Introduction to
Information Retrieval

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Lecture 16: Flat Clustering

K-means

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

Document representations in clustering

- Vector space model
- As in vector space classification, we measure relatedness between vectors by Euclidean distance . . .
- . . .which is almost equivalent to cosine similarity.
- Almost: centroids are not length-normalized.

Introduction to Information Retrieval

K-means

- 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:

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

where we use ω to denote a cluster.

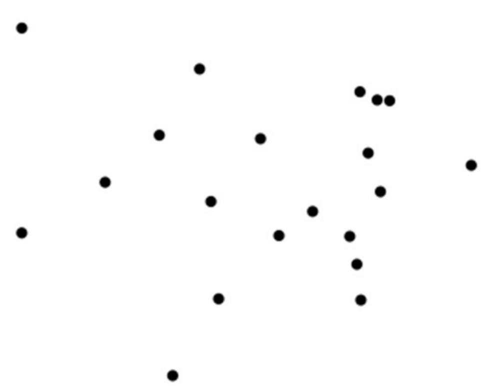
- We try to find the minimum average squared difference by iterating two steps:
  - reassignment: assign each vector to its closest centroid
  - recomputation: recompute each centroid as the average of the vectors that were assigned to it in reassignment

K-means algorithm

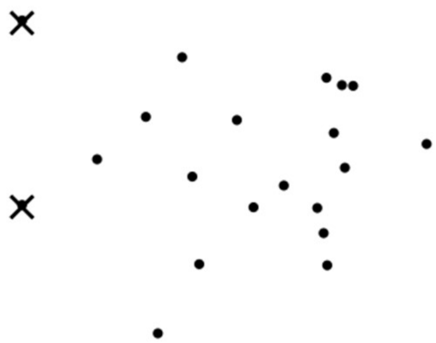
K-MEANS$(\{\vec{x}_1, \ldots, \vec{x}_N\}, K)$

$(\vec{s}_1, \vec{s}_2, \ldots, \vec{s}_K) \leftarrow$ 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 $\{\vec{\mu}_1, \ldots, \vec{\mu}_K\}$

Worked Example: Set of to be clustered

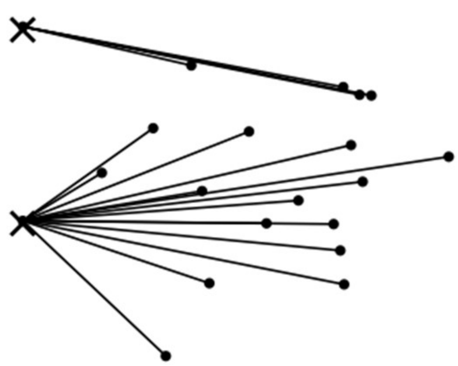


Worked Example: Random selection of initial centroids

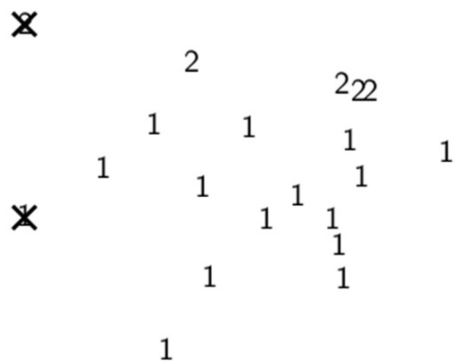


Exercise: (i) Guess what the optimal clustering into two clusters is in this case; (ii) compute the centroids of the clusters

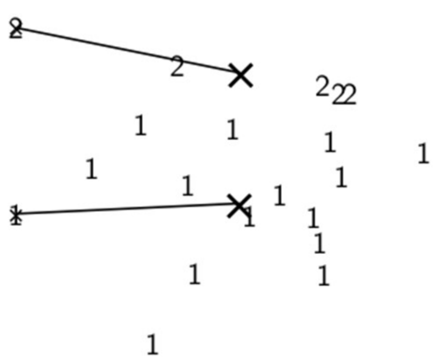
Worked Example: Assign points to closest center



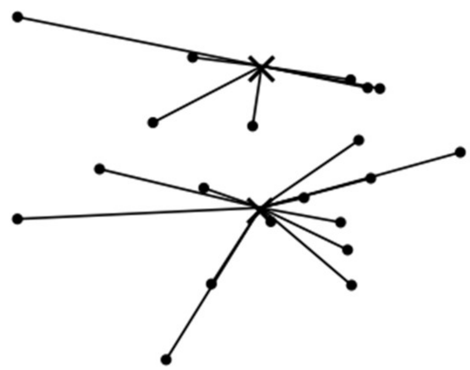
Worked Example: Assignment



Worked Example: Recompute cluster centroids



Worked Example: Assign points to closest centroid



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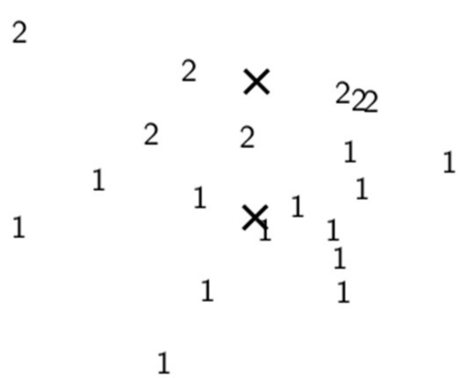

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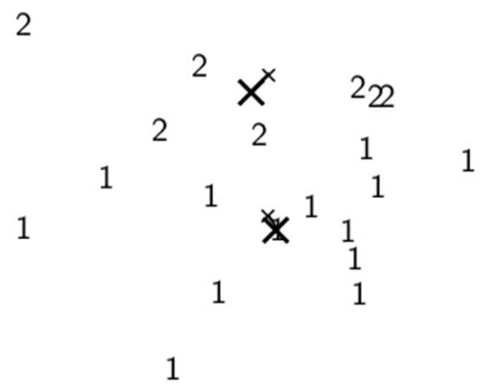

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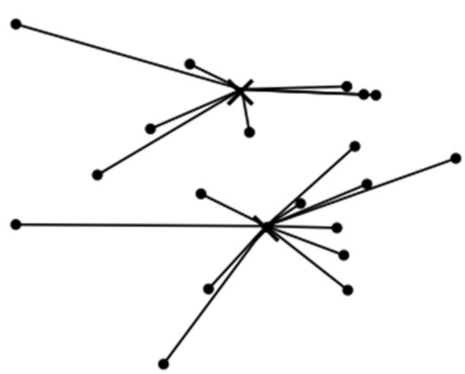

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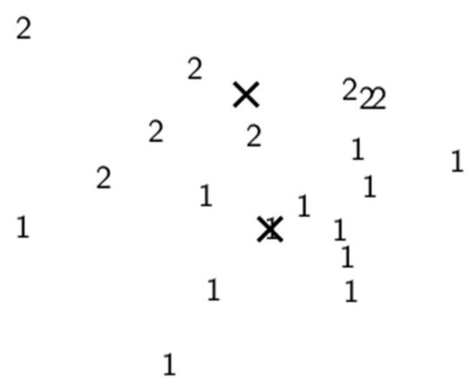

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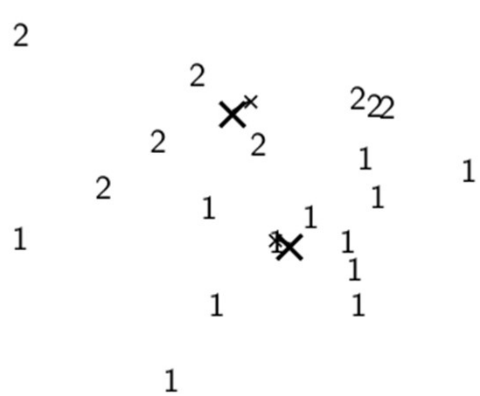

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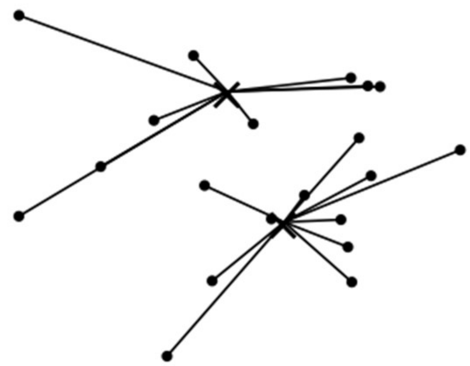

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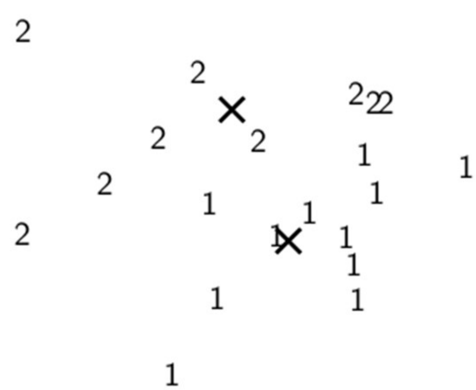

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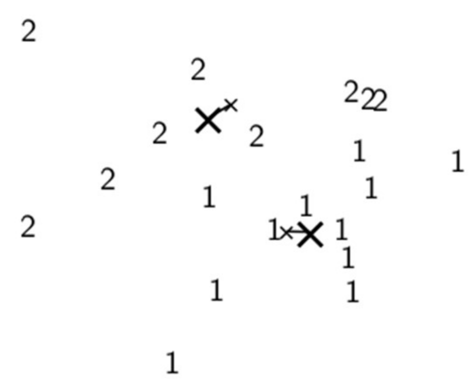

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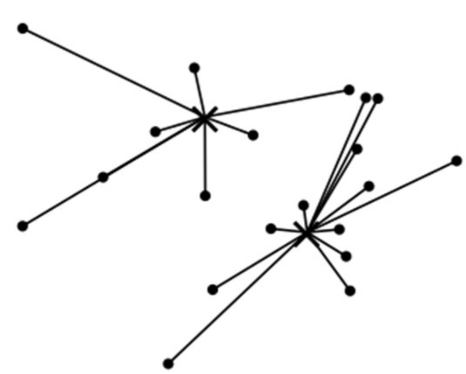

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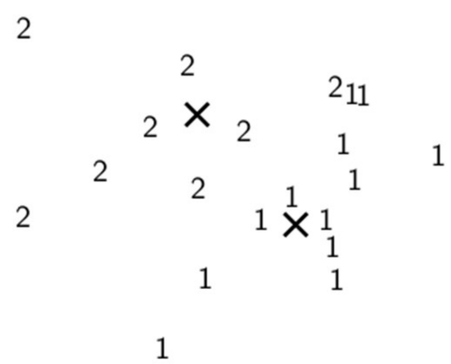

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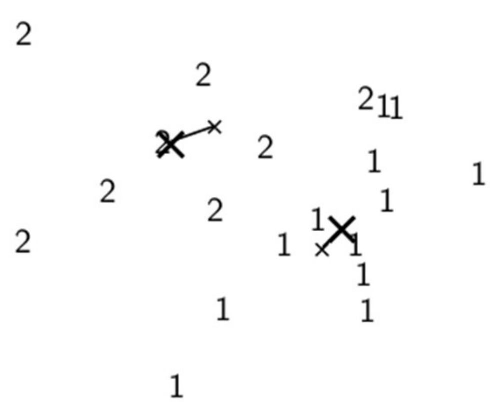

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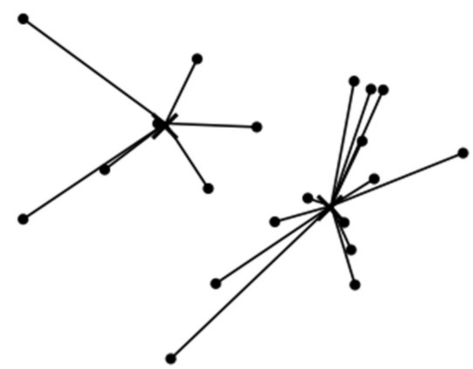

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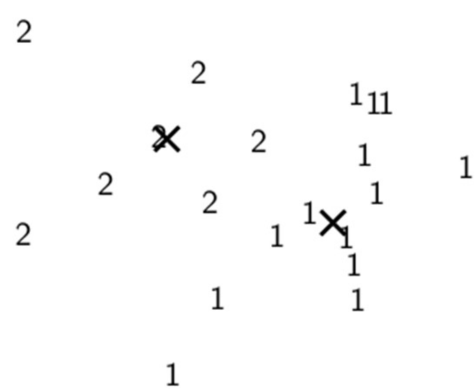

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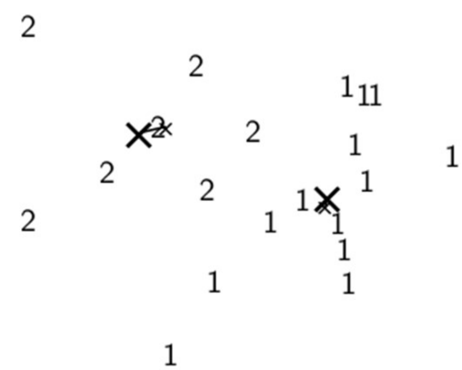

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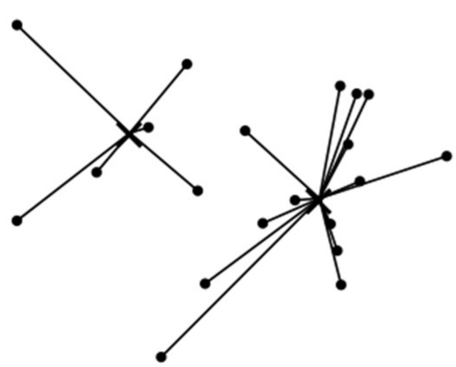

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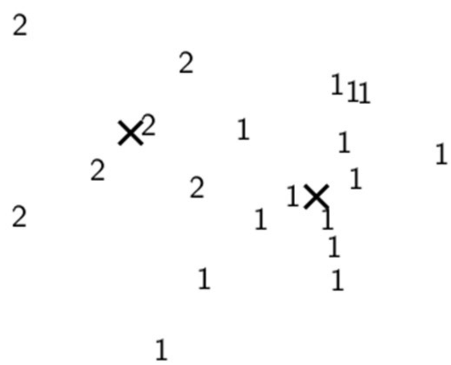
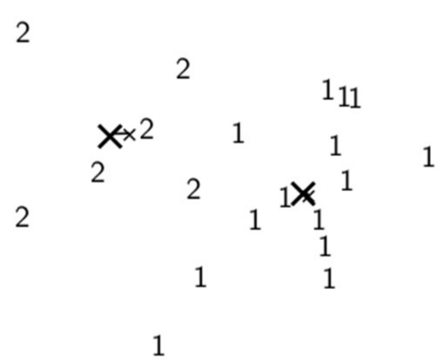
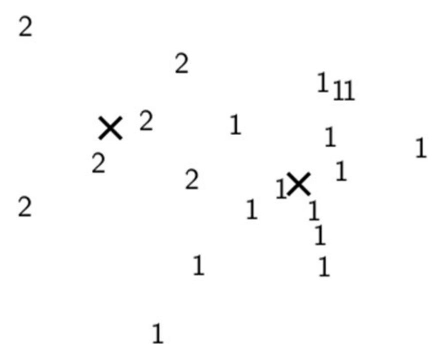


Worked Example: Recompute cluster caentroids



Worked Ex.: Centroids and assignments after convergence



K-means is guaranteed to converge: Proof

- RSS = sum of all squared distances between document vector and closest centroid
- RSS decreases during each reassignment step.
  - because each vector is moved to a closer centroid
- RSS decreases during each recomputation step.
  - see next slide
- There is only a finite number of clusterings.
- Thus: We must reach a fixed point.
- Assumption: Ties are broken consistently.

Recomputation decreases average distance

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

$$\mathrm{RSS}_k(\vec{v}) = \sum_{\vec{x}\in\omega_k} \|\vec{v}-\vec{x}\|^2 = \sum_{\vec{x}\in\omega_k} \sum_{m=1}^{M} (v_m - x_m)^2$$

$$\frac{\partial \mathrm{RSS}_k(\vec{v})}{\partial v_m} = \sum_{\vec{x}\in\omega_k} 2(v_m - x_m) = 0$$

$$v_m = \frac{1}{|\omega_k|} \sum_{\vec{x}\in\omega_k} x_m$$

The last line is the componentwise definition of the centroid! We minimize RSSk when the old centroid is replaced with the new centroid. RSS, the sum of the RSSk , must then also decrease during recomputation.

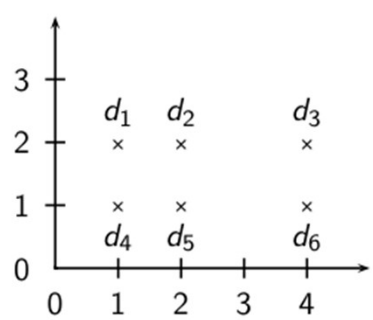
K-means is guaranteed to converge

- But we don't know how long convergence will take!
- If we don't care about a few docs switching back and forth, then convergence is usually fast (< 10-20 iterations).
- However, complete convergence can take many more iterations.

Optimality of *K*-means

- Convergence does not mean that we converge to the optimal clustering!
- This is the great weakness of K-means.
- If we start with a bad set of seeds, the resulting clustering can be horrible.

Convergence Exercise: Suboptimal clustering



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

Initialization of *K*-means

- Random seed selection is just one of many ways K-means can be initialized.
- Random seed selection is not very robust: It's easy to get a suboptimal clustering.
- Better ways of computing initial centroids:
  - Select seeds not randomly, but using some heuristic (e.g., filter out outliers or find a set of seeds that has "good coverage" of the document space)
  - Use hierarchical clustering to find good seeds
  - Select i (e.g., $i = 10$) different random sets of seeds, do a K-means clustering for each, select the clustering with lowest RSS

Time complexity of *K*-means

- Computing one distance of two vectors is $O(M)$.
- Reassignment step: $O(KNM)$ (we need to compute KN document-centroid distances)
- Recomputation step: $O(NM)$ (we need to add each of the document's < M values to one of the centroids)
- Assume number of iterations bounded by I
- Overall complexity: $O(IKNM)$ – linear in all important dimensions
- However: This is not a real worst-case analysis.
- 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?

What is a good clustering?

- Internal criteria
  - Example of an internal criterion: RSS in *K*-means
- But an internal criterion often does not evaluate the actual utility of a clustering in the application.
- Alternative: External criteria
  - Evaluate with respect to a human-defined classification

External criteria for clustering quality

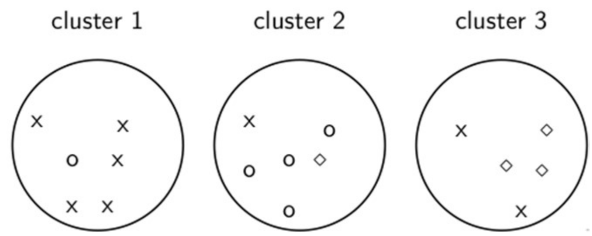
- Based on a gold standard data set, e.g., the Reuters collection we also used for the evaluation of classification
- Goal: Clustering should reproduce the classes in the gold standard
- (But we only want to reproduce how documents are divided into groups, not the class labels.)
- First measure for how 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.
- 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



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 ⋄, cluster 3). Purity is $(1/17) \times (5 + 4 + 3) \approx 0.71$.

Rand index

- Definition: $\mathrm{RI} = \frac{\mathrm{TP}+\mathrm{TN}}{\mathrm{TP}+\mathrm{FP}+\mathrm{FN}+\mathrm{TN}}$
- Based on 2x2 contingency table of all pairs of documents:

	same cluster	different clusters
same class	true positives (TP)	false negatives (FN)
different classes	false positives (FP)	true negatives (TN)

- TP+FN+FP+TN is the total number of pairs.
- There are $\binom{N}{2}$ pairs 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

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:

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

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:

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

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) ≈ 0.68.

Two other external evaluation measures

- Two other measures
- Normalized mutual information (NMI)
  - How much information does the clustering contain about the classification?
  - Singleton clusters (number of clusters = number of docs) have maximum MI
  - 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

	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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How many clusters?

- Number of clusters K is given in many applications.
  - E.g., there may be an external constraint on K. Example: In the case of Scatter-Gather, it was hard to show more than 10–20 clusters on a monitor in the 90s.
- What if there is no external constraint? Is there a "right" number of clusters?
- One way to go: define an optimization criterion
  - Given docs, find K for which the optimum is reached.
  - What optimiation criterion can we use?
  - We can't use RSS or average squared distance from centroid as criterion: always chooses $K = N$ clusters.

Exercise

- Your job is to develop the clustering algorithms for a competitor to news.google.com
- You want to use *K*-means clustering.
- How would you determine *K*?

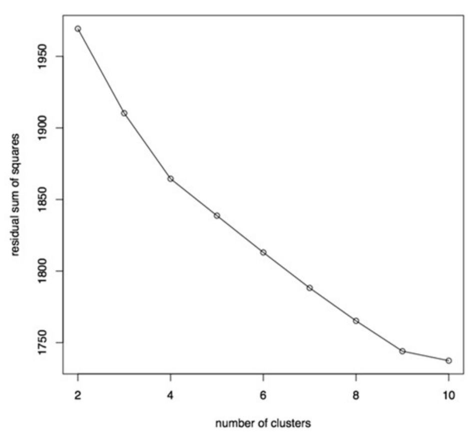
Simple objective function for *K* (1)

- Basic idea:
  - Start with 1 cluster ($K = 1$)
  - Keep adding clusters (= keep increasing *K*)
  - Add a penalty for each new cluster
- Trade off cluster penalties against average squared distance from centroid
- Choose the value of *K* with the best tradeoff

Simple objective function for *K* (2)

- Given a clustering, define the cost for a document as (squared) distance to centroid
- Define total distortion RSS(K) as sum of all individual document costs (corresponds to average distance)
- Then: penalize each cluster with a cost λ
- Thus for a clustering with *K* clusters, total cluster penalty is *K*λ
- Define the total cost of a clustering as distortion plus total cluster penalty: RSS(K) + *K*λ
- Select K that minimizes (RSS(K) + *K*λ)
- 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.

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://ifnlp.org/ir
  - *K*-means example
  - Keith van Rijsbergen on the cluster hypothesis (he was one of
  - the originators)
  - Bing/Carrot2/Clusty: search result clustering