Maschinelle Sprachverarbeitung

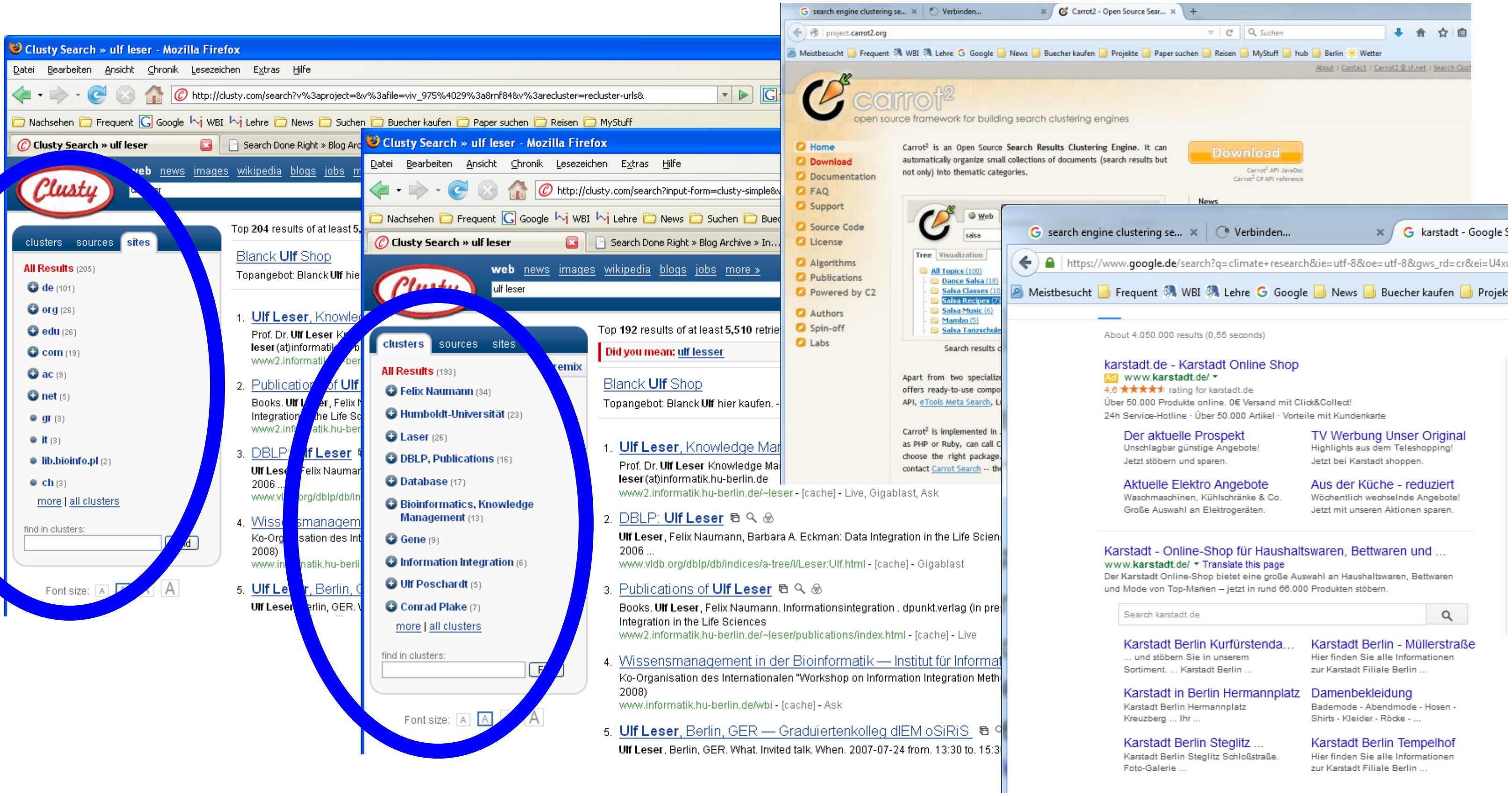
Text Clustering

Ulf Leser

Content of this Lecture

- (Text) clustering
- Cluster quality
- Clustering algorithms
- Application

Processing Search Results



Clusty Search » ulf leser - Mozilla Firefox

Datei Bearbeiten Ansicht Chronik Lesezeichen Extras Hilfe

http://clusty.com/search?input-form=clusty-simple&v

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clusters sources sites

All Results (193)

- Felix Naumann (34)
- Humboldt-Universität (23)
- Laser (26)
- DBLP, Publications (16)
- Database (17)
- Bioinformatics, Knowledge Management (13)
- Gene (9)
- Information Integration (6)
- Ulf Poschardt (5)
- Conrad Plake (7)

more | all clusters

find in clusters:

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Top 192 results of at least 5,510 retrie

Did you mean: ulf lesser

Blanck Ulf Shop
Topangebot: Blanck Ulf hier kaufen.

1. Ulf Leser, Knowledge Mar
Prof. Dr. Ulf Leser Knowledge Ma
leser (at)informatik.hu-berlin.de
www2.informatik.hu-berlin.de/~leser - [cache] - Live, Gigablast, Ask

2. DBLP: Ulf Leser
Ulf Leser, Felix Naumann, Barbara A. Eckman: Data Integration in the Life Scien
2006 ...
www.vldb.org/dblp/db/indices/a-tree/l/Leser:Ulf.html - [cache] - Gigablast

3. Publications of Ulf Leser
Books. Ulf Leser, Felix Naumann. Informationsintegration . dpunkt.verlag (in pre
Integration in the Life Sciences
www2.informatik.hu-berlin.de/~leser/publications/index.html - [cache] - Live

4. Wissensmanagement in der Bioinformatik — Institut für Informat
Ko-Organisation des Internationalen "Workshop on Information Integration Meth
2008)
www.informatik.hu-berlin.de/wbi - [cache] - Ask

5. Ulf Leser, Berlin, GER — Graduiertenkolleg dIEM oSiRiS
Ulf Leser, Berlin, GER. What. Invited talk. When. 2007-07-24 from. 13:30 to. 15:3

Clusty Search » ulf leser - Mozilla Firefox

http://clusty.com/search?v%3aproject=&v%3afile=viz_975%4029%3a8rnf84&v%3arecluster=recluster-urls&

Nachsehen Frequent Google WBI Lehre News Suchen Buecher kaufen Paper suchen Reisen MyStuff

All Results (205)

- de (101)
- org (26)
- edu (26)
- com (19)
- ac (9)
- net (5)
- gr (3)
- it (3)
- lib.bioinfo.pl (2)
- ch (3)

more | all clusters

Top 204 results of at least 5,

Carrot2 - Open Source Sear...

project.carrot2.org

carrot2
open source framework for building search clustering engines

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Labs

Carrot² is an Open Source Search Results Clustering Engine. It can automatically organize small collections of documents (search results but not only) into thematic categories.

Download

Tree | Visualization
All Topics (100)
Dance Salsa (18)
Salsa Classes (10)
Salsa Recipes (7)
Salsa Music (6)
Mambo (5)
Salsa Tanzschule

karstadt - Google S

https://www.google.de/search?q=climate+research&ie=utf-8&oe=utf-8&gws_rd=cr&ei=U4x

About 4.050.000 results (0,55 seconds)

karstadt.de - Karstadt Online Shop
Ad www.karstadt.de/
4,6 ★★★★★ rating for karstadt.de
Über 50.000 Produkte online. 0€ Versand mit Click&Collect!
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Search karstadt.de

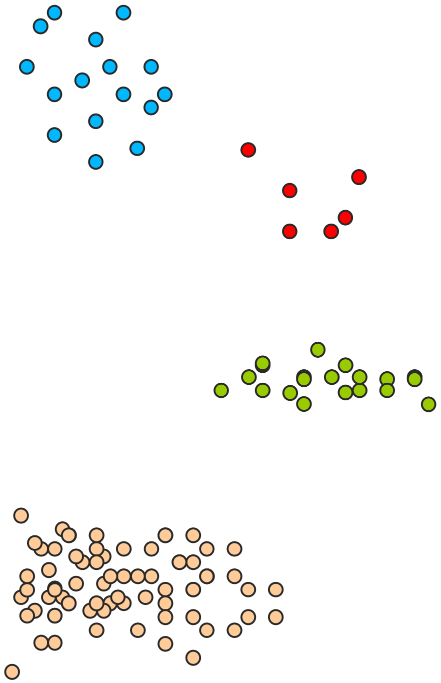
Karstadt Berlin Kurfürstenda...
Karstadt Berlin - Müllerstraße
Karstadt in Berlin Hermannplatz
Damenbekleidung
Karstadt Berlin Steglitz ...
Karstadt Berlin Tempelhof

- "… The research breakthrough was labeling the clusters, i.e., grouping search results into folder topics …"
  - [Clusty.com blog]

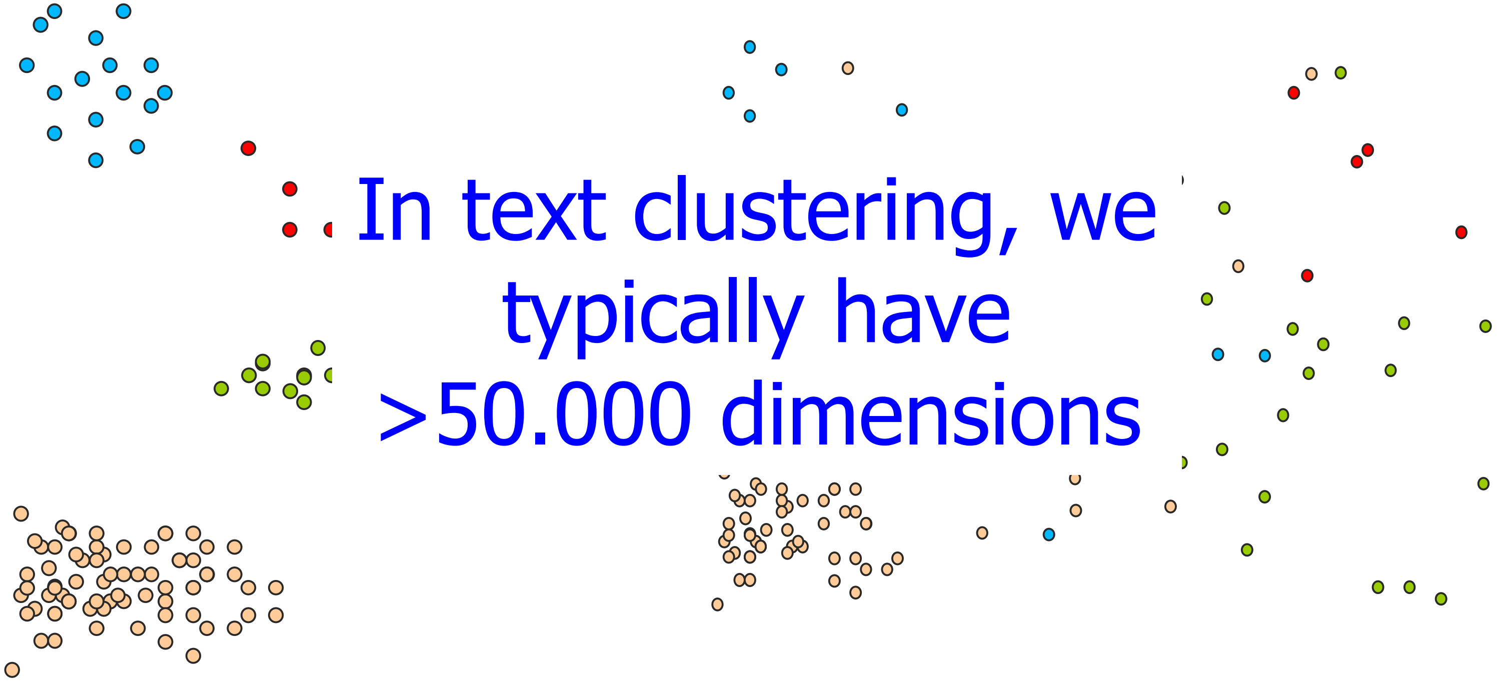
Clustering

- Clustering groups objects (docs) into (usually disjoint) sets
- Intuitively, each set should contain objects that are similar to each other and dissimilar to objects in any other set
  - We need a similarity or distance function
  - That is the only text-specific bit – the rest is "just" clustering
- Often called "unsupervised learning"
  - We don't know how many sets/classes/clusters exist
  - We don't know how those sets should look like
  - We don't know if homogeneous sets exist at all

Nice



Nice – Not Nice



In text clustering, we typically have >50.000 dimensions

Text Clustering Applications

- Explorative data analysis
  - Learn about the structure within your document collection
- Corpus preprocessing
  - Clustering provides a “semantic index” to a corpus
  - Group docs into clusters to ease navigation
  - Retrieval speed: Index only one representative per cluster (e.g. kNN)
- Processing of search results
  - Cluster all hits into groups of similar hits (in particular: duplicates)
- Improving recall
  - Return doc and all members of its cluster
  - Has similarity to automatic relevance feedback using top-k docs
- Word sense disambiguation
  - The different senses of a word should appear as clusters
- Assess “classifyability”
  - Cluster training data and compare clusters to predefined classes
- …

Similarity between Documents

- Clustering requires a distance function
  - Should always be a metric
  - d(x,x)=0, d(x,y)=d(y,x), d(x,y)≤d(x,z)+d(z,y)
- In contrast to search, we compare two docs
  - And not a document and a query
- Nevertheless, often the same methods are used
  - Vector space , TF*IDF, cosine distance, feature selection, …

$$sim(d_1,d_2)=\cos(d_1,d_2)=\frac{d_1\circ d_2}{|d_1|*|d_2|}=\frac{\sum\left(d_1[i]*d_2[i]\right)}{\sqrt{\sum d_1[i]^2}*\sqrt{\sum d_2[i]^2}}$$

Clustering Speed

- In Information Retrieval
  - We compare a vector of 100K dimensions with very few (<3?) non-null values (nnv) with one with many more (500?) nnvs
  - Use inverted index to pick docs that have an overlap with the query
- In clustering
  - We compare a vector with ~500 nnv with one with ~500 nnv
  - We need to compare many (all) docs with many (all) docs
    - Depends on the clustering algorithm
  - Inverted indexes offer much less, if any, speed-up
- Feature selection or dimensionality reduction is essential
  - E.g., use the 1.000 “most descriptive” terms
  - E.g., perform Latent Semantic Indexing (LSI) before clustering

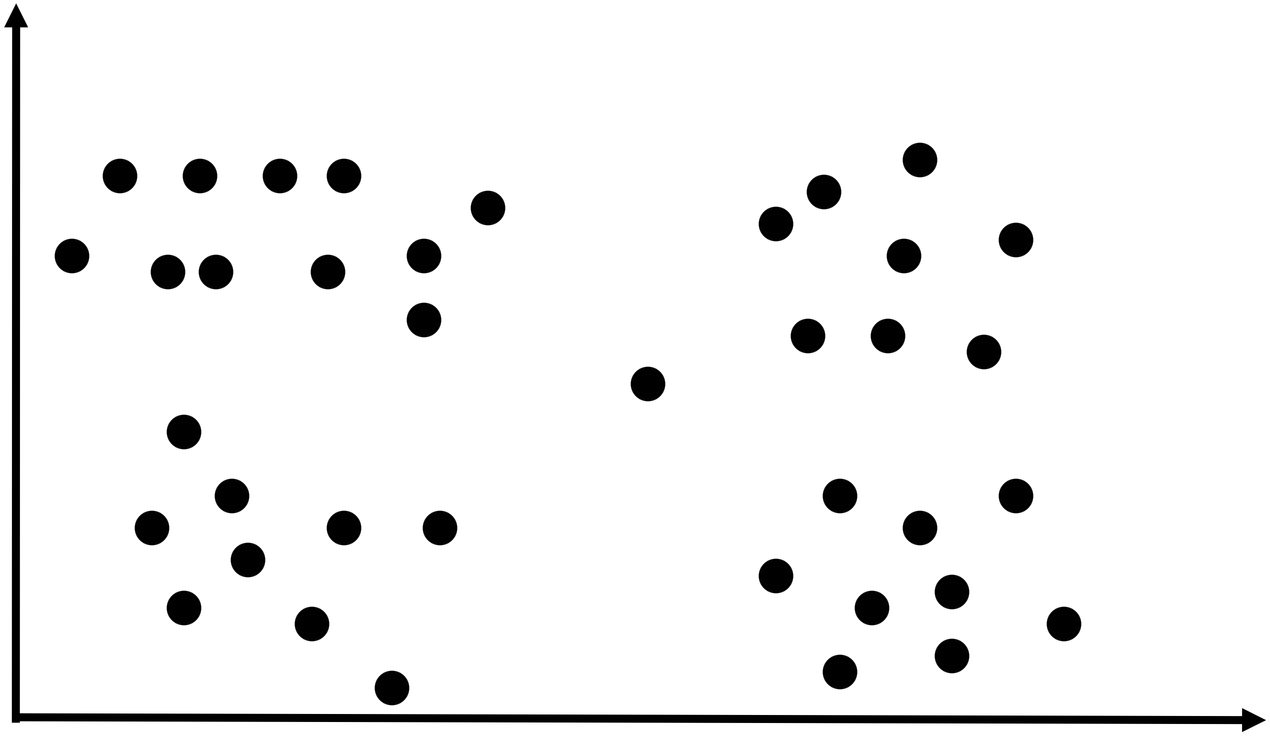
Cluster Labels (Finding Key Phrases)

- For user interaction, clusters need to have a name
- Names should capture the topic (semantic) of the cluster
- Some possibilities
  - Chose term (or n-gram) with highest TF*IDF value in cluster
    - E.g. TF computed as average or considering all docs in cluster as one
  - Chose term with highest TF*IDF value in cluster centre
  - Apply statistical method to find terms whose TF*IDF distribution deviates the most between clusters
    - E.g. Chi^2-Test, Kullback–Leibler divergence
    - Requires comparison of each cluster with each cluster for each term
    - Only possible when strict term-pre-filtering was applied
  - Report top-K token or top-K terms (by whatever method)
  - …

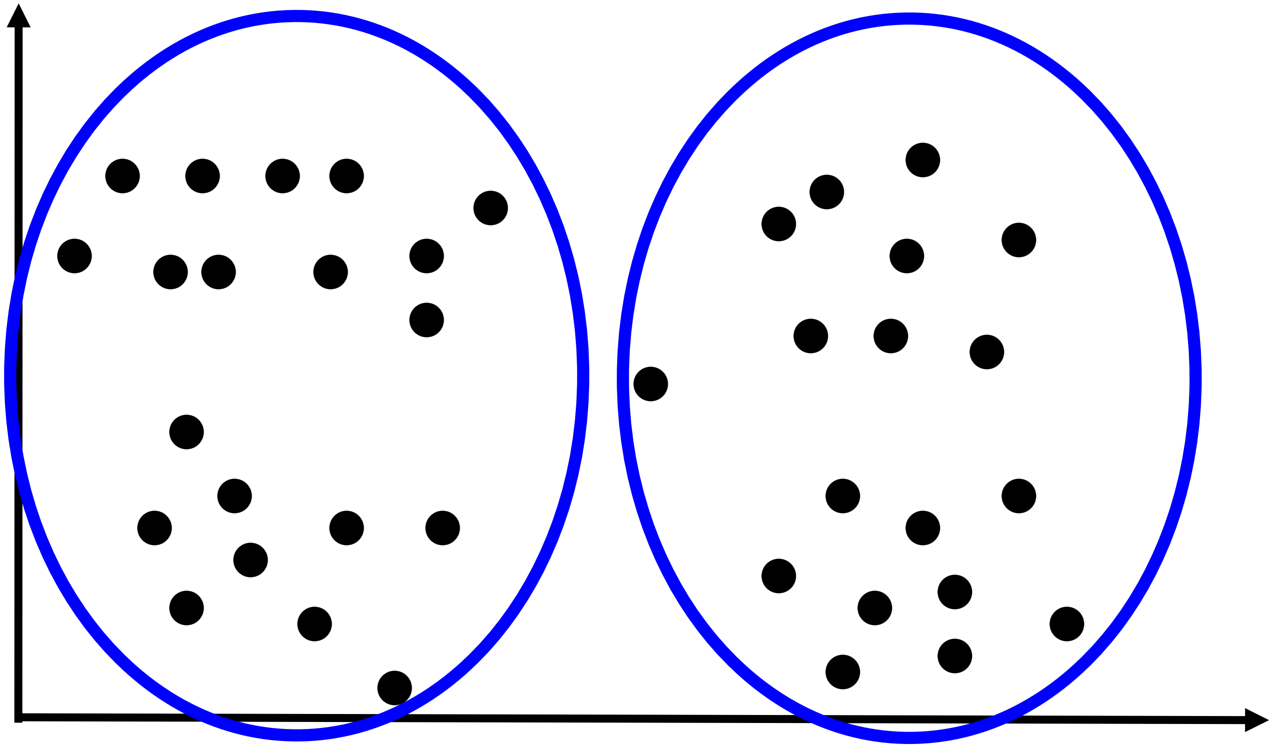
Content of this Lecture

- (Text) clustering
- Cluster quality
- Clustering algorithms
- Application

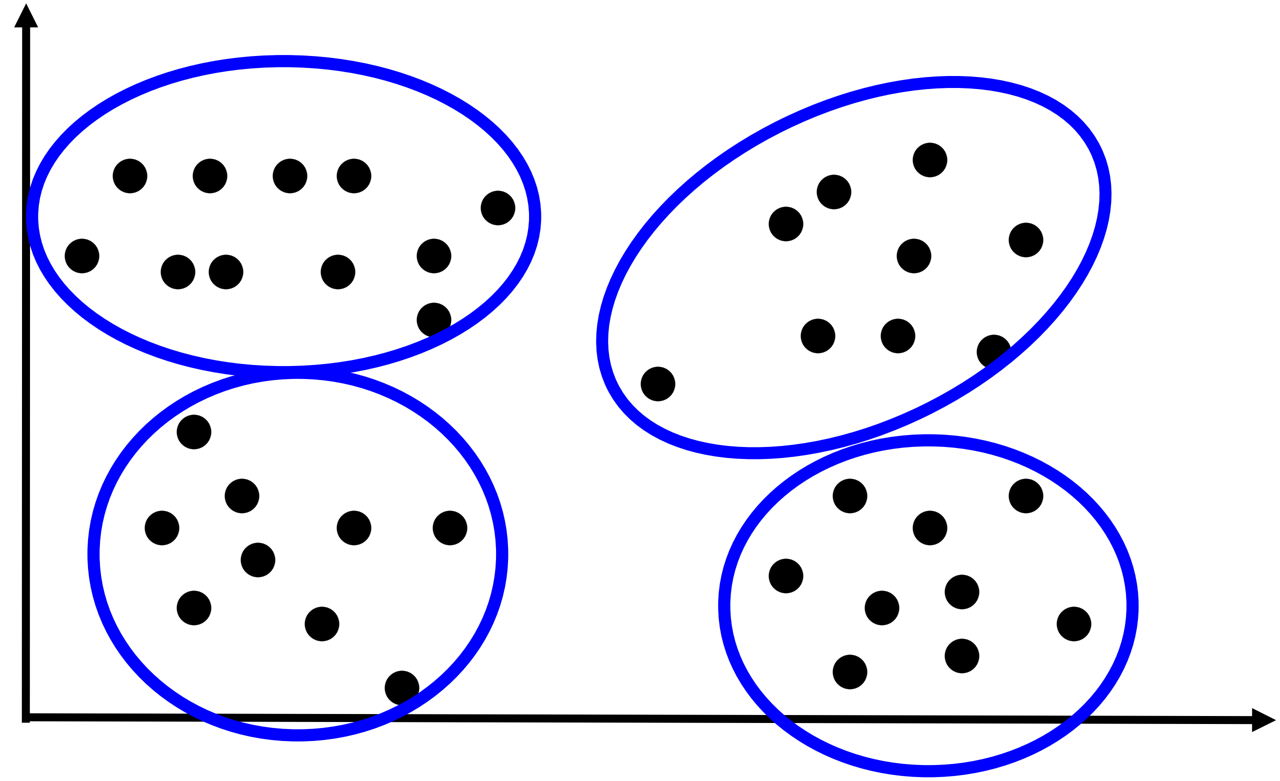
How many Clusters?



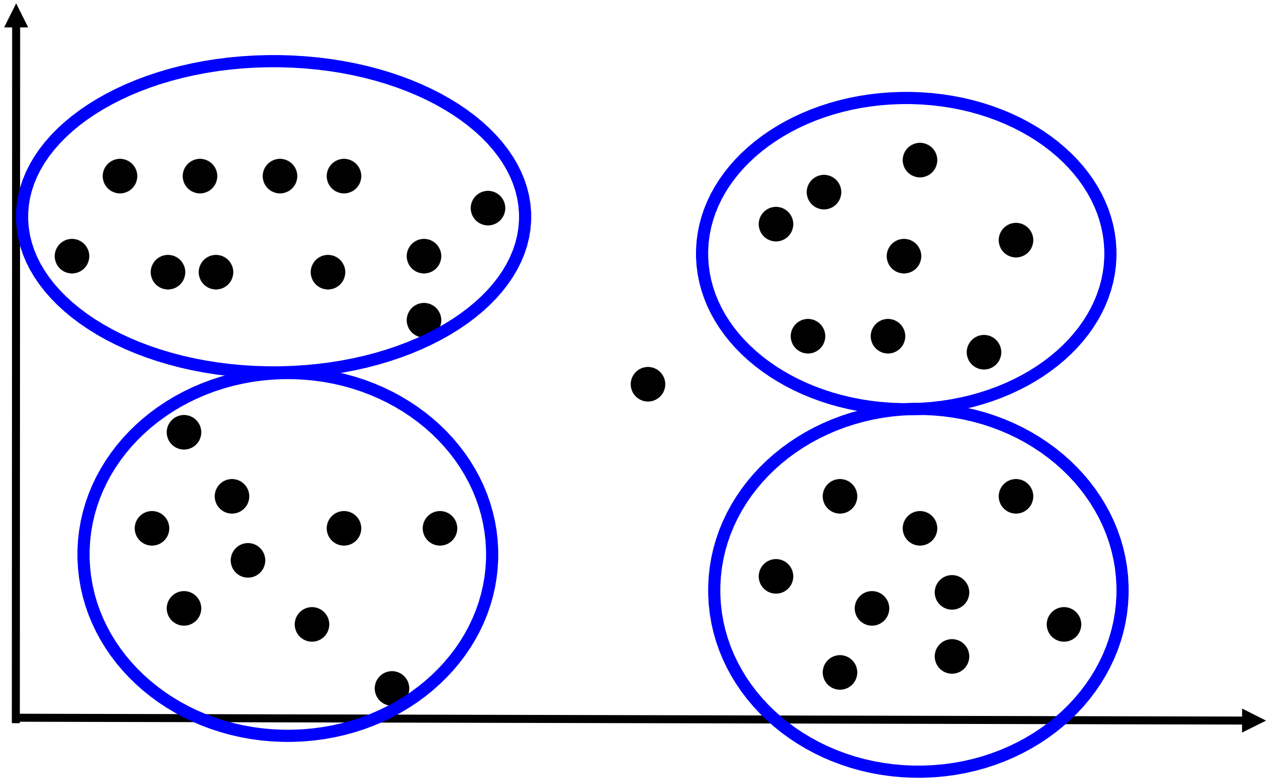
Maybe 2?



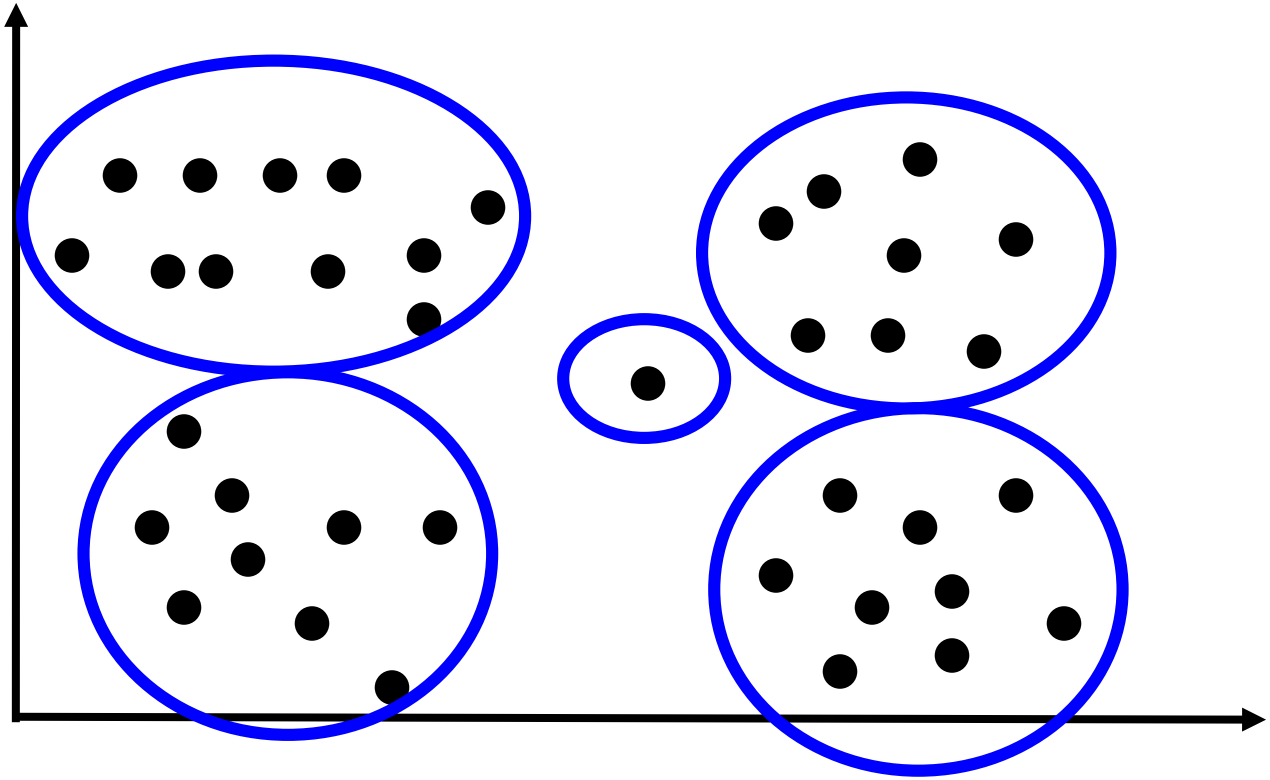
Maybe 4?



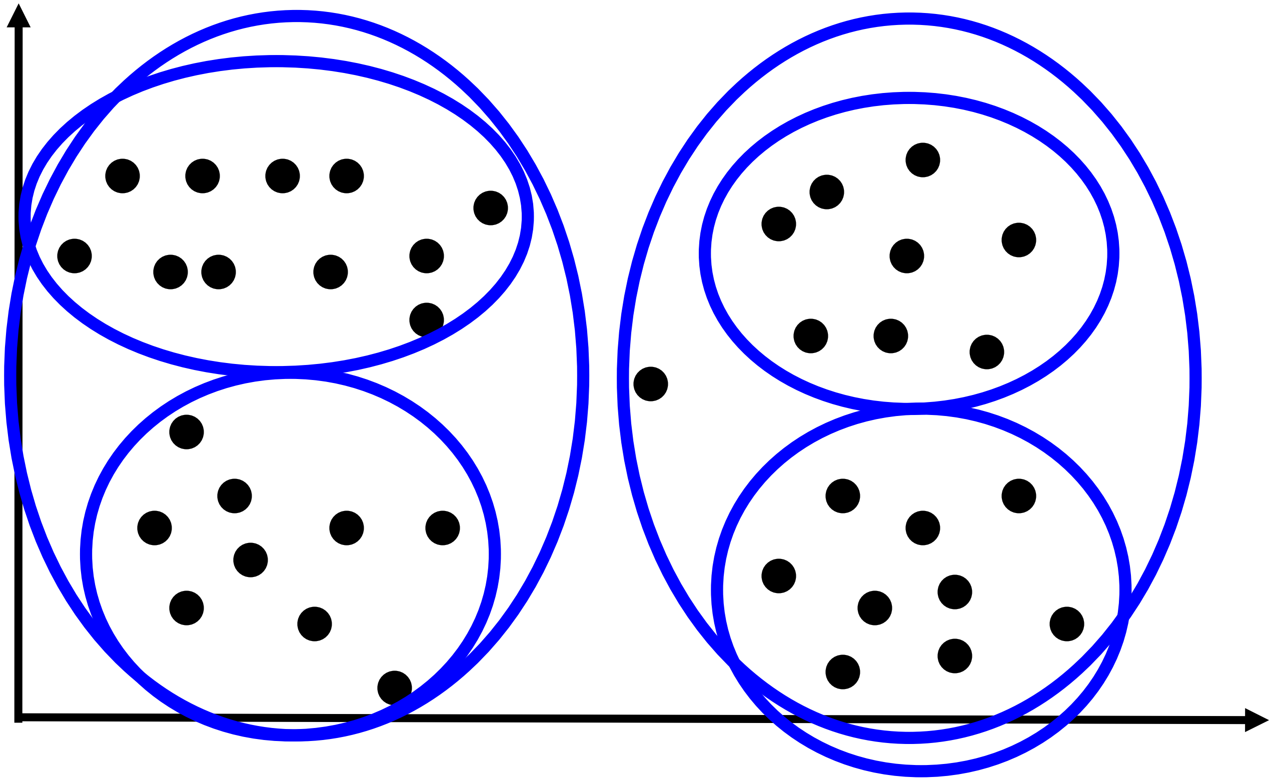
Maybe 4 and One Outlier?



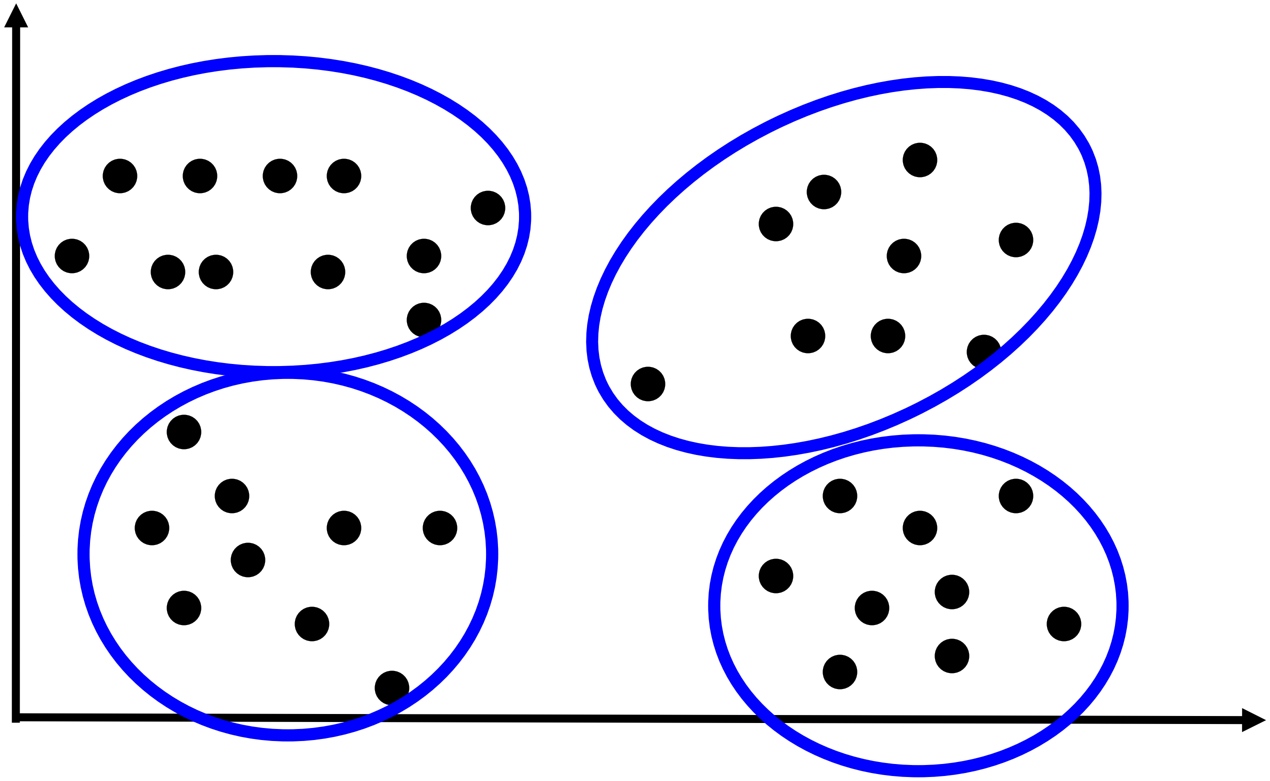
Maybe 5?



Maybe 4 and 2 – at Different Levels?



Which Distance Measure did you Use?



Quality of a Clustering

- There is no “true” number of clusters
- In real data sets, one cannot determine the number of clusters by “looking at the data”
  - Too many dimensions
  - Distance function need not map nicely to visualization
  - Clustering should help you in looking at the data
- We need to define the quality of a clustering
- Ideally, this quality score peaks at the intuitively best number of clusters

Distance to a Cluster

- We frequently will have to compute the distance between a point o (a doc) and a cluster c, d(o,c)
  - And sometimes distances between clusters – later
- Various methods
  - Distance to numerical center of a cluster
  - Distance to the most central point of a cluster
  - Average distance to all points in cluster

$$d(o,c) = d(o, c_{mean})$$

$$d(o,c) = d(o, c_{median})$$

$$d(o,c) = \sum_{p \in c} d(o,p) * {}^{1}\!/_{|c|}$$

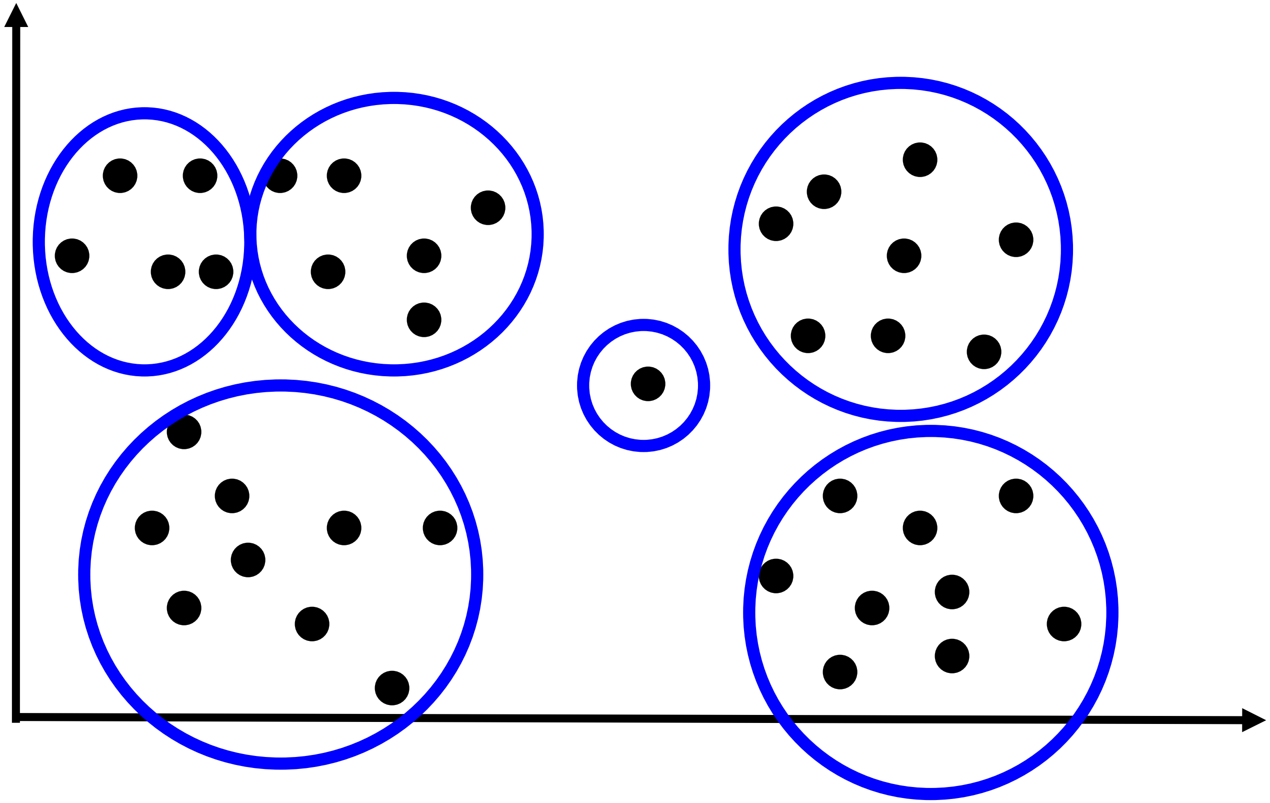
Quality of a Clustering – First Approach

- Compute average distance between all cluster members (objects = docs) in all clusters
- Definition
  Let f be a clustering of a set of objects O into a set C of classes with |C|=k. The k-score q_k of f is

$$q_k(f) = \sum_{i=1..k} d(o, f(o))$$

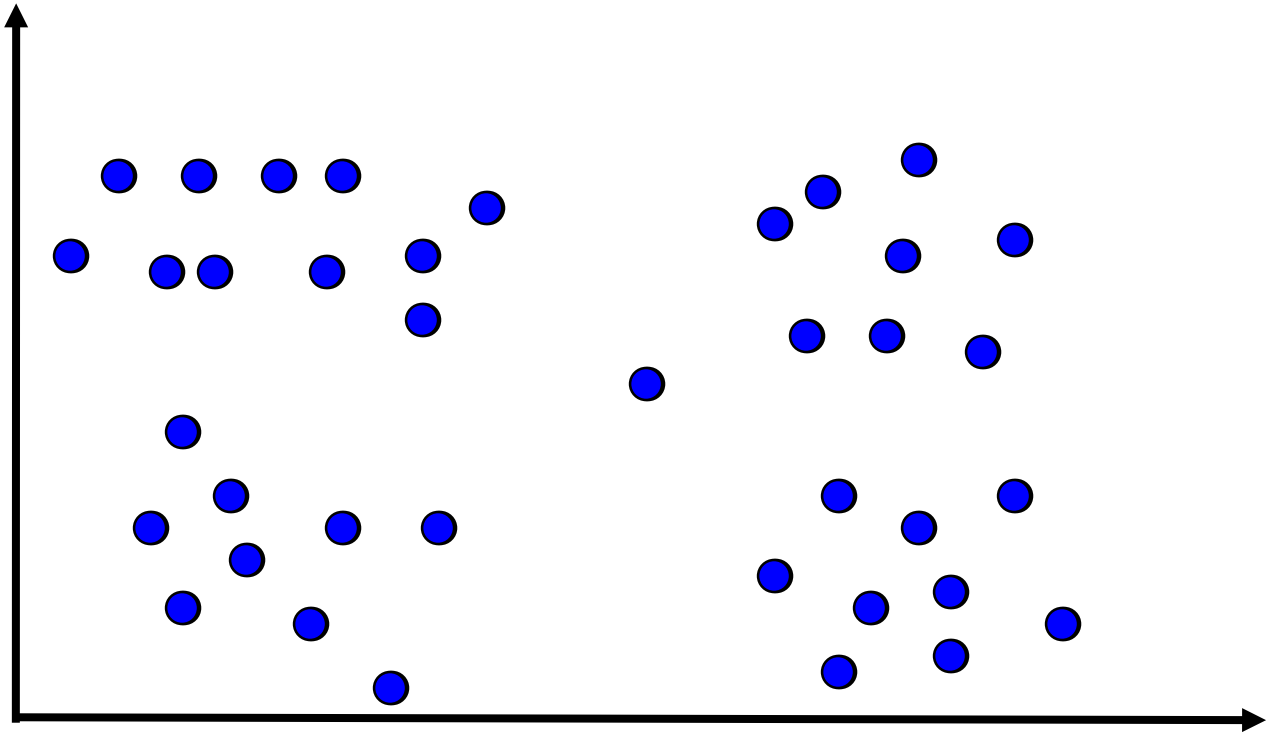
  - Any measure for point-to-cluster distance may be used

6-Score



- Certainly better than the 2/4/5-score we have seen
- Thus: Chose the k with the best k-score?

Disadvantage



- Always has a trivially optimal solution: k=|O|
- Points in a cluster should be close to each other but also far away from points in other clusters
- Still useful to compare different clusterings for the same k

Silhouette

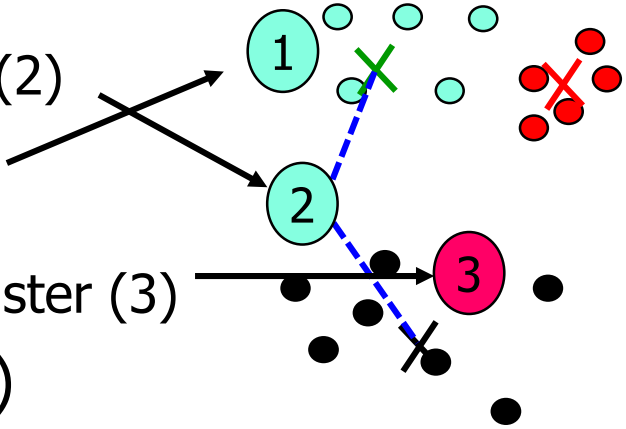
- Alternative: Silhouette
  - Punish points that are not “clearly” assigned to one cluster
- Definition

  Let $f: O \rightarrow C$ with $|C|$ arbitrary. We define
  - *Inner score: $in(o) = d(o, f(o))$*
  - *Outer score: $out(o) = \min(d(o,c_i))$ with $c_i \neq f(o)$*
  - *The silhouette of o, s(o), is defined as* $$s(o) = \frac{out(o) - in(o)}{\max(in(o), out(o))}$$
  - *The silhouette of f, s(f), is defined as* $$s(f) = \sum s(o)$$

Intuition

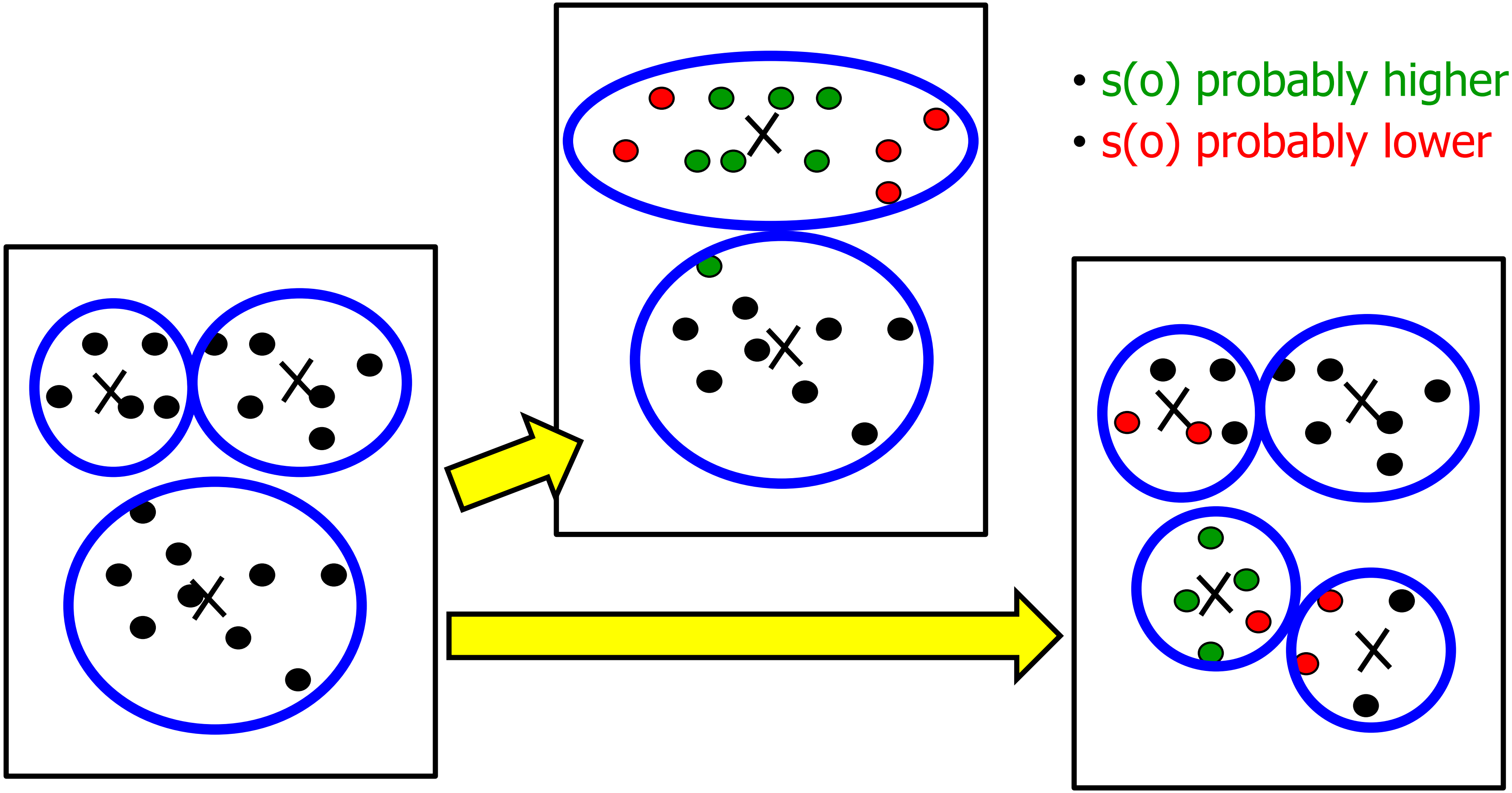
$$s(o) = \frac{out(o) - in(o)}{\max(in(o), out(o))}$$

- It holds: -1 ≤ s(o) ≤1
  - s(o) ≈ 0: Point right between two cluster (2)
  - s(o) ~ 1: Point very close to only one (1) (its own) cluster
  - s(o) ~ -1: Point far away from its own cluster (3)
- Computing the silhouette is in O(kmn)
  - If clusters are represented by centroids
  - m: Dimensionality, n: Number of objects, k: Number of clusters
  - Compare each object to each centroid



Behavior

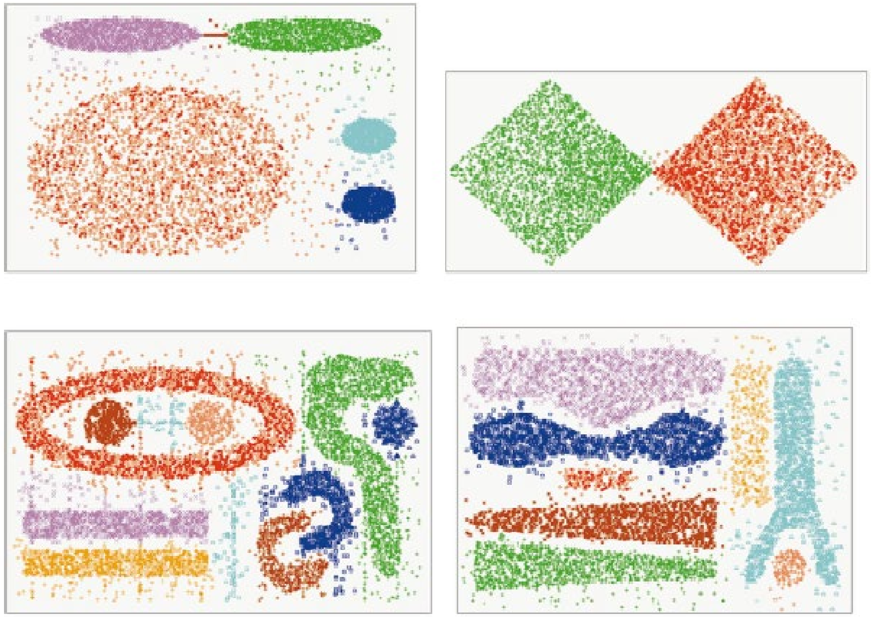
- Silhouette is not always better / worse for more clusters



- s(o) probably higher
- s(o) probably lower

Not the End

- In general, clusters need not be hyper-spheres
- Clusters need not even have convex shapes
- Cluster centre need not be part of a cluster
- Requires completely different quality metrics
- Definition must fit to the data/application
- Not used in text clustering
  - To my knowledge



Source: [FPPS96]

Content of this Lecture

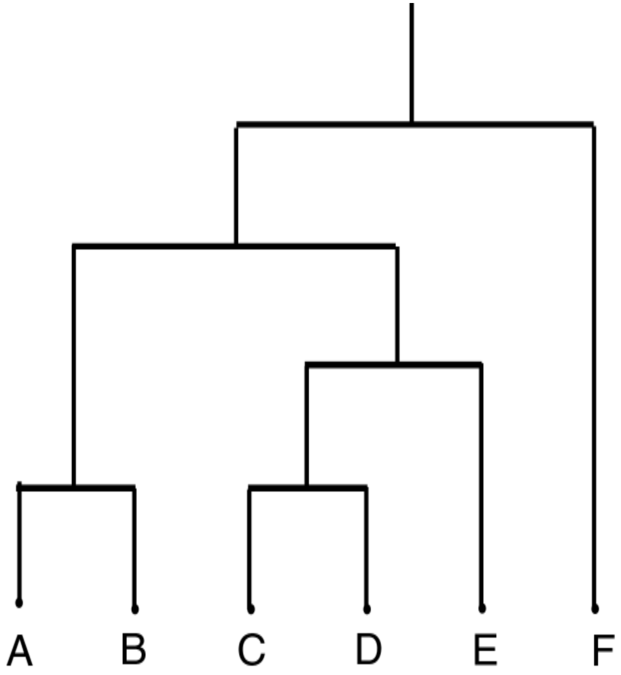
- Text clustering
- Cluster quality
- Clustering algorithms
  - Hierarchical clustering
  - K-means
  - Soft clustering: EM algorithm
- Application

Classes of Cluster Algorithms

- Hierarchical clustering
  - Iteratively creates a hierarchy of clusters
  - Bottom-Up: Start from |O| cluster and merge until only 1 remains
  - Top-Down: Start from one cluster and split
  - (… or until some stop criterion is met)
- Partitioning
  - Heuristically partition all objects in k clusters
  - Guess a first partitioning and improve iteratively
  - k is a parameter of the method, not a result
- Other
  - Graph-Theoretic: Min-Cut (optimal partitioning) etc.
  - Density-base clustering
  - …

Hierarchical Clustering

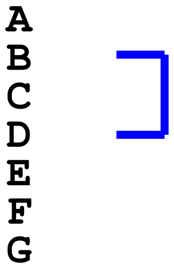
- Also called UPGMA: Unweighted Pair-group method with arithmetic mean
- Computes a binary tree (dendrogram)
- Algorithm
  - Compute distance matrix M (expensive)
  - Choose pair d_1, d_2 with smallest distance
  - Define x as centre point of d_1 and d_2
    - Coordinates need not be computed
  - Remove d_1, d_2 from M
  - Insert x into M
    - Distance between x and any d in M: Average distance between d_1 and d and d_2 and d
  - Loop until M has size 2x2



Example

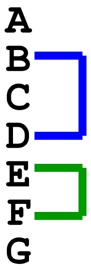
	A	B	C	D	E	F	G
A							
B	.						
C	.	.					
D	.	.	.				
E	.	.	.	.			
F	.	.	.	.	.		
G	.	.	.	.	.	.	

(B,D)→a



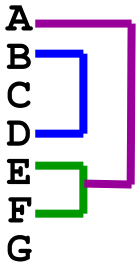
	A	C	E	F	G	a
A						
C	.					
E	.	.				
F	.	.	.			
G	.	.	.	.		
a	.	.	.	.	.	

(E,F)→b



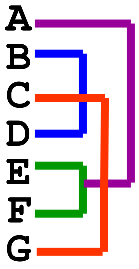
	A	C	G	a	b
A					
C	.				
G	.	.			
a	.	.	.		
b	.	.	.	.	

(A,b)→c



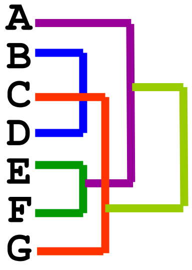
	C	G	a	c
C				
G	.			
a	.	.		
c	.	.	.	

(C,G)→d



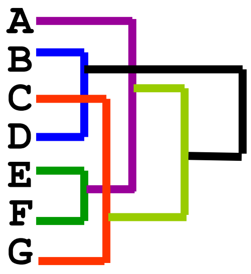
	a	c	d
a			
c	.		
d	.	.	

(d,c)→e

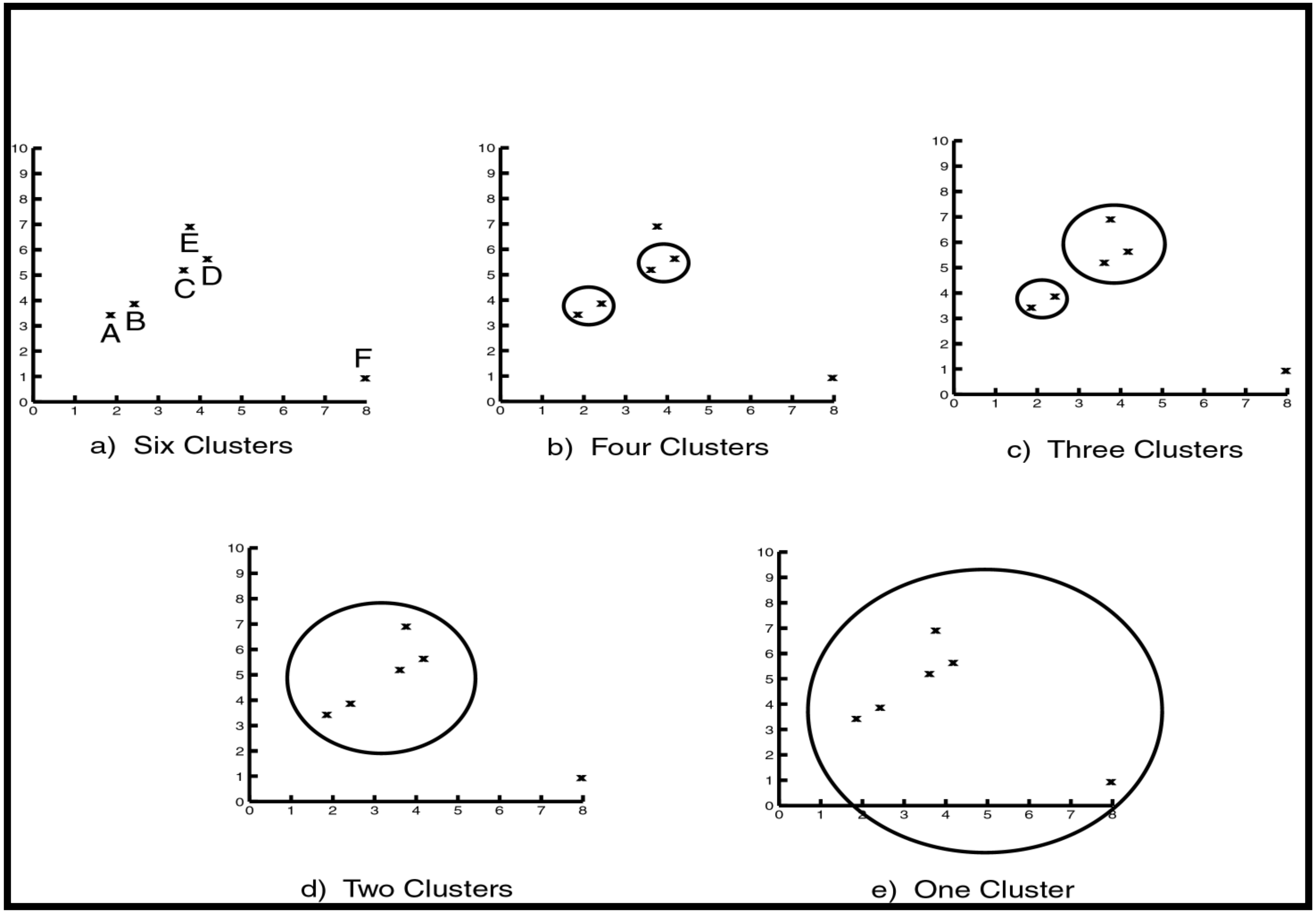


	a	e
a		
e	.	

(a,e)→f



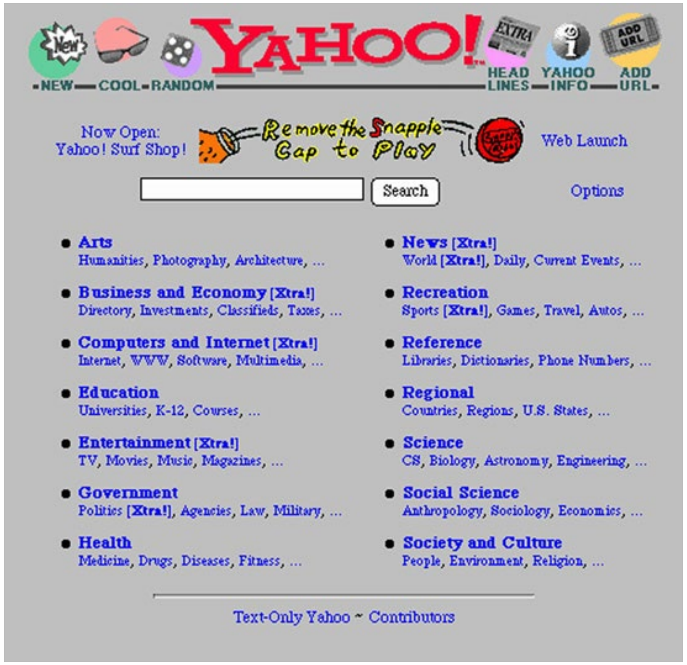
Visual



A
B
C
D
E
F
0
1
2
3
4
5
6
7
8
9
10
a) Six Clusters
b) Four Clusters
c) Three Clusters
d) Two Clusters
e) One Cluster

Intuition

- Hierarchical clustering organizes a doc collection
- Ideally, hierarchical clustering directly creates a hierarchical and intuitive directory of the corpus
- Not easy
  - Many, many ways to group objects – hierarchical clustering will choose just one
  - No guarantee that clusters make sense semantically
  - Problem of finding labels (= directory names)

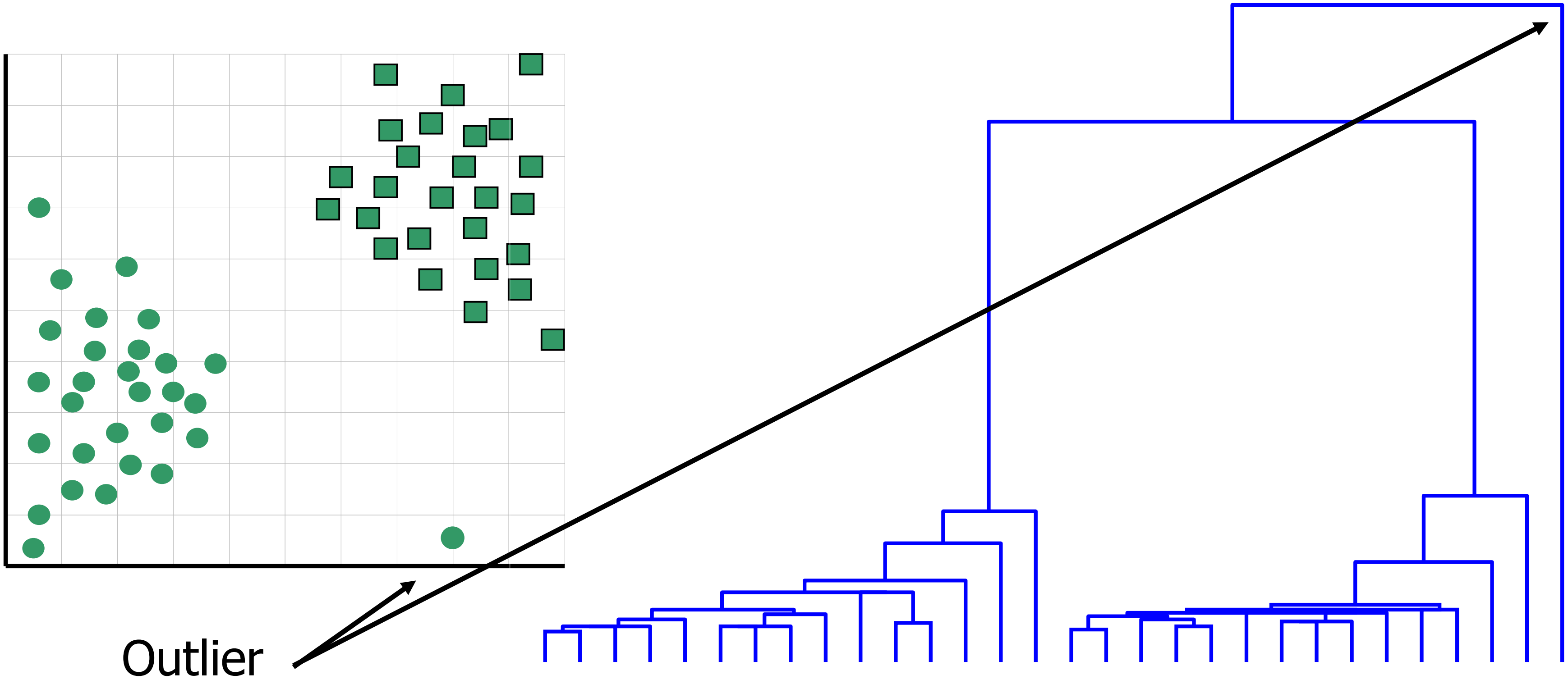


- **Arts** Humanities, Photography, Architecture, ...
- **Business and Economy** [Xtra!] Directory, Investments, Classifieds, Taxes, ...
- **Computers and Internet** [Xtra!] Internet, WWW, Software, Multimedia, ...
- **Education** Universities, K-12, Courses, ...
- **Entertainment** [Xtra!] TV, Movies, Music, Magazines, ...
- **Government** Politics [Xtra!], Agencies, Law, Military, ...
- **Health** Medicine, Drugs, Diseases, Fitness, ...
- **News** [Xtra!] World [Xtra!], Daily, Current Events, ...
- **Recreation** Sports [Xtra!], Games, Travel, Autos, ...
- **Reference** Libraries, Dictionaries, Phone Numbers, ...
- **Regional** Countries, Regions, U.S. States, ...
- **Science** CS, Biology, Astronomy, Engineering, ...
- **Social Science** Anthropology, Sociology, Economics, ...
- **Society and Culture** People, Environment, Religion, ...

Text-Only Yahoo ~ Contributors

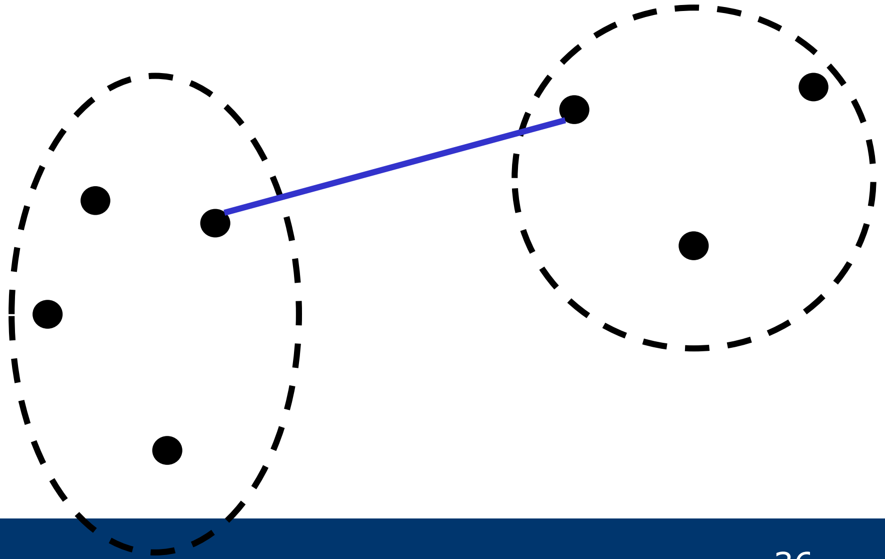
Visualization: Branch Length

- Use branch length to symbolize distance
- Outlier detection



Variations

- We used the distance between the centers of two clusters to decide about distance between clusters
- Other alternatives (incurring different complexities)
  - Single Link: Distance of the two closest docs in both clusters
  - Complete Link: Distance of the two furthest docs
  - Average Link: Average distance between pairs of docs from both clusters
  - Centroid: Distance between centre points



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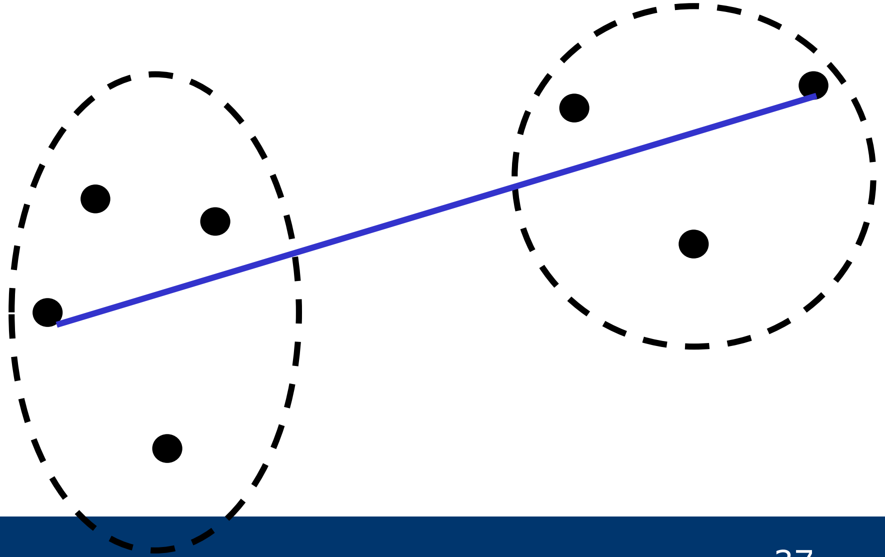

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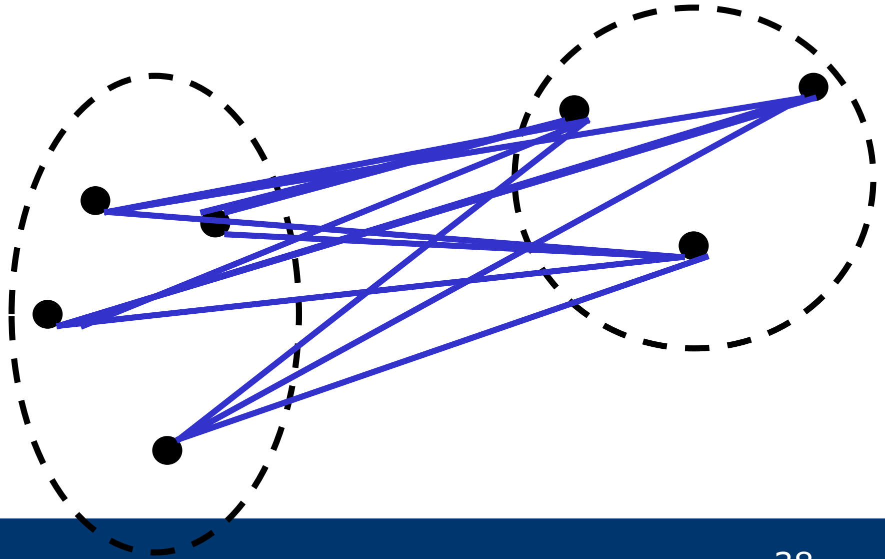

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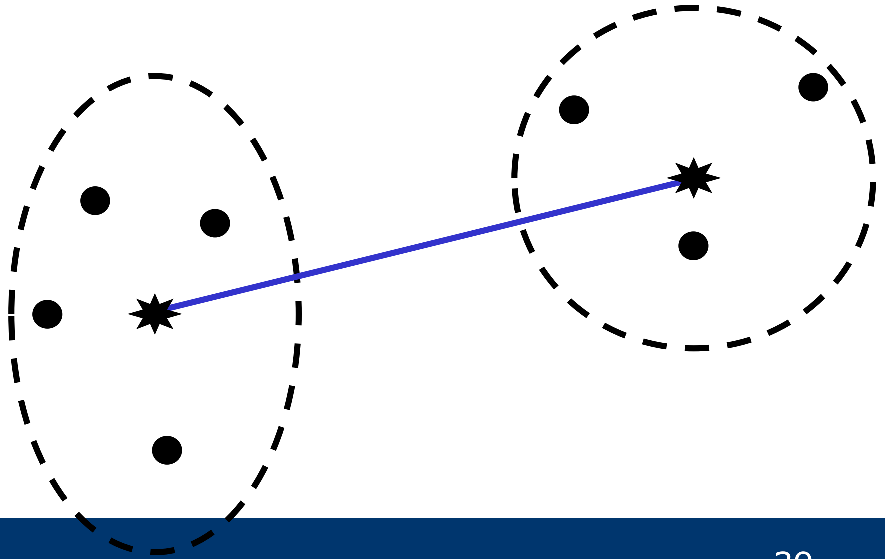
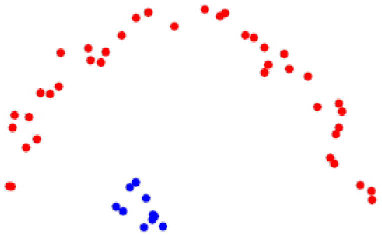
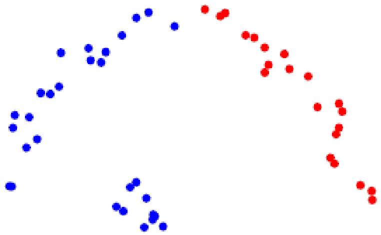


Comparison

- Single-link
  - Optimizes a local criterion
    - Only look at the closest pair – clusters must be similar in some point
  - Similar to computing a minimal spanning tree
  - Creates elongated clusters (chaining effect)
- Complete-link
  - Optimizes a global criterion
    - Look at the worst pair – all points within clusters must be similar
  - Creates more compact, “more” convex, spherical clusters

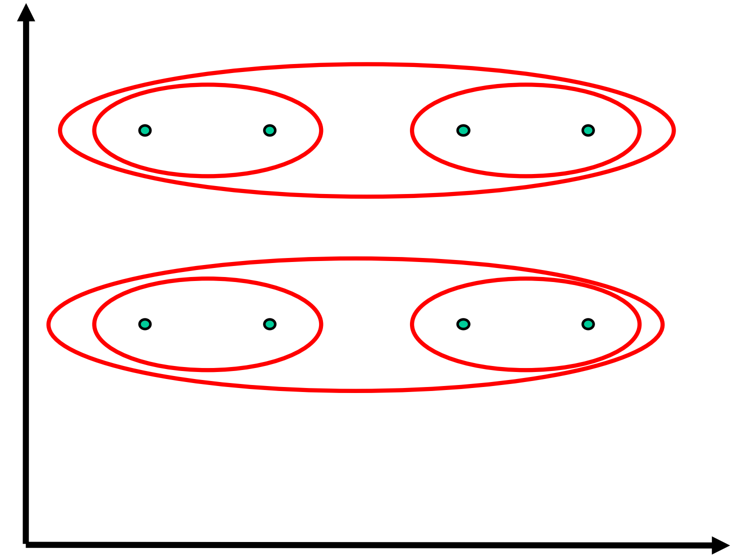


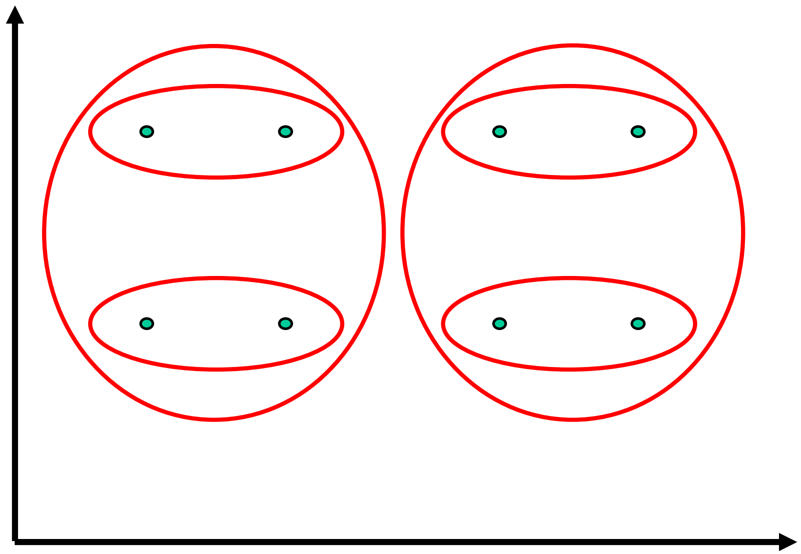
Single Linkage



Complete Linkage

Single-link versus Complete-link





Properties of Hierarchical Clustering

- Advantages
  - Simple and intuitive
  - Number of clusters is not an input of the method
  - Usually good quality clusters (which clusters?)
- Disadvantage
  - Does not really generate clusters
  - Very expensive; let n=|O|, m: dimensionality|
    - Computing M requires $O(n^2)$ space and $O(mn^2)$ time
    - Naïve implementation is in $O(m*n^2*log(n))$
    - Can be achieved in $O(m*n^2)$ (for single-link and complete-link)
  - Not applicable as such to large doc sets

Content of this Lecture

- Text clustering
- Cluster quality
- Clustering algorithms
  - Hierarchical clustering
  - K-means
  - Soft clustering: EM algorithm
- Application

Min-k-Cut Clustering

- Clustering in graph-theoretic concepts
- Definition

  Let G=(V,E) be a complete, weighted, undirected graph with V=O and w(<o_1,o_2>) = sim(o_1, o_2).

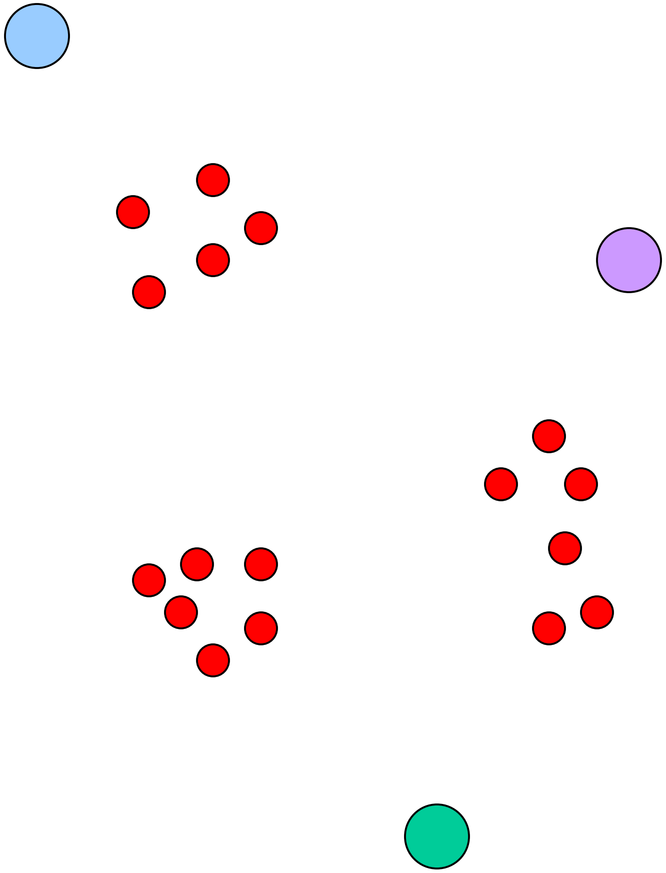
  - *A k-cut of G is a set S of edges such G'=(V,E\S) has k connected components.*
  - *A min-k-cut of G is a k-cut of G such that w(S) is minimal*
- Notes
  - Every k-cut is a clustering of G into k clusters
    - We use distance, not similarity, and maximize, not minimize
  - Finding a min-k-cut is in $O(|V|^{k\text{^}2})$
  - Not feasible in practice

Partitioning: K-Means

- Probably the most popular clustering algorithm
- Heuristic for solving the min-k-cut problem
- Requires the number k of clusters to be predefined
- Algorithm
  - Fix k
  - Guess k cluster centers
    - Can use k randomly chosen docs or k random points in feature-space
  - Loop forever
    - Assign all docs to their closest cluster center
    - If no doc has changed its assignment, stop
      - K-Means always converges, but possibly very slowly
      - Alternative: Stop once sufficiently few docs have changed their assignment
    - Otherwise, compute new cluster centers

Example 1

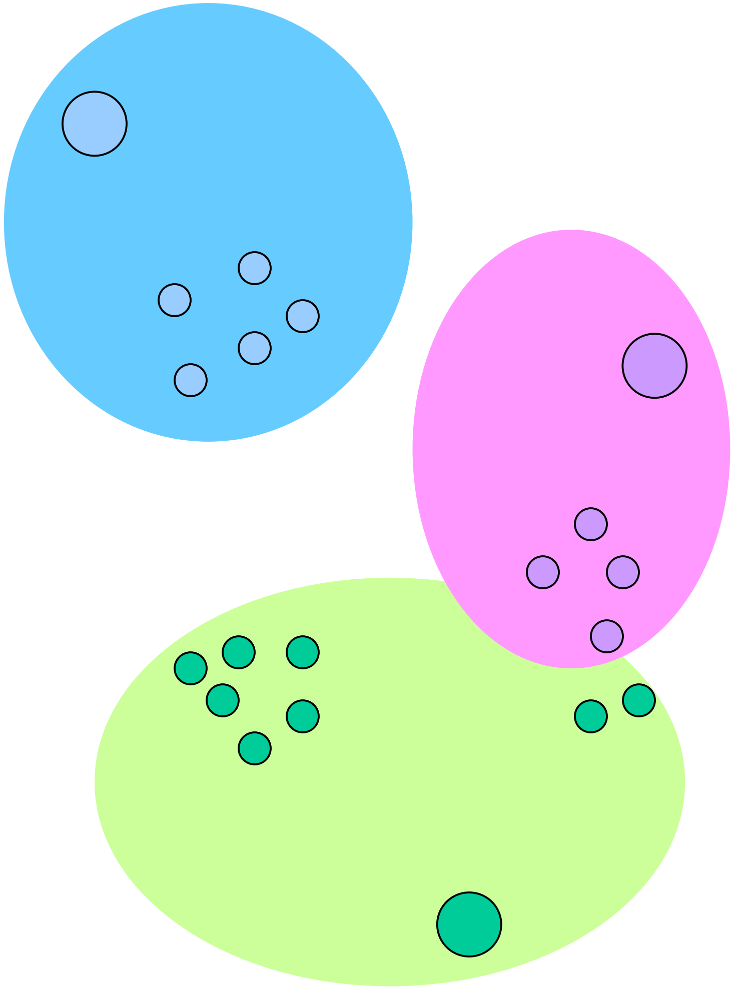
- k=3
- Choose random start points



Quelle: Stanford, CS 262
Computational Genomics

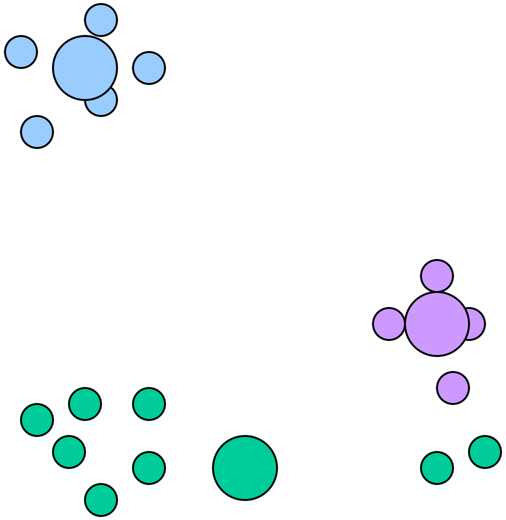
Example 2

- Assign docs to closest cluster centre

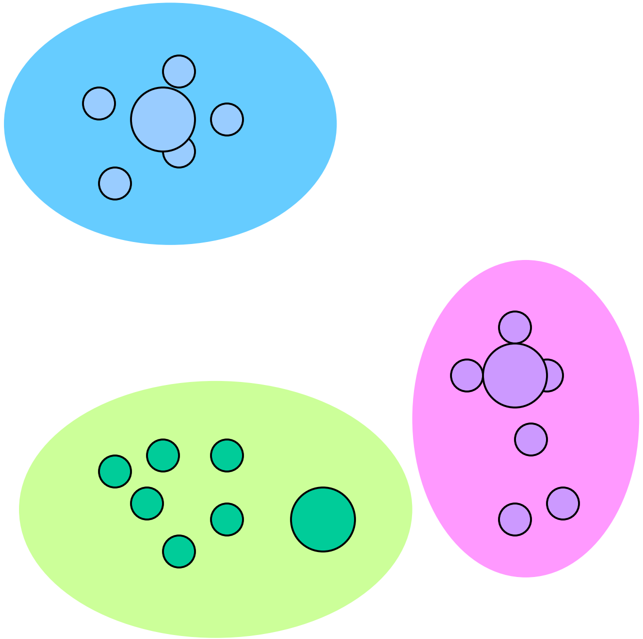


Example 3

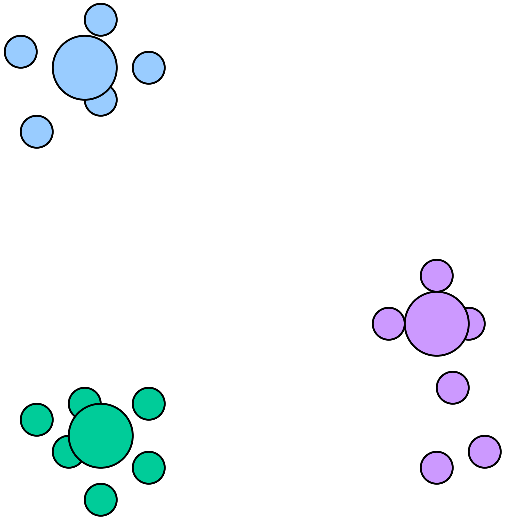
- Compute new cluster centre



Example 4

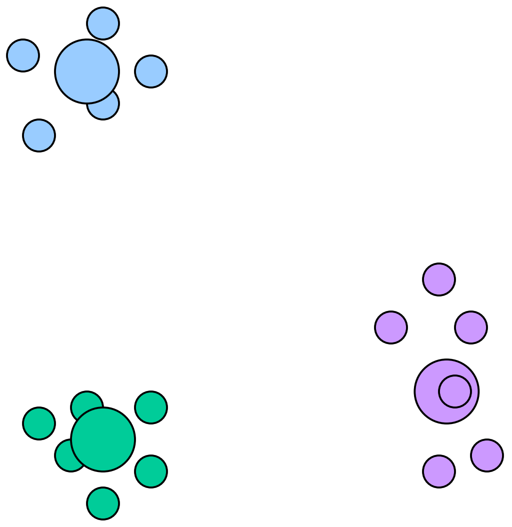


Example 5



Example 6

- Converged

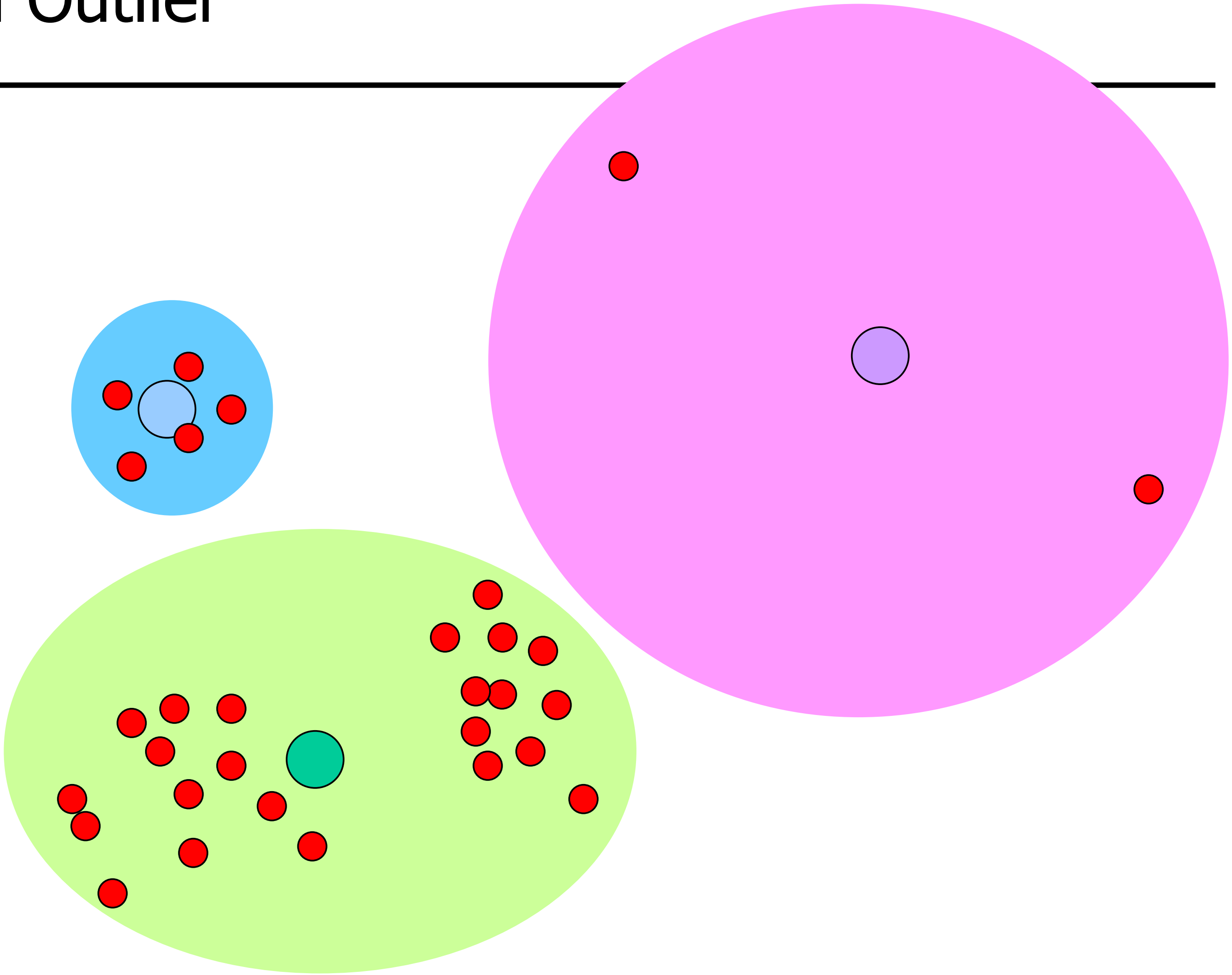


Properties

- Usually, k-Means converges quite fast
- Reasonable complexity: O(l*k*n*m)
  - Let l be the number of iterations
  - Assignment: n*k distance computations with O(m) each
  - New centers: Summing up n vectors of size m in k partitions
  - l is in principle unbounded, but small in practice (<100)
- Choosing the "right" start points is important
  - k-Means is a greedy heuristic and only finds local optima
  - Option 1: Start several times with different start points
  - Option 2: Compute hierarchical clustering on small random sample and choose cluster centers as start points ("Buckshot" algorithm)
- How to choose k?
  - Try for different k and compare quality score(s)

k-Means and Outlier

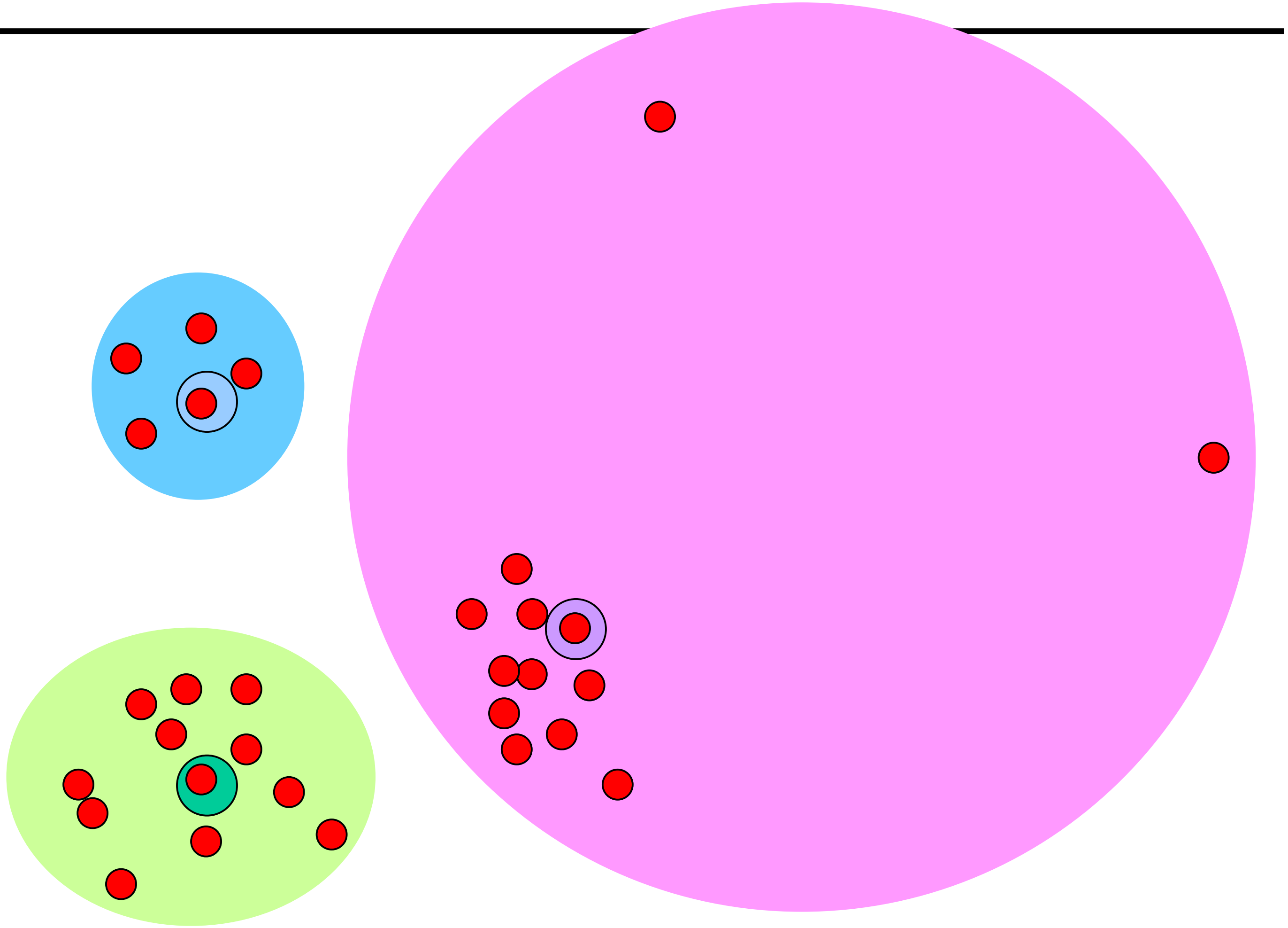
Assume k=3



Help: K-Medoid

- Chose the doc in the middle of a cluster as representative
  - Kaufman, Rousseeuw (1990): "Partitioning around medoids (pam)." in *Finding groups in data: an introduction to cluster analysis*
- Advantage
  - Less sensitive to outliers
  - Also works for non-metric spaces as no “new” center point need to be computed
- Disadvantage: Increased complexity
  - Finding the median doc requires computing all pair-wise distances in each cluster in each round
  - Complexity is $O(n^3)$ in each step
    - We can save re-computations at the expense of more space

k-Medoid and Outlier



Content of this Lecture

- Text clustering
- Cluster quality
- Clustering algorithms
  - Hierarchical clustering
  - K-means
  - Soft clustering: EM algorithm
- Application

Soft Clustering

- We assumed docs are assigned to exactly one cluster
- Probabilistic interpretation: All docs pertain to all clusters with a certain probability
- Generative model
  - Assume we have k "doc-producing" devices
    - Such as authors, topics, …
  - Each device produces docs that are normally distributed in feature space with device-specific mean and variance
  - Assume that k devices produced |D| documents
  - Clustering: Re-discovery of mean and variance of each device
- Solution: Expectation Maximization Algorithm (EM)

Expectation Maximization (rough sketch)

- EM optimizes set of parameters P of a multivariate normal distribution (mean and variance, k clusters) given the data
- Iterative process with two phases
  - Guess an initial P
  - Expectation: Assign all docs its most likely generator based on P
  - Maximization: Compute new optimal P based on assignment
    - Using MLE or other estimation techniques
  - Iterate through both steps until convergence
- Finds a local optimum, convergence guaranteed
- K-Means: Special case of EM
  - Clusters with different means but equal variance
  - K-Means assumes all clusters have the same error model

Content of this Lecture

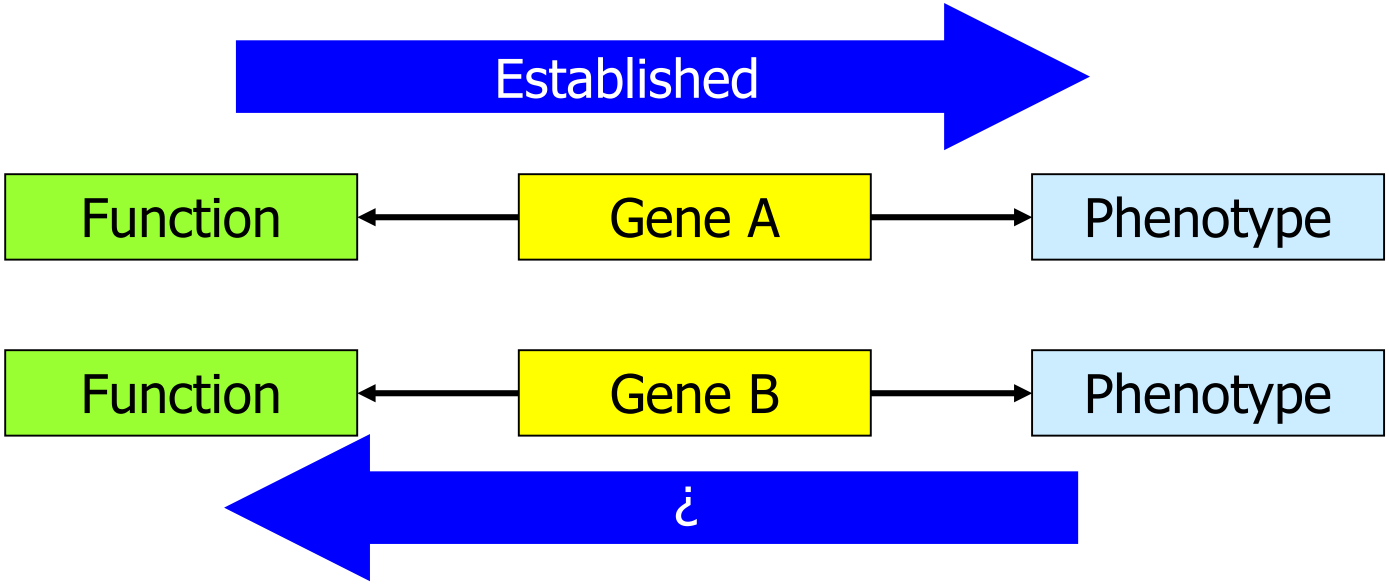
- Text clustering
- Cluster quality
- Clustering algorithms
- Application
  - Clustering Phenotypes

Mining Phenotypes for Function Prediction

Or …

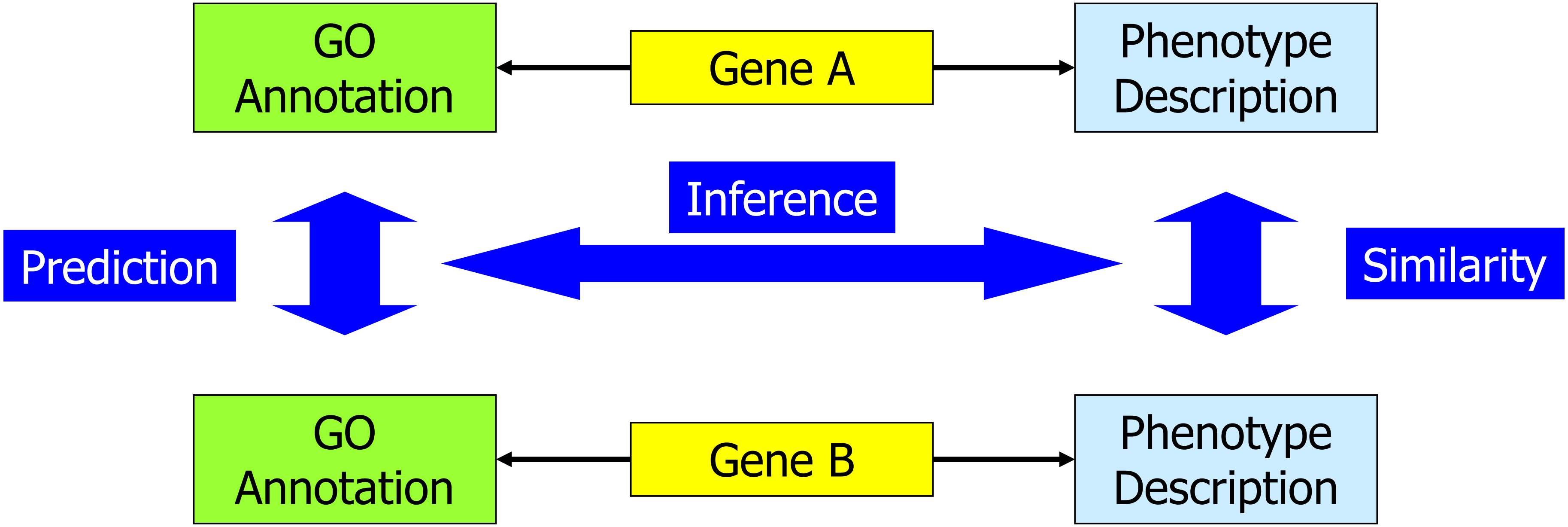
Source: http://www.guy-sports.com/humor/videos/powerpoint_presentation_dogs.htm

Mining Phenotypes: General Idea



- Known: Genes with sim. functions produce sim. phenotypes
- Question: If genes generate very similar phenotypes – do they have the same functions?
  - Groth et al. (2008). "Mining phenotypes for gene function prediction." BMC Bioinformatics 9: 136.

Approach


GO Annotation
Gene A
Phenotype Description
Inference
Prediction
Similarity
GO Annotation
Gene B
Phenotype Description

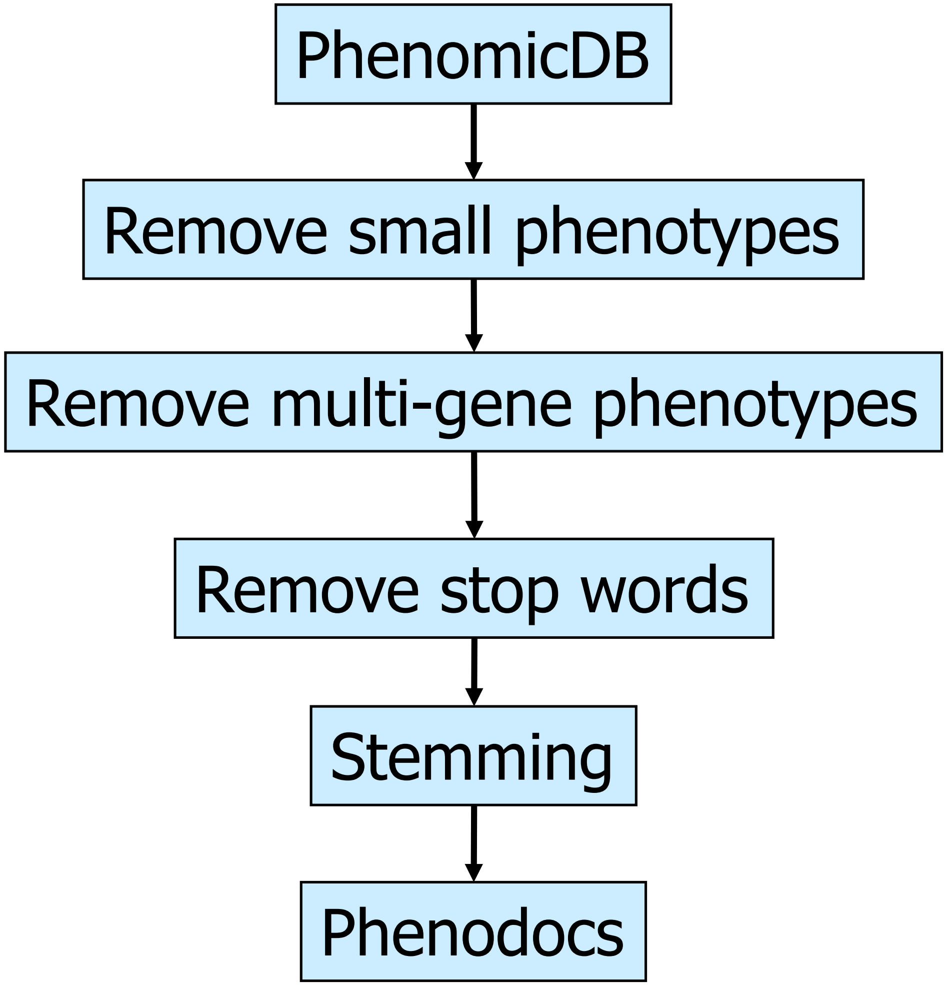
Phenodocs

411,102 phenotype texts

Short: <250 words

Remove all phenotypes associated to more than one gene (~500)

39,610 ‘phenodocs’ for 15,426 genes



PhenomicDB

Remove small phenotypes

Remove multi-gene phenotypes

Remove stop words

Stemming

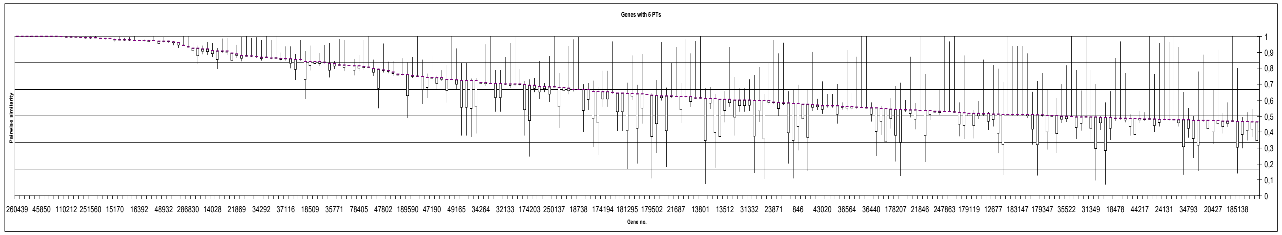
Phenodocs

K-Means Clustering

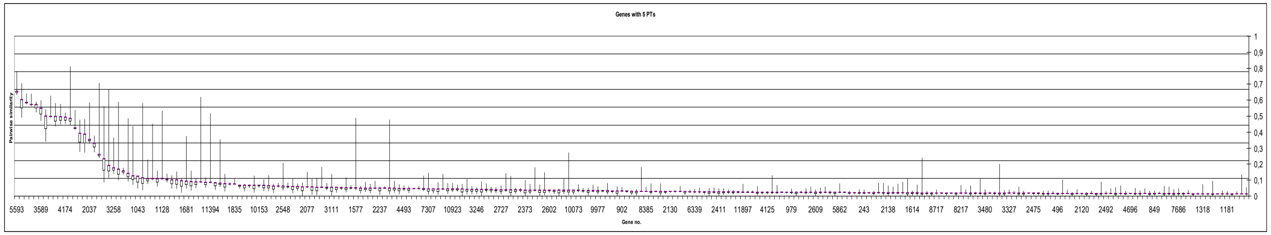
- Hierarchical clustering would require
  ~ 40.000*40.000 = 1.600.000.000 comparisons
- K-Means: Simple, iterative algorithm
- Number of clusters must be predefined
  - We experimented with 250 … 3000 clusters

Properties: Phenodoc Similarity of Genes

Genes in phenoclusters



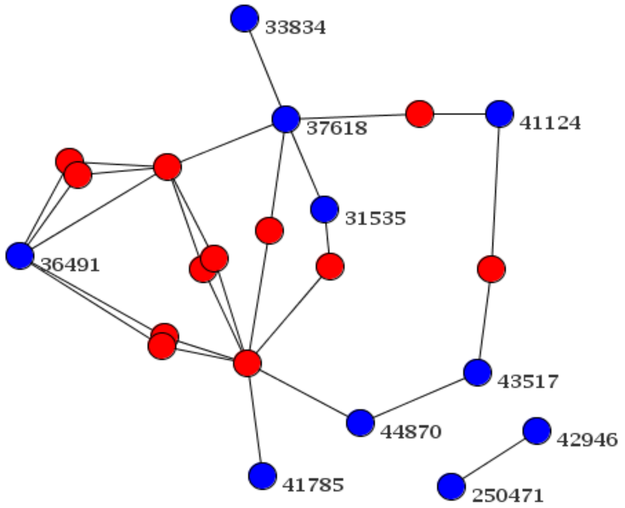
Control (Random selection)



- Pair-wise similarity scores of phenodocs of genes in the same cluster, sorted by score
- Result: Phenodocs of genes in phenoclusters are highly similar to each other

PPI: Inter-Connectedness

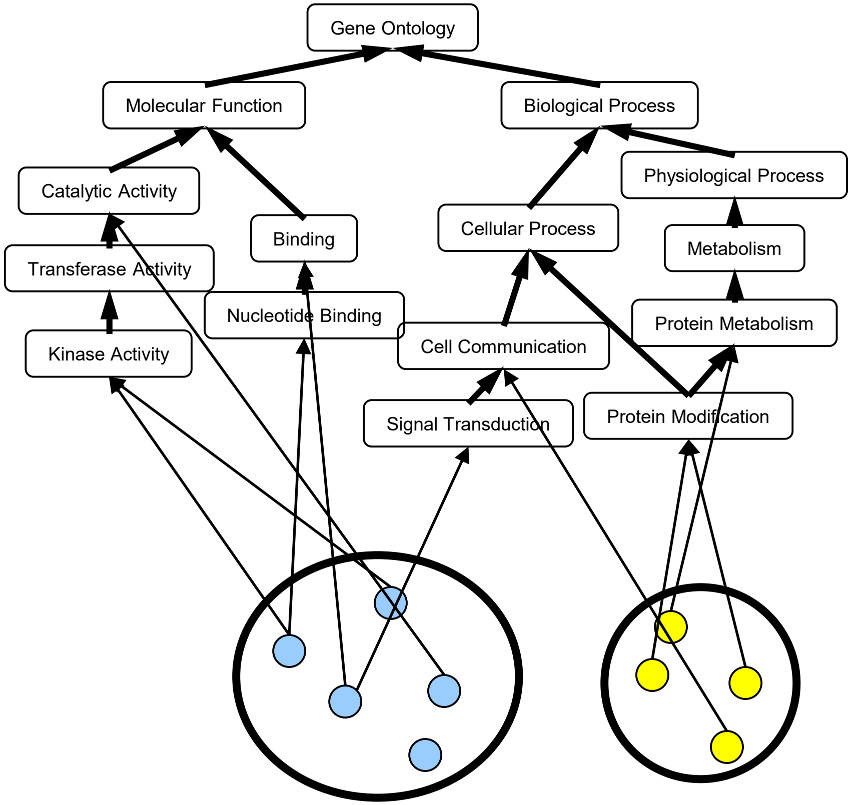
- Interacting proteins often share function
- PPI from BIOGRID database
  - Not at all a complete dataset
- In >200 clusters, >30% of genes interact with each other
- Control (random groups): 3 clusters
- Result: Genes in phenoclusters interact with each other much more often than expected by chance



Proteins and interactions from BioGrid. Red proteins have no phenotypes in PhenomicDB

Coherence of Functional Annotation

- Comparison of GO annotation of genes in phenoclusters
  - Data from Entrez Gene
  - Similarity of two GO terms: Normalized number of shared ancestors
  - Similarity of two genes: Average of the top-k GO pairs
- >200 clusters with score >0.4
  - Control: 2 clusters
- Results: Genes in phenoclusters have a much higher coherence in functional annotation than expected by chance

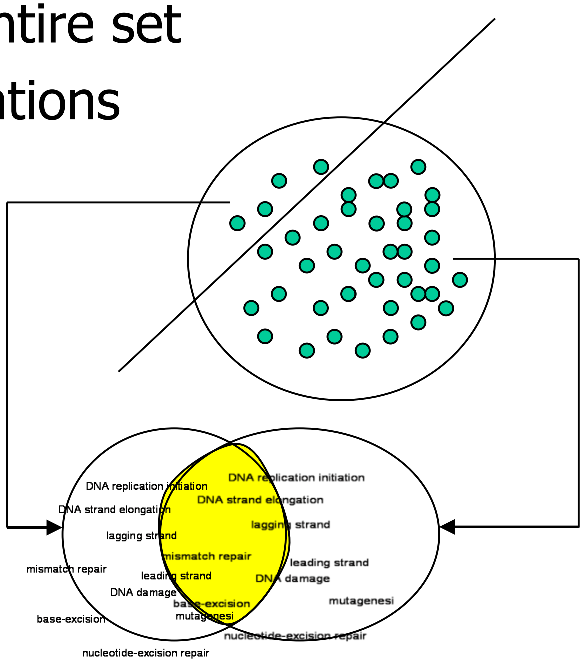


Function Prediction

- Can increased functional coherence of clusters be exploited for function prediction?
- Approach
  - Compute phenoclusters
  - For each cluster, compute set of associated genes (gene cluster)
  - In each gene cluster, predict frequent GO terms to all genes
    - Frequent: annotated to >50% of genes in the cluster
- Some filtering of clusters required / useful
  - Filter 1: Only clusters with >2 members and at least one common GO term
  - Filter 2: Only clusters with GO coherence>0.4
  - Filter 3: Only clusters with PPI-connectedness >33%
  - …

Evaluation

- How can we know how good we are?
- Cross-validation
  - Separate genes in training (90%) and test (10%)
  - Remove annotation from genes in test set
  - Build clusters and predict functions on entire set
  - Compare predicted with removed annotations
    - Precision and recall
  - Repeat and average results
    - Macro-average
- Note: This punishes new and potentially valid annotations



Results for Different Filters

	(Filter 1)	(Filter 1 & Filter 2)	(Filter 1 & Filter 3)
# of clusters	196	74	53
# of terms	345	159	102
# of genes	3213	711	409
Precision	67.91%	62.52%	60.52%
Recall	22.98%	26.16%	19.78%

- What if we consider predicted terms to be correct that are a little more general than the removed terms (filter 1)?
  - One step more general: 75.6% precision, 28.7% recall
  - Two steps: 76.3% precision, 30.7% recall
- The less stringent "GO equality", the better the results
  - This is a common "trick" in studies using GO

Results for Different Cluster Sizes

K	250	500	750	1,000		2,750	3,000
Cluster w/ GO-Sim ≥ 1	14 (5.6%)	26 (5.2%)	44 (5.9%)	71 (7.1%)		273 (9.9%)	309 (10.3%)
# Genes	561	781	943	1155		2094	2221
Cluster w/ PPi ≥ 75%	12 (4.8%)	34 (6.8%)	65 (8.7%)	88 (8.8%)		314 (11.4%)	353 (11.8%)
# Genes	785	988	1166	1263		1810	1914
Cluster w/ PPi ≥ 33%	49 (19.6%)	119 (23.8%)	193 (25.7%)	252 (25.2%)		662 (24.1%)	717 (23.9%)
# Genes	3362	4044	4296	4417		4811	4833
Cluster for GO-Pred.	73 (29.2%)	153 (30.6%)	230 (30.7%)	295 (29.5%)	...	748 (27.2%)	816 (27.2%)
# Genes	3465	4139	4344	4438		5016	5115
# Terms	123	247	383	489		1436	1557
Precision	81.53%	77.16%	74.26%	71.73%		63.92%	62.89%
Recall	16.90%	20.22%	24.45%	26.36%		34.64%	34.61%
Avg. Genes/Cluster	52	26	17	13		4	4

- With increasing k
  - Clusters are smaller
  - Number of predicted terms increases
    - Clusters are more homogeneous
  - Number of genes which receive annotations increases
  - Precision decreases slowly, recall increases
    - Effect of the rapid increase in number of predictions

Selbsttest

- Gegeben der folgende Datensatz. Wenden Sie den hierarchischen Cluster-Algorithmus an und zeichnen Sie die entstandenen Cluster. Verwenden Sie Euklidischen Abstand
- Welche Komplexität hat hierarchisches Clustering? Begründen Sie.
- Beschreiben Sie drei verschiedene Methoden, mit denen man den k-Means Algorithmus initialisieren kann. Was sind Vor-/Nachteile?
- Was ist der Unterschied zwischen k-Means und k-Mediod? Wie ändert sich die Komplexität von k-Means zu k-Medoid – und warum?