Introduction to Information Retrieval
`http://informationretrieval.org`

IIR 16: Flat Clustering

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Overview

Outline

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:

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

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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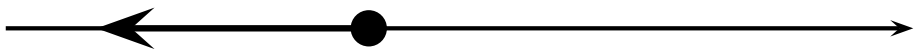

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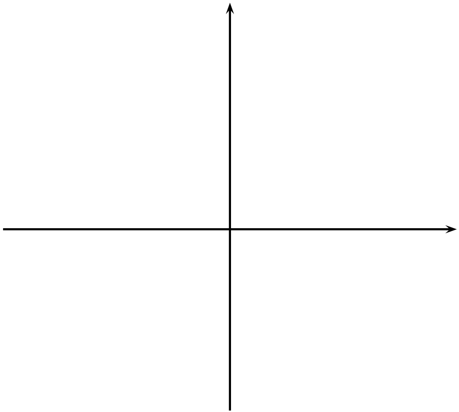

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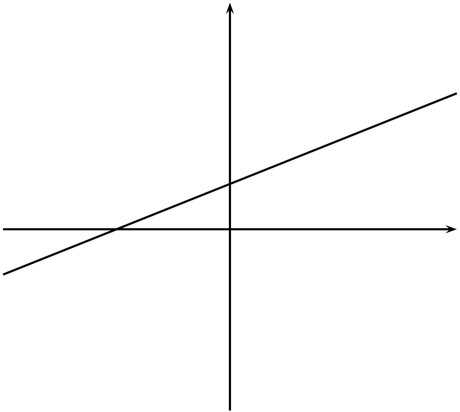

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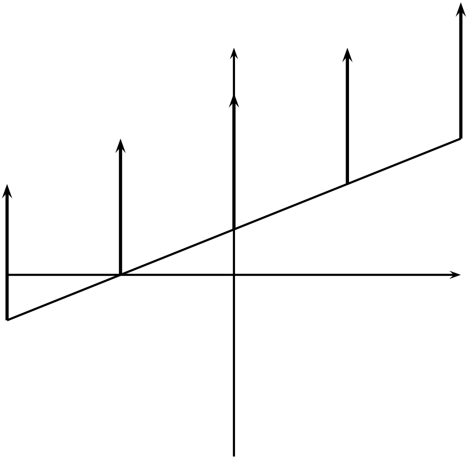

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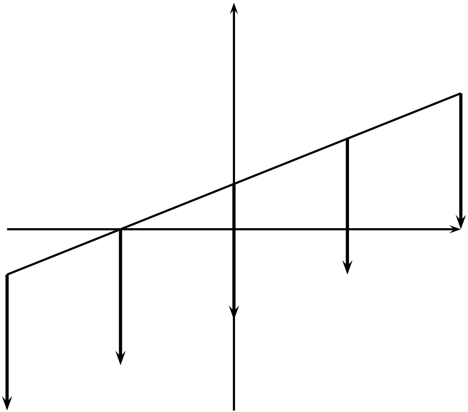

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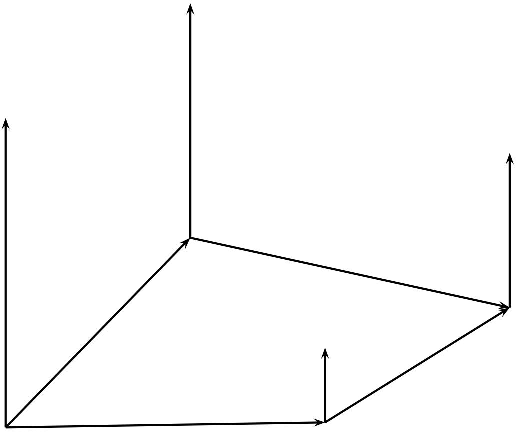

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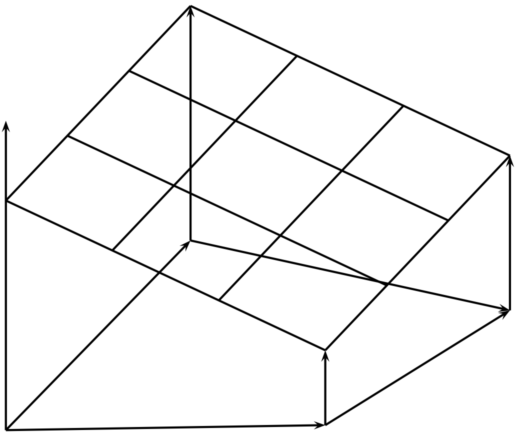

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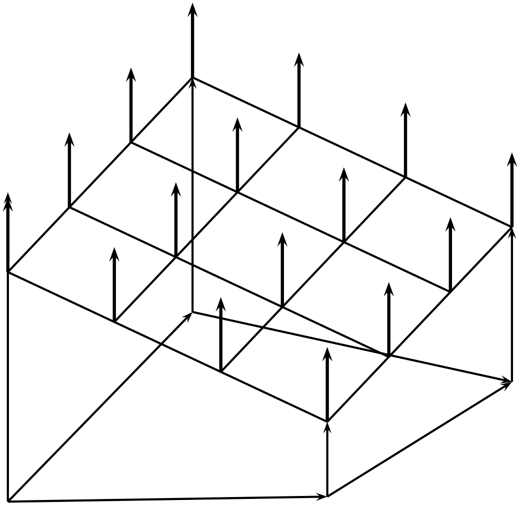

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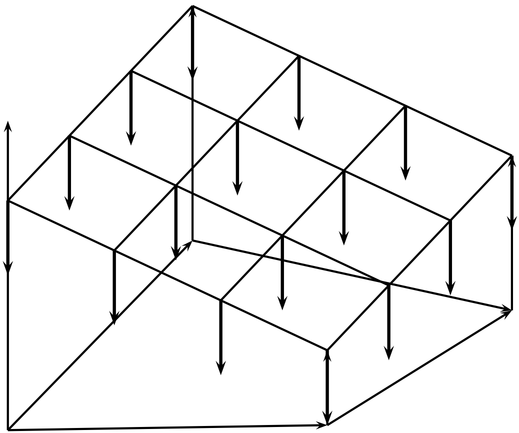

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Rocchio as a linear classifier

- 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 $\theta = 0.5 * (|\vec{\mu}(c_1)|^2 - |\vec{\mu}(c_2)|^2)$.

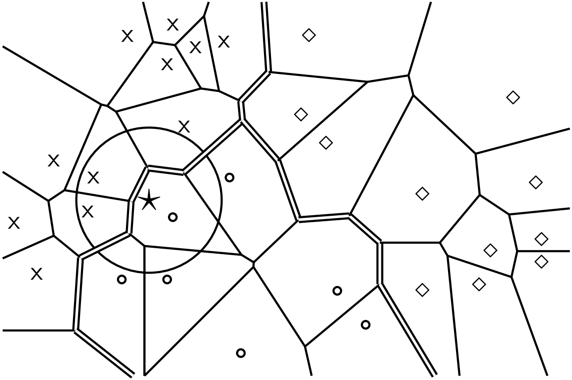
Naive Bayes as a linear classifier

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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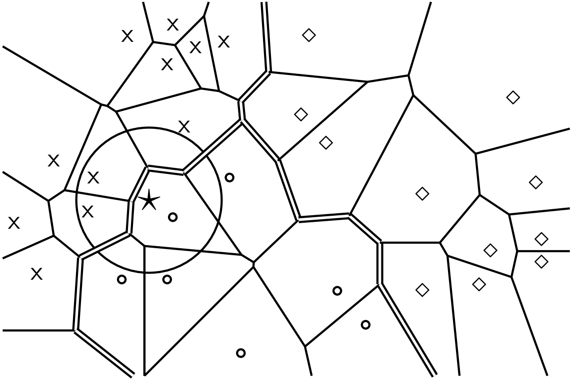

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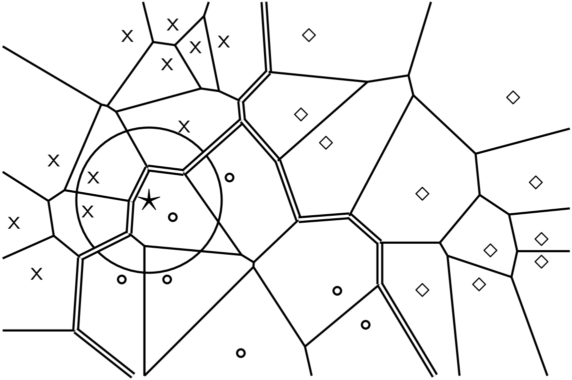

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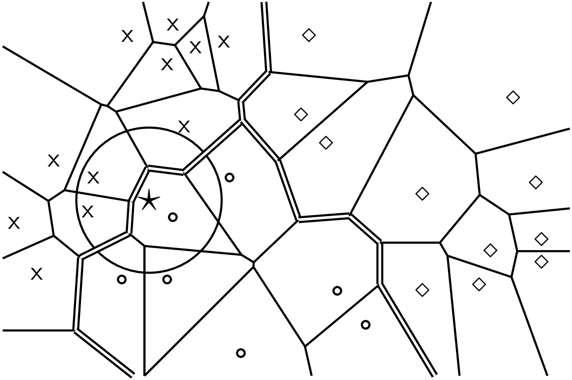

- Classification decision based on majority of k nearest neighbors.
- The decision boundaries between classes are piecewise linear ...
- ... but they are not linear separators that can be described as $\sum_{i=1}^{M} w_i d_i = \theta$.

Outline

What is clustering?

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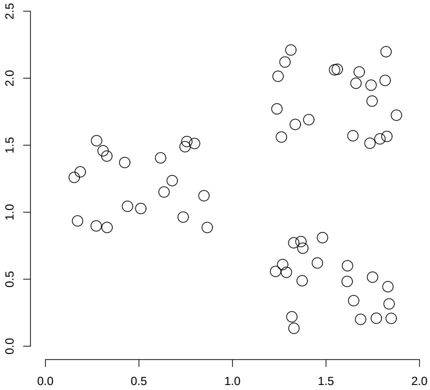
- Clustering is the most common form of unsupervised learning.
- Unsupervised = there are no labeled or annotated data.

Data set with clear cluster structure



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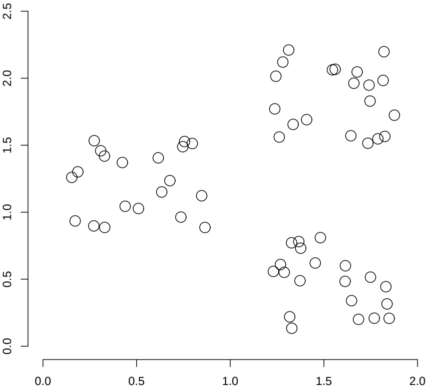

How would you design an algorithm for finding the three clusters in this case?

Classification vs. Clustering

- Classification: supervised learning

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- Classification: 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, ...

Outline

The cluster hypothesis

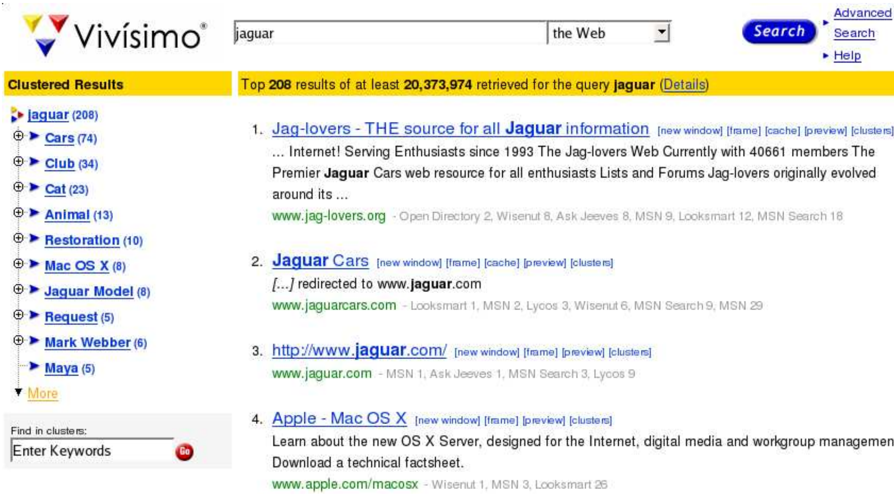
Cluster hypothesis. Documents in the same cluster behave similarly with respect to relevance to information needs.

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

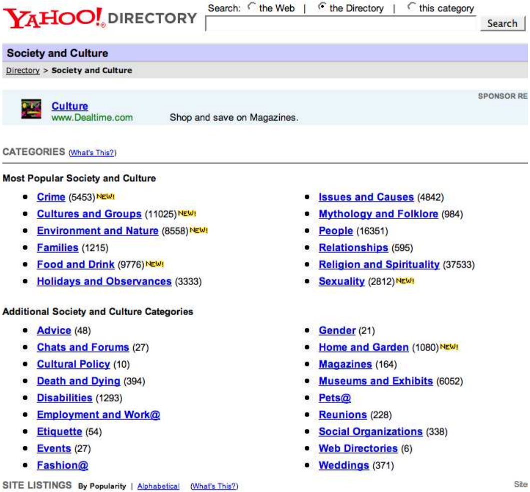
Applications of clustering in IR

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)

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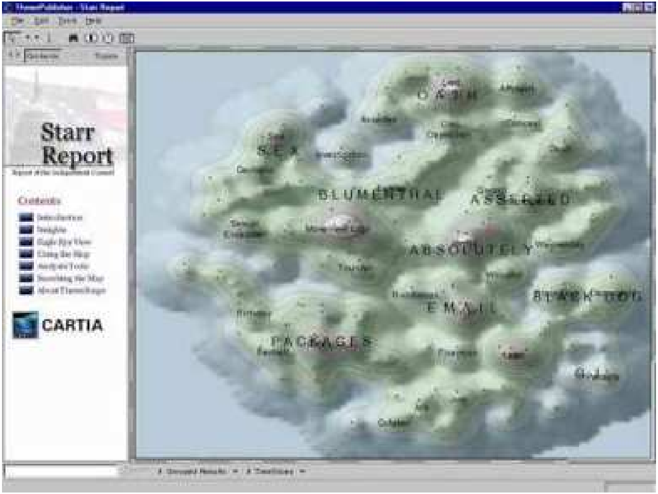
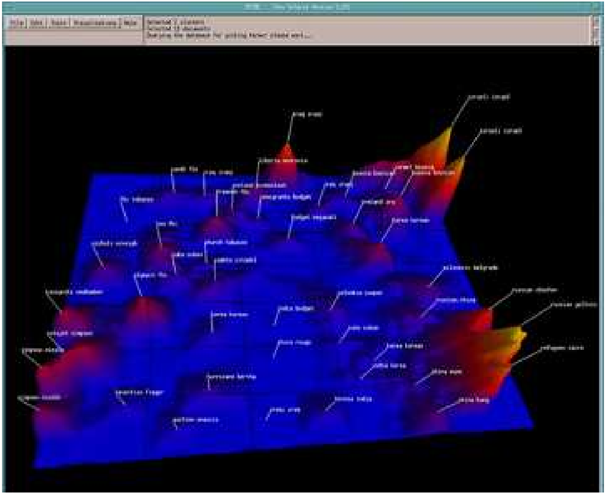
Global navigation combined with visualization (1)



Global navigation combined with visualization (2)



Global clustering for navigation: Google News

http://news.google.com

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- Recall: centroids are not length-normalized.
- For centroids, distance and cosine give different results.

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    - Example: avoid very small and very large clusters

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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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- Effective heuristic method: K-means algorithm

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  - 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

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

$(\vec{s}_1, \vec{s}_2, \ldots, \vec{s}_K) \leftarrow \text{SELECTRANDOMSEEDS}(\{\vec{x}_1, \ldots, \vec{x}_N\}, K)$

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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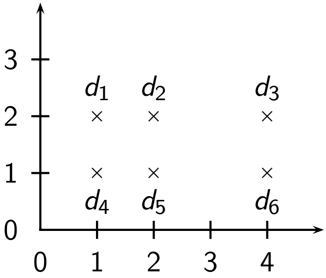
- If we start with a bad set of seeds, the resulting clustering can be horrible.

Example for suboptimal clustering



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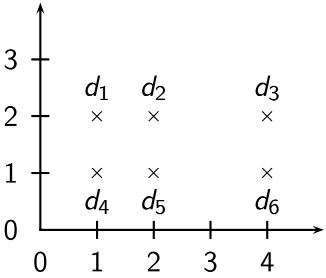

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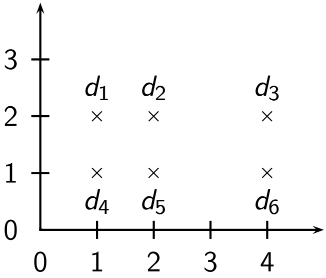

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- Do we converge on this clustering for arbitrary seeds d_{i_1}, d_{i_2}?

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- In pathological cases, the number of iterations can be much higher than linear in the number of documents.

Outline

What is a good clustering?

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  - Evaluate with respect to a human-defined classification

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- Goal: Clustering should reproduce the classes in the gold standard
- (But we only want to reproduce how documents are divided into groups, not the class labels.)
- First measure for how well we were able to reproduce the classes: purity

External criterion: Purity

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

- $\Omega = \{\omega_1, \omega_2, \ldots, \omega_K\}$ is the set of clusters and $C = \{c_1, c_2, \ldots, c_J\}$ is the set of classes.

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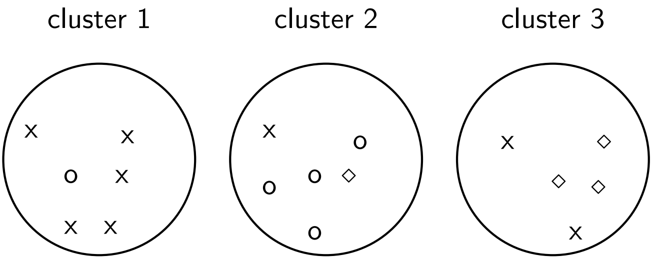
- For each cluster ω_k: find class c_j with most members n_{kj} in ω_k
- Sum all n_{kj} and divide by total number of points

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/◇/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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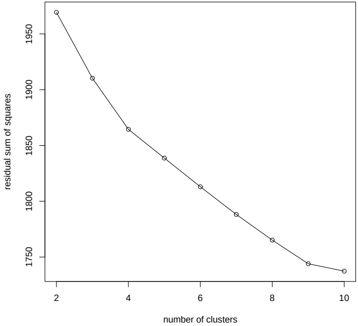
- Still need to determine good value for λ ...

Finding the "knee" in the curve



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

Resources

- Chapter 16 of IIR

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- Clusty/Vivisimo: search result clustering