

Introduction to Information Retrieval

<http://informationretrieval.org>

IIR 16: Flat Clustering

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2014-06-11

Overview

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

Outline

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Learning to rank for zone scoring

Given query q and document d , weighted zone scoring assigns to the pair (q, d) a score in the interval $[0,1]$ by computing a **linear combination** of document zone scores, where each zone contributes a value.

- Consider a set of documents, which have l zones
- Let $g_1, \dots, g_l \in [0, 1]$, such that $\sum_{i=1}^l g_i = 1$
- For $1 \leq i \leq l$, let s_i be the Boolean score denoting a match (or non-match) between q and the i^{th} zone
 - $s_i = 1$ if a query term occurs in zone i , 0 otherwise

Weighted zone scoring aka ranked Boolean retrieval

Rank documents according to $\sum_{i=1}^l g_i s_i$

Learning to rank approach: learn the weights g_i from training data

Training set for learning to rank

Φ_j	d_j	q_j	s_T	s_B	$r(d_j, q_j)$
Φ_1	37	linux	1	1	Relevant
Φ_2	37	penguin	0	1	Nonrelevant
Φ_3	238	system	0	1	Relevant
Φ_4	238	penguin	0	0	Nonrelevant
Φ_5	1741	kernel	1	1	Relevant
Φ_6	2094	driver	0	1	Relevant
Φ_7	3194	driver	1	0	Nonrelevant

Summary of learning to rank approach

- The problem of making a binary relevant/nonrelevant judgment is cast as a classification or regression problem, based on a training set of query-document pairs and associated relevance judgments.
- In principle, any method learning a classifier (including least squares regression) can be used to find this line.
- Big advantage of learning to rank: we can avoid hand-tuning scoring functions and simply learn them from training data.
- Bottleneck of learning to rank: the cost of maintaining a representative set of training examples whose relevance assessments must be made by humans.

LTR features used by Microsoft Research (1)

- Zones: body, anchor, title, url, whole document
- Features derived from standard IR models: query term number, query term ratio, length, idf, sum of term frequency, min of term frequency, max of term frequency, mean of term frequency, variance of term frequency, sum of length normalized term frequency, min of length normalized term frequency, max of length normalized term frequency, mean of length normalized term frequency, variance of length normalized term frequency, sum of tf-idf, min of tf-idf, max of tf-idf, mean of tf-idf, variance of tf-idf, boolean model, BM25

LTR features used by Microsoft Research (2)

- Language model features: LMIR.ABS, LMIR.DIR, LMIR.JM
- Web-specific features: number of slashes in url, length of url, inlink number, outlink number, PageRank, SiteRank
- Spam features: QualityScore
- Usage-based features: query-url click count, url click count, url dwell time

Ranking SVMs

- Vector of feature differences: $\Phi(d_i, d_j, q) = \psi(d_i, q) - \psi(d_j, q)$
- By hypothesis, one of d_i and d_j has been judged more relevant.
- Notation: We write $d_i \prec d_j$ for “ d_i precedes d_j in the results ordering”.
- If d_i is judged more relevant than d_j , then we will assign the vector $\Phi(d_i, d_j, q)$ the class $y_{ijq} = +1$; otherwise -1 .
- This gives us a training set of pairs of vectors and “precedence indicators”. Each of the vectors is computed as the difference of two document-query vectors.
- We can then train an SVM on this training set with the goal of obtaining a classifier that returns

$$\vec{w}^T \Phi(d_i, d_j, q) > 0 \quad \text{iff} \quad d_i \prec d_j$$

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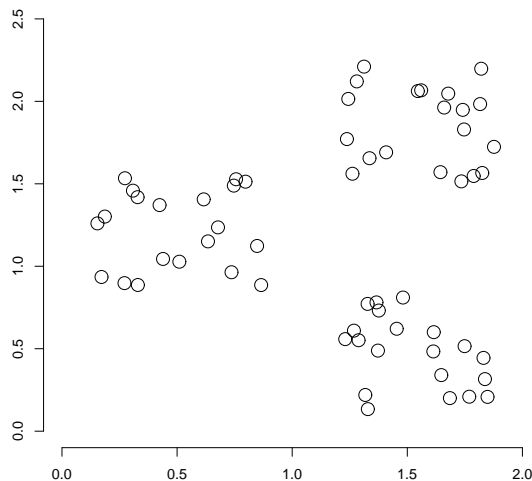
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- Clustering is the most common form of **unsupervised** learning.
- Unsupervised = there are no labeled or annotated data. □

Data set with clear cluster structure



Classification vs. Clustering

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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, ...



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Van Rijsbergen's original wording (1979): "closely associated documents tend to be relevant to the same requests". □

Applications of clustering in IR

Applications of clustering in IR

application	what is clustered?	benefit
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
cluster-based retrieval	collection	higher efficiency: faster search

Search result clustering for better navigation

Search result clustering for better navigation

The screenshot shows the Vivísimo search engine interface. At the top, there is a search bar with the query "jaguar" and a dropdown menu set to "the Web". A blue "Search" button is to the right, along with links for "Advanced Search" and "Help".

Below the search bar, a yellow banner displays "Clustered Results" and "Top 208 results of at least 20,373,974 retrieved for the query jaguar (Details)".

On the left side, a vertical list of clusters is shown, each with a plus icon and a link to the cluster:

- [jaguar](#) (208)
- [Cars](#) (74)
- [Club](#) (34)
- [Cat](#) (23)
- [Animal](#) (13)
- [Restoration](#) (10)
- [Mac OS X](#) (8)
- [Jaguar Model](#) (8)
- [Request](#) (5)
- [Mark Webber](#) (6)
- [Maya](#) (5)
- [More](#)

At the bottom left, there is a "Find in clusters:" search box with the text "Enter Keywords" and a red "Go" button.

The main content area displays the top search results:

- [Jag-lovers - THE source for all Jaguar information](#) [new window] [frame] [cache] [preview] [clusters]

... Internet! Serving Enthusiasts since 1993 The Jag-lovers Web Currently with 40661 members The Premier **Jaguar** Cars web resource for all enthusiasts Lists and Forums Jag-lovers originally evolved around its ...

[www.jag-lovers.org](#) - Open Directory 2, Wisenut 8, Ask Jeeves 8, MSN 9, Looksmart 12, MSN Search 18
- [Jaguar Cars](#) [new window] [frame] [cache] [preview] [clusters]

[...] redirected to [www.jaguar.com](#)

[www.jaguarcars.com](#) - Looksmart 1, MSN 2, Lycos 3, Wisenut 6, MSN Search 9, MSN 29
- [http://www.jaguar.com/](#) [new window] [frame] [preview] [clusters]

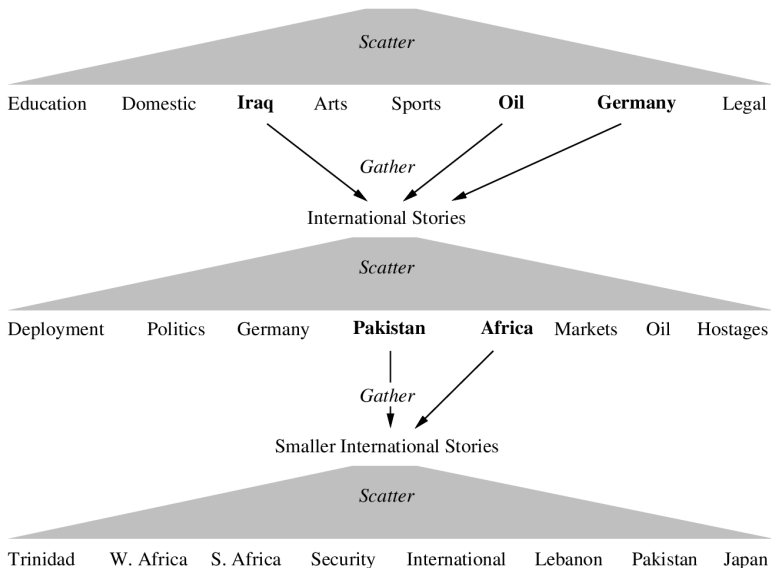
[www.jaguar.com](#) - MSN 1, Ask Jeeves 1, MSN Search 3, Lycos 9
- [Apple - Mac OS X](#) [new window] [frame] [preview] [clusters]

Learn about the new OS X Server, designed for the Internet, digital media and workgroup management. Download a technical factsheet.

[www.apple.com/macosx](#) - Wisenut 1, MSN 3, Looksmart 25

Scatter-Gather

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Global navigation: Yahoo

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YAHOO! DIRECTORY Search: the Web | the Directory | this category

Society and Culture

Directory > Society and Culture

 **Culture** SPONSOR RE
www.Dealtime.com Shop and save on Magazines.

CATEGORIES [\(What's This?\)](#)

Most Popular Society and Culture

- [Crime](#) (5453) NEW!
- [Cultures and Groups](#) (11025) NEW!
- [Environment and Nature](#) (8558) NEW!
- [Families](#) (1215)
- [Food and Drink](#) (9776) NEW!
- [Holidays and Observances](#) (3333)
- [Issues and Causes](#) (4842)
- [Mythology and Folklore](#) (984)
- [People](#) (16351)
- [Relationships](#) (595)
- [Religion and Spirituality](#) (37533)
- [Sexuality](#) (2812) NEW!

Additional Society and Culture Categories

- [Advice](#) (48)
- [Chats and Forums](#) (27)
- [Cultural Policy](#) (10)
- [Death and Dying](#) (394)
- [Disabilities](#) (1293)
- [Employment and Work@](#)
- [Etiquette](#) (54)
- [Events](#) (27)
- [Fashion@](#)
- [Gender](#) (21)
- [Home and Garden](#) (1080) NEW!
- [Magazines](#) (164)
- [Museums and Exhibits](#) (6052)
- [Pets@](#)
- [Reunions](#) (228)
- [Social Organizations](#) (338)
- [Web Directories](#) (6)
- [Weddings](#) (371)

SITE LISTINGS By Popularity | [Alphabetical](#) | [\(What's This?\)](#) Site

Global navigation: MESH (upper level)

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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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[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 \[C04.925\] +](#)

Navigational hierarchies: Manual vs. automatic creation

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- Next week: latent semantic indexing, a form of soft clustering



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- Effective heuristic method: K -means algorithm □

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- Perhaps the best known clustering algorithm
- Simple, works well in many cases
- Use as default / baseline for clustering documents



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- . . . which is almost equivalent to cosine similarity.
- Almost: centroids are not length-normalized. □

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where we use ω to denote a cluster.

- We try to find the minimum average squared difference by iterating two steps:

K-means: Basic idea

- Each cluster in K-means is defined by a **centroid**.
- Objective/partitioning criterion: **minimize the average squared difference from the centroid**
- Recall definition of centroid:

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

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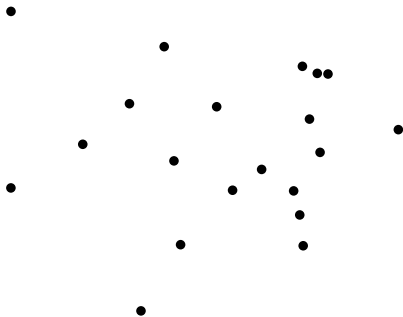
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 - **reassignment**: assign each vector to its closest centroid
 - **recomputation**: recompute each centroid as the average of the vectors that were assigned to it in reassignment □

K-means pseudocode (μ_k is centroid of ω_k)

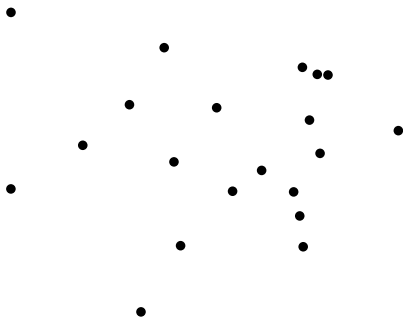
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```
K-MEANS( $\{\vec{x}_1, \dots, \vec{x}_N\}, K$ )
1   $(\vec{s}_1, \vec{s}_2, \dots, \vec{s}_K) \leftarrow \text{SELECTRANDOMSEEDS}(\{\vec{x}_1, \dots, \vec{x}_N\}, K)$ 
2  for  $k \leftarrow 1$  to  $K$ 
3  do  $\vec{\mu}_k \leftarrow \vec{s}_k$ 
4  while stopping criterion has not been met
5  do for  $k \leftarrow 1$  to  $K$ 
6      do  $\omega_k \leftarrow \{\}$ 
7      for  $n \leftarrow 1$  to  $N$ 
8          do  $j \leftarrow \arg \min_{j'} |\vec{\mu}_{j'} - \vec{x}_n|$ 
9               $\omega_j \leftarrow \omega_j \cup \{\vec{x}_n\}$  (reassignment of vectors)
10     for  $k \leftarrow 1$  to  $K$ 
11         do  $\vec{\mu}_k \leftarrow \frac{1}{|\omega_k|} \sum_{\vec{x} \in \omega_k} \vec{x}$  (recomputation of centroids)
12 return  $\{\vec{\mu}_1, \dots, \vec{\mu}_K\}$ 
```

Worked Example: Set of points to be clustered

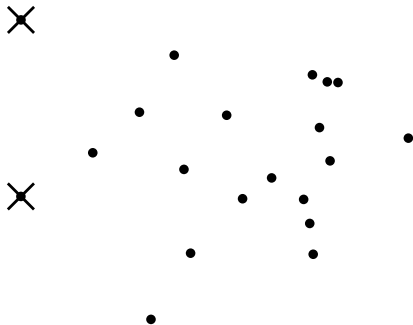


Worked Example

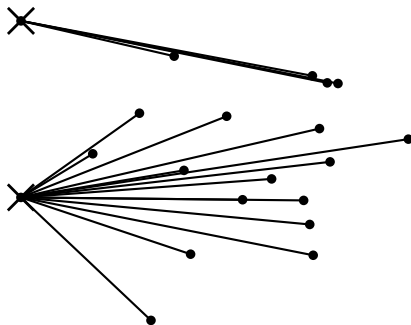


Exercise: (i) Guess what the optimal clustering into two clusters is in this case; (ii) compute the centroids of the clusters □

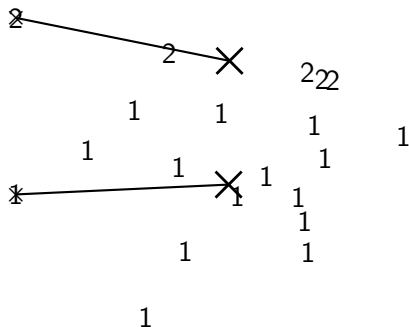
Worked Example: Random selection of initial centroids



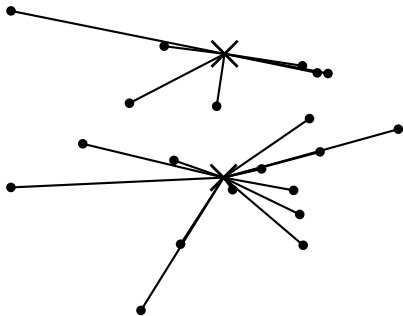
Worked Example: Assign points to closest center



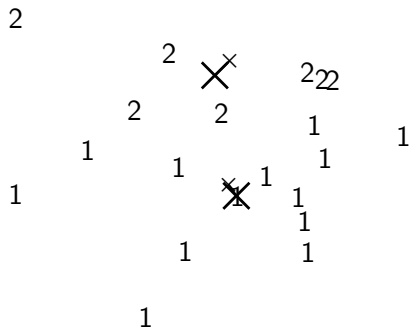
Worked Example: Recompute cluster centroids



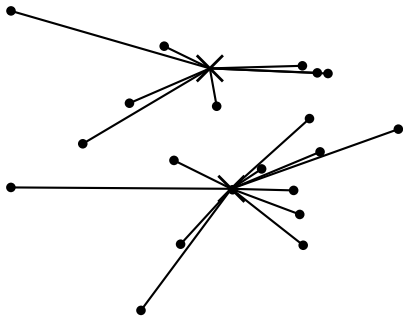
Worked Example: Assign points to closest centroid



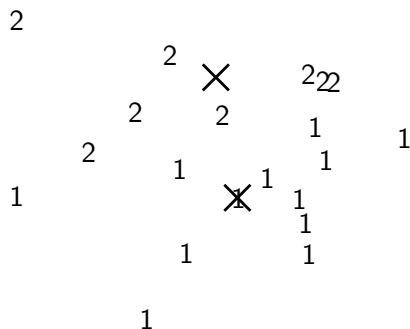
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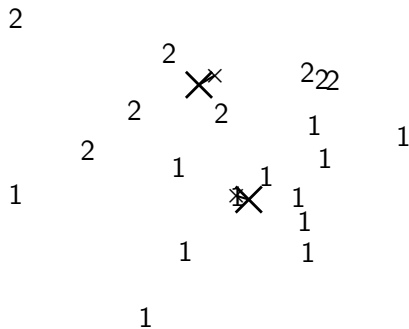
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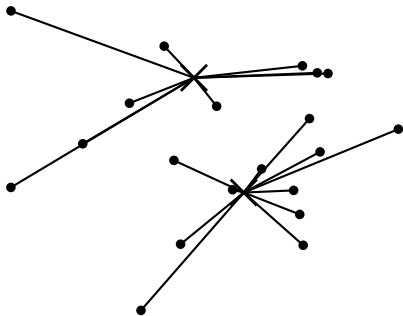
Worked Example: Assignment



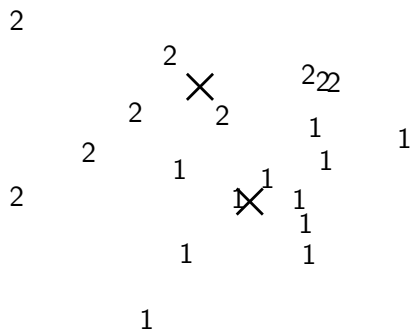
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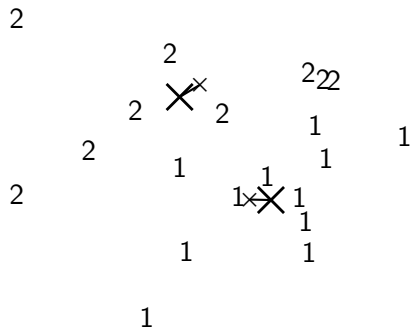
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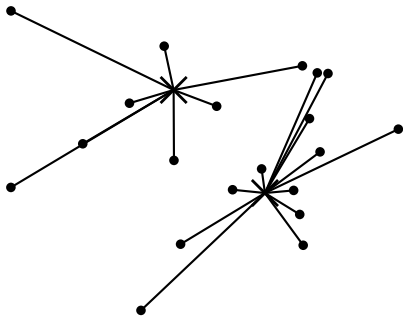
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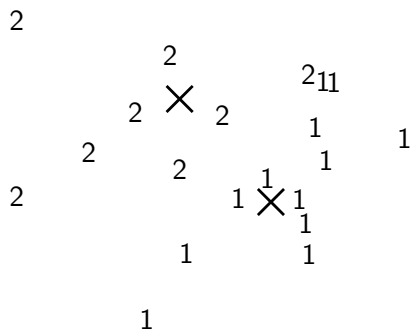
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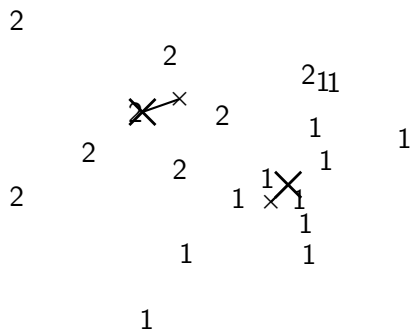
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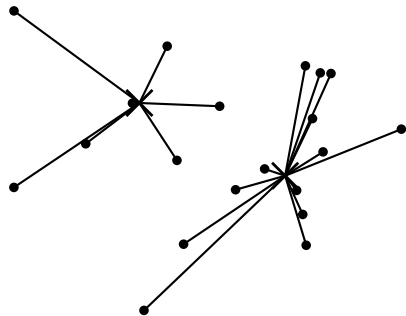
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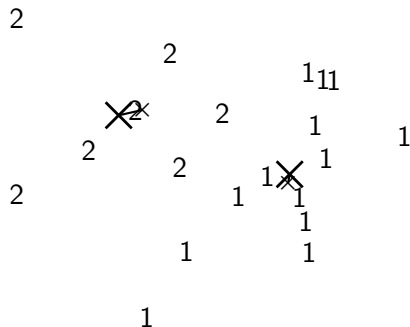
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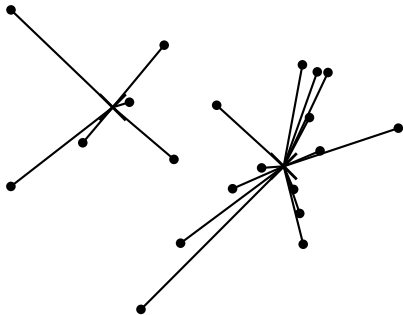
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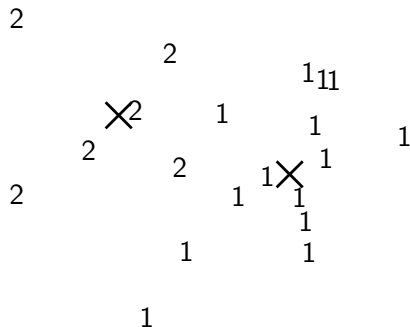
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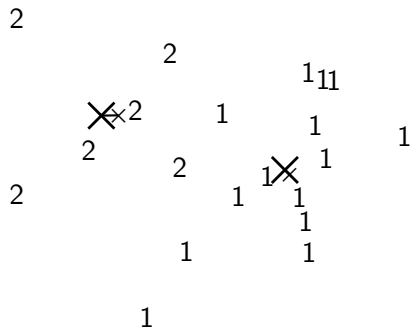
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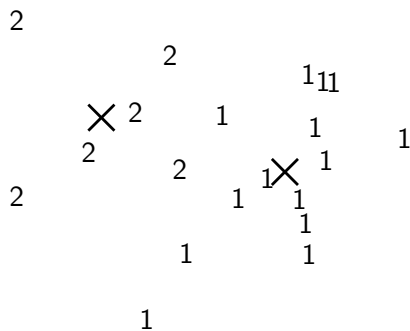
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Worked Ex.: Centroids and assignments after convergence



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- Finite set & monotonically decreasing \rightarrow convergence □

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$$RSS_k(\vec{v}) = \sum_{\vec{x} \in \omega_k} \|\vec{v} - \vec{x}\|^2 = \sum_{\vec{x} \in \omega_k} \sum_{m=1}^M (v_m - x_m)^2$$
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- However, complete convergence can take many more iterations.



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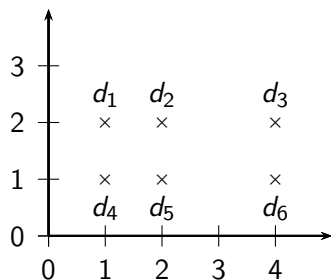
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- If we start with a bad set of seeds, the resulting clustering can be horrible. □

Exercise: Suboptimal clustering

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- What is the optimal clustering for $K = 2$?
- Do we converge on this clustering for arbitrary seeds d_i, d_j ?



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- In pathological cases, complexity can be worse than linear. □

Outline

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

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 - (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**
- 

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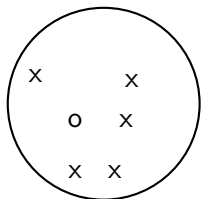
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- For each cluster ω_k : find class c_j with most members n_{kj} in ω_k
- Sum all n_{kj} and divide by total number of points □

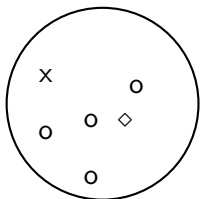
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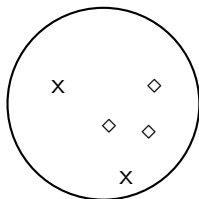
cluster 1



cluster 2



cluster 3



To compute purity: $5 = \max_j |\omega_1 \cap c_j|$ (class x, cluster 1); $4 = \max_j |\omega_2 \cap c_j|$ (class o, cluster 2); and $3 = \max_j |\omega_3 \cap c_j|$ (class \diamond , cluster 3). Purity is $(1/17) \times (5 + 4 + 3) \approx 0.71$. □

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- $TP+FN+FP+TN = \binom{N}{2}$ for N documents.
- Example: $\binom{17}{2} = 136$ in o/◇/x example
- Each pair is either positive or negative (the clustering puts the two documents in the same or in different clusters) ...
- ...and either “true” (correct) or “false” (incorrect): the clustering decision is correct or incorrect. □

Rand Index: Example

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As an example, we compute RI for the o/◇/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:

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

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

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

Thus, $FP = 40 - 20 = 20$.

FN and TN are computed similarly. □

Rand measure for the o/◇/x example

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



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 - Therefore: normalize by entropy of clusters and classes
- F measure
 - Like Rand, but “precision” and “recall” can be weighted □

Evaluation results for the o/◇/x example

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	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). □

Outline

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

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 - Given docs, find K for which the optimum is reached.
 - What optimization criterion can we use?
 - We can't use RSS or average squared distance from centroid as criterion: always chooses $K = N$ clusters. □

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- You want to use K -means clustering.
- How would you determine K ?



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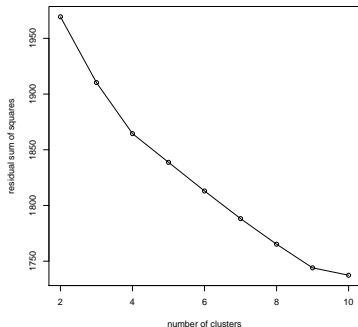
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- Select K that minimizes $(RSS(K) + K\lambda)$
- Still need to determine good value for $\lambda \dots$



Finding the “knee” in the curve

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Pick the number of clusters where curve “flattens”. Here: 4 or 9. □

Take-away today

- What is clustering?
- Applications of clustering in information retrieval
- *K*-means algorithm
- Evaluation of clustering
- How many clusters?



Resources

- Chapter 16 of IIR
- Resources at <http://cis1mu.org>
 - Keith van Rijsbergen on the cluster hypothesis (he was one of the originators)
 - Bing/Carrot2/Clusty: search result clustering systems
 - Stirling number: the number of distinct k -clusterings of n items