal vector $\vec{w} = \vec{\mu}(c_1) - \vec{\mu}(c_2)$ and $\theta = 0.5 * (|\vec{\mu}(c_1)|^2 - |\vec{\mu}(c_2)|^2)$.

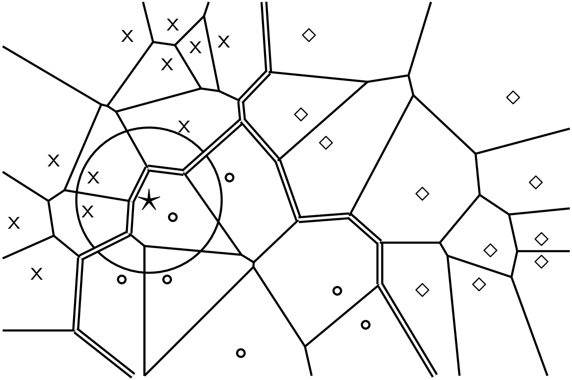
Naive Bayes as a linear classifier

Naive Bayes is a linear separator defined by:

$$\sum_{i=1}^{M} w_i d_i = \theta$$

where $w_i = \log[\hat{P}(t_i|c)/\hat{P}(t_i|\bar{c})]$, d_i = number of occurrences of t_i in d, and $\theta = -\log[\hat{P}(c)/\hat{P}(\bar{c})]$. Here, the index i, $1 \leq i \leq M$, refers to terms of the vocabulary (not to positions in d as k did in our original definition of Naive Bayes)

kNN is not a linear classifier



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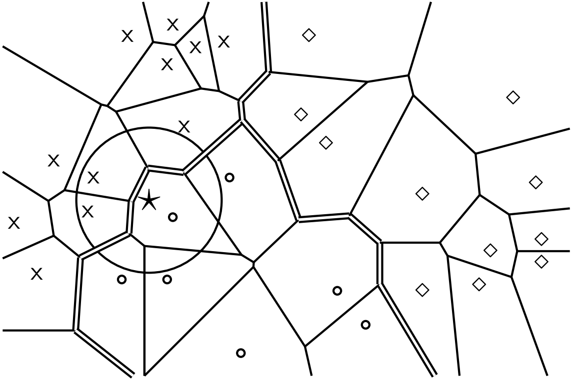

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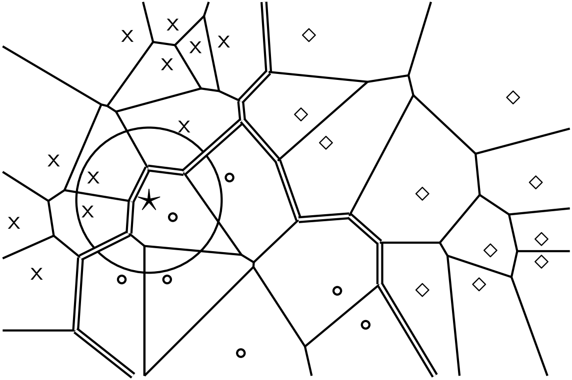

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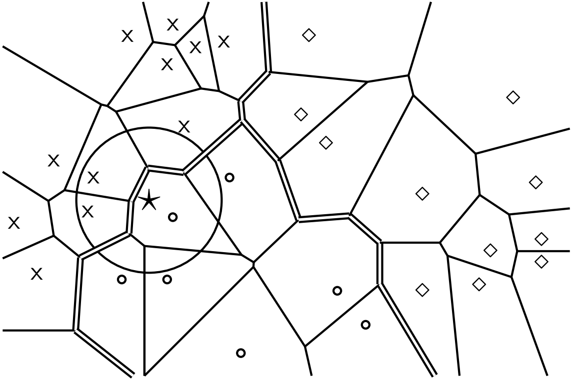

- Classification decision based on majority of k nearest neighbors.
- The decision boundaries between classes are piecewise linear . . .
- . . . but they are not linear separators that can be described as $\sum_{i=1}^{M} w_i d_i = \theta$.

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What is clustering?

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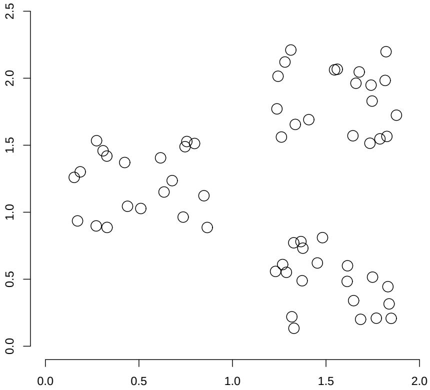
- Clustering is the most common form of unsupervised learning.
- Unsupervised = there are no labeled or annotated data.

Data set with clear cluster structure



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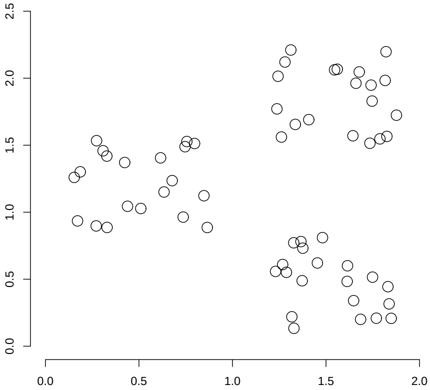

How would you design an algorithm for finding the three clusters in this case?

Classification vs. Clustering

- Classification: supervised learning

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- Classification: supervised learning
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- Classification: supervised learning
- Clustering: unsupervised learning
- Classification: Classes are human-defined and part of the input to the learning algorithm.
- Clustering: Clusters are inferred from the data without human input.
  - However, there are many ways of influencing the outcome of clustering: number of clusters, similarity measure, representation of documents, ...

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The cluster hypothesis

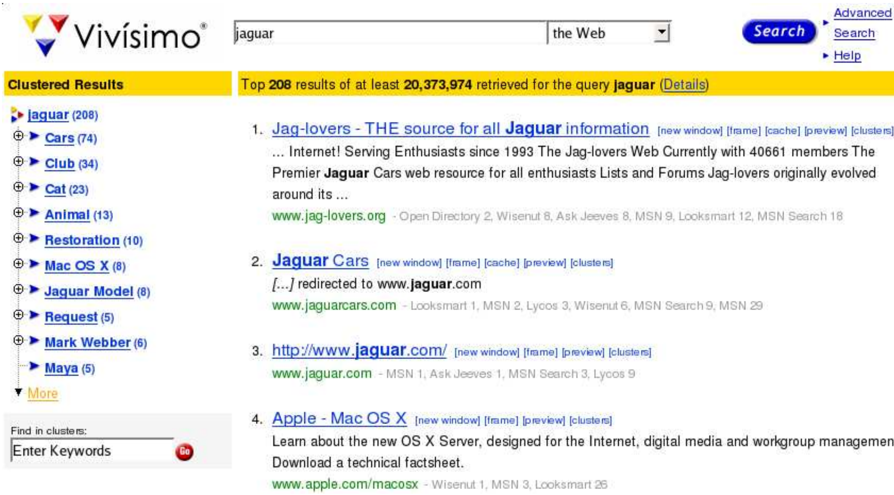
Cluster hypothesis. Documents in the same cluster behave similarly with respect to relevance to information needs.

All applications in IR are based (directly or indirectly) on the cluster hypothesis.

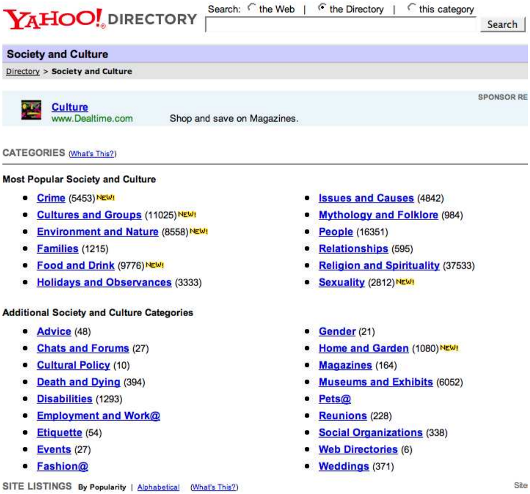
Applications of clustering in IR

Application	What is clustered?	Benefit	Example
Search result clustering	search results	more effective information presentation to user	
Scatter-Gather	(subsets of) collection	alternative user interface: "search without typing"	
Collection clustering	collection	effective information presentation for exploratory browsing	McKeown et al. 2002, http://news.google.com
Language modeling	collection	increased precision and/or recall	Liu&Croft 2004
Cluster-based retrieval	collection	higher efficiency: faster search	Salton 1971

Search result clustering for better navigation



Global navigation: Yahoo



Global navigation: MESH (upper level)

MeSH Tree Structures - 2008

Return to Entry Page

1. Anatomy [A]
2. Organisms [B]
3. Diseases [C]
   - Bacterial Infections and Mycoses [C01] +
   - Virus Diseases [C02] +
   - Parasitic Diseases [C03] +
   - Neoplasms [C04] +
   - Musculoskeletal Diseases [C05] +
   - Digestive System Diseases [C06] +
   - Stomatognathic Diseases [C07] +
   - Respiratory Tract Diseases [C08] +
   - Otorhinolaryngologic Diseases [C09] +
   - Nervous System Diseases [C10] +
   - Eye Diseases [C11] +
   - Male Urogenital Diseases [C12] +
   - Female Urogenital Diseases and Pregnancy Complications [C13] +
   - Cardiovascular Diseases [C14] +
   - Hemic and Lymphatic Diseases [C15] +
   - Congenital, Hereditary, and Neonatal Diseases and Abnormalities [C16] +
   - Skin and Connective Tissue Diseases [C17] +
   - Nutritional and Metabolic Diseases [C18] +
   - Endocrine System Diseases [C19] +
   - Immune System Diseases [C20] +
   - Disorders of Environmental Origin [C21] +
   - Animal Diseases [C22] +
   - Pathological Conditions, Signs and Symptoms [C23] +
4. Chemicals and Drugs [D]
5. Analytical, Diagnostic and Therapeutic Techniques and Equipment [E]
6. Psychiatry and Psychology [F]
7. Biological Sciences [G]
8. Natural Sciences [H]
9. Anthropology, Education, Sociology and Social Phenomena [I]
10. Technology, Industry, Agriculture [J]
11. Humanities [K]

Global navigation: MESH (lower level)

- Neoplasms [C04]
  - Cysts [C04.182] +
  - Hamartoma [C04.445] +
  - ➤ Neoplasms by Histologic Type [C04.557]
    - Histiocytic Disorders, Malignant [C04.557.227] +
    - Leukemia [C04.557.337] +
    - Lymphatic Vessel Tumors [C04.557.375] +
    - Lymphoma [C04.557.386] +
    - Neoplasms, Complex and Mixed [C04.557.435] +
    - Neoplasms, Connective and Soft Tissue [C04.557.450] +
    - Neoplasms, Germ Cell and Embryonal [C04.557.465] +
    - Neoplasms, Glandular and Epithelial [C04.557.470] +
    - Neoplasms, Gonadal Tissue [C04.557.475] +
    - Neoplasms, Nerve Tissue [C04.557.580] +
    - Neoplasms, Plasma Cell [C04.557.595] +
    - Neoplasms, Vascular Tissue [C04.557.645] +
    - Nevi and Melanomas [C04.557.665] +
    - Odontogenic Tumors [C04.557.695] +
  - Neoplasms by Site [C04.588] +
  - Neoplasms, Experimental [C04.619] +
  - Neoplasms, Hormone-Dependent [C04.626]
  - Neoplasms, Multiple Primary [C04.651] +
  - Neoplasms, Post-Traumatic [C04.666]
  - Neoplasms, Radiation-Induced [C04.682] +
  - Neoplasms, Second Primary [C04.692]
  - Neoplastic Processes [C04.697] +
  - Neoplastic Syndromes, Hereditary [C04.700] +
  - Paraneoplastic Syndromes [C04.730] +
  - Precancerous Conditions [C04.834] +
  - Pregnancy Complications, Neoplastic [C04.850] +
  - Tumor Virus Infections [C04.925] +

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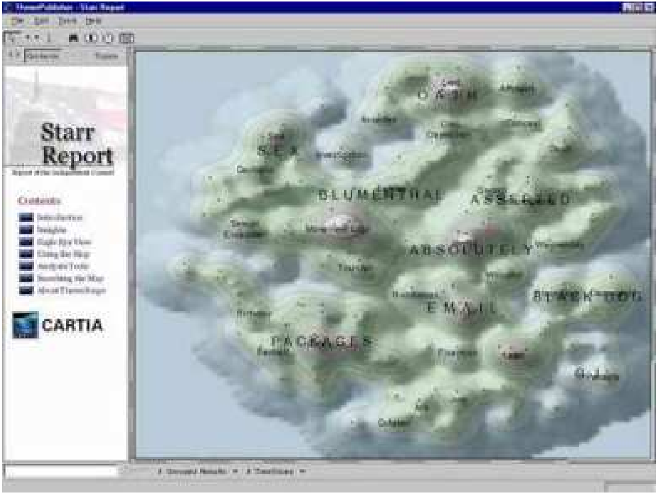
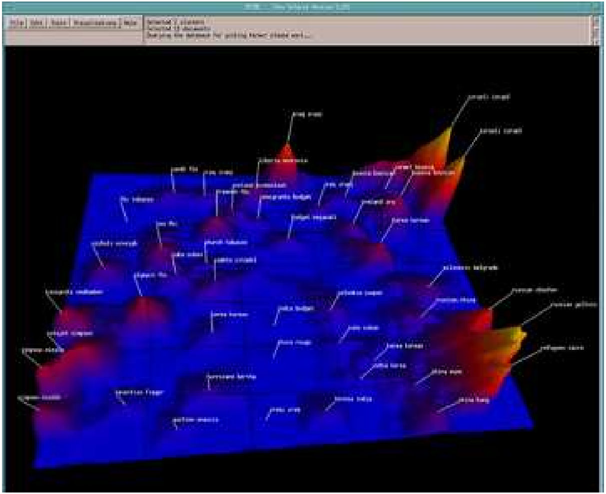
  - Google News

Global navigation combined with visualization (1)



Global navigation combined with visualization (2)



Global clustering for navigation: Google News

http://news.google.com

Clustering for improving recall

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Document representations in clustering

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Document representations in clustering

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- As in vector space classification, we measure relatedness between vectors by Euclidean distance ...
- ... which is equivalent to cosine similarity.
- Recall: centroids are not length-normalized.
- For centroids, distance and cosine give different results.

Issues in clustering

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- Often: secondary goals in clustering
  - Example: avoid very small and very large clusters

Flat vs. Hierarchical clustering

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- We won't have time for soft clustering. See IIR 16.5, IIR 18

Our plan

- This lecture: Flat, hard clustering

Our plan

- This lecture: Flat, hard clustering
- Next lecture: Hierarchical, hard clustering

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- Global optimization: exhaustively enumerate partitions, pick optimal one
  - Not tractable

Flat algorithms

- Flat algorithms compute a partition of N documents into a set of K clusters.
- Given: a set of documents and the number K
- Find: a partition in K clusters that optimizes the chosen partitioning criterion
- Global optimization: exhaustively enumerate partitions, pick optimal one
  - Not tractable
- Effective heuristic method: K-means algorithm

Outline

1. Recap
2. Introduction
3. Clustering in IR
4. K-means
5. Evaluation
6. How many clusters?

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- We try to find the minimum average squared difference by iterating two steps:
  - reassignment: assign each vector to its closest centroid
  - recomputation: recompute each centroid as the average of the vectors that were assigned to it in reassignment

K-means algorithm

K-MEANS$(\{\vec{x}_1, \ldots, \vec{x}_N\}, K)$

$(\vec{s}_1, \vec{s}_2, \ldots, \vec{s}_K) \leftarrow$ SELECTRANDOMSEEDS$(\{\vec{x}_1, \ldots, \vec{x}_N\}, K)$
for $k \leftarrow 1$ **to** K
do $\vec{\mu}_k \leftarrow \vec{s}_k$
while stopping criterion has not been met
do for $k \leftarrow 1$ **to** K
    do $\omega_k \leftarrow \{\}$
    for $n \leftarrow 1$ **to** N
    do $j \leftarrow \arg\min_{j'} |\vec{\mu}_{j'} - \vec{x}_n|$
        $\omega_j \leftarrow \omega_j \cup \{\vec{x}_n\}$ *(reassignment of vectors)*
    for $k \leftarrow 1$ **to** K
    do $\vec{\mu}_k \leftarrow \frac{1}{|\omega_k|} \sum_{\vec{x} \in \omega_k} \vec{x}$ *(recomputation of centroids)*
return $\{\vec{\mu}_1, \ldots, \vec{\mu}_K\}$

K-means example

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- But complete convergence can take many more iterations.

Recomputation decreases average distance

$\text{RSS} = \sum_{k=1}^{K} \text{RSS}_k$ – the residual sum of squares (the “goodness” measure)

$$\begin{aligned} \text{RSS}_k(\vec{v}) &= \sum_{\vec{x} \in \omega_k} \|\vec{v} - \vec{x}\|^2 = \sum_{\vec{x} \in \omega_k} \sum_{m=1}^{M} (v_m - x_m)^2 \\ \frac{\partial \text{RSS}_k(\vec{v})}{\partial v_m} &= \sum_{\vec{x} \in \omega_k} 2(v_m - x_m) = 0 \end{aligned}$$

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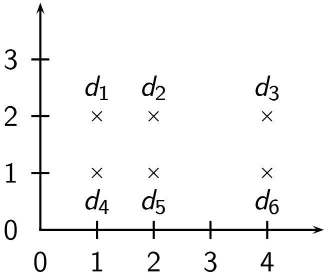
- This is the great weakness of K-means.
- If we start with a bad set of seeds, the resulting clustering can be horrible.

Example for suboptimal clustering



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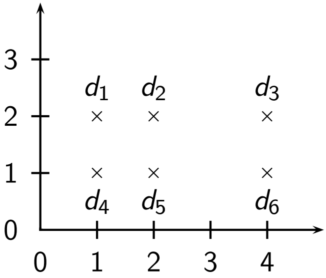

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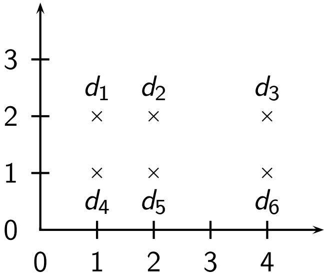

- What is the optimal clustering for $K = 2$?
- Do we converge on this clustering for arbitrary seeds d_{i_1}, d_{i_2}?

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  - Select i (e.g., $i = 10$) different sets of seeds, do a K-means clustering for each, select the clustering with lowest RSS

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- However: This is not a real worst-case analysis.
- In pathological cases, the number of iterations can be much higher than linear in the number of documents.

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- First measure for how well we were able to reproduce the classes: purity

External criterion: Purity

$$\text{purity}(\Omega, C) = \frac{1}{N} \sum_k \max_j |\omega_k \cap c_j|$$

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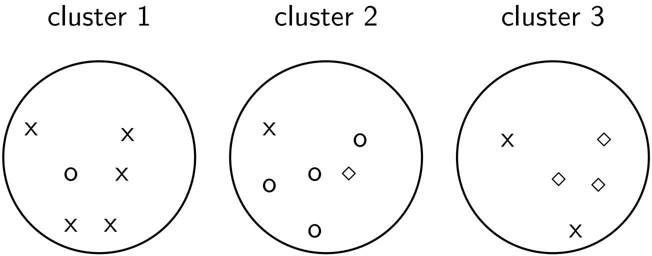
- For each cluster ω_k: find class c_j with most members n_{kj} in ω_k
- Sum all n_{kj} and divide by total number of points

Example for computing purity



Majority class and number of members of the majority class for the three clusters are: x, 5 (cluster 1); o, 4 (cluster 2); and $\diamond$, 3 (cluster 3). Purity is $(1/17) \times (5 + 4 + 3) \approx 0.71$.

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- ... and either "true" (correct) or "false" (incorrect): the clustering decision is correct or incorrect.

As an example, we compute RI for the o/$\diamond$/x example. We first compute TP + FP. The three clusters contain 6, 6, and 5 points, respectively, so the total number of "positives" or pairs of documents that are in the same cluster is:

$$\text{TP} + \text{FP} = \binom{6}{2} + \binom{6}{2} + \binom{5}{2} = 40$$

Of these, the x pairs in cluster 1, the o pairs in cluster 2, the $\diamond$ pairs in cluster 3, and the x pair in cluster 3 are true positives:

$$\text{TP} = \binom{5}{2} + \binom{4}{2} + \binom{3}{2} + \binom{2}{2} = 20$$

Thus, FP $= 40 - 20 = 20$.
FN and TN are computed similarly.

Rand measure for the o/$\diamond$/x example

	same cluster	different clusters
same class	TP = 20	FN = 24
different classes	FP = 20	TN = 72

RI is then $(20 + 72)/(20 + 20 + 24 + 72) \approx 0.68$.

Evaluation results for the o/$\diamond$/x example

	purity	NMI	RI	F_5
lower bound	0.0	0.0	0.0	0.0
maximum	1.0	1.0	1.0	1.0
value for example	0.71	0.36	0.68	0.46

All four measures range from 0 (really bad clustering) to 1 (perfect clustering).

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    - Like Rand, but "precision" and "recall" can be weighted

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  - Why can't we use RSS or average squared distance from centroid?

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  - Start with 1 cluster ($K = 1$)
  - Keep adding clusters (= keep increasing K)
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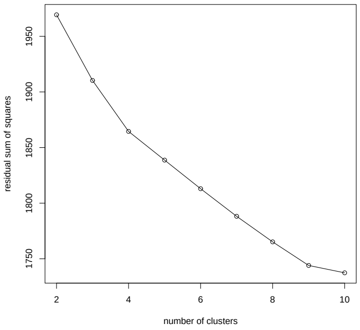
- Still need to determine good value for λ ...

Finding the "knee" in the curve



Pick the number of clusters where curve "flattens". Here: 4 or 9.

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- Clusty/Vivisimo: search result clustering