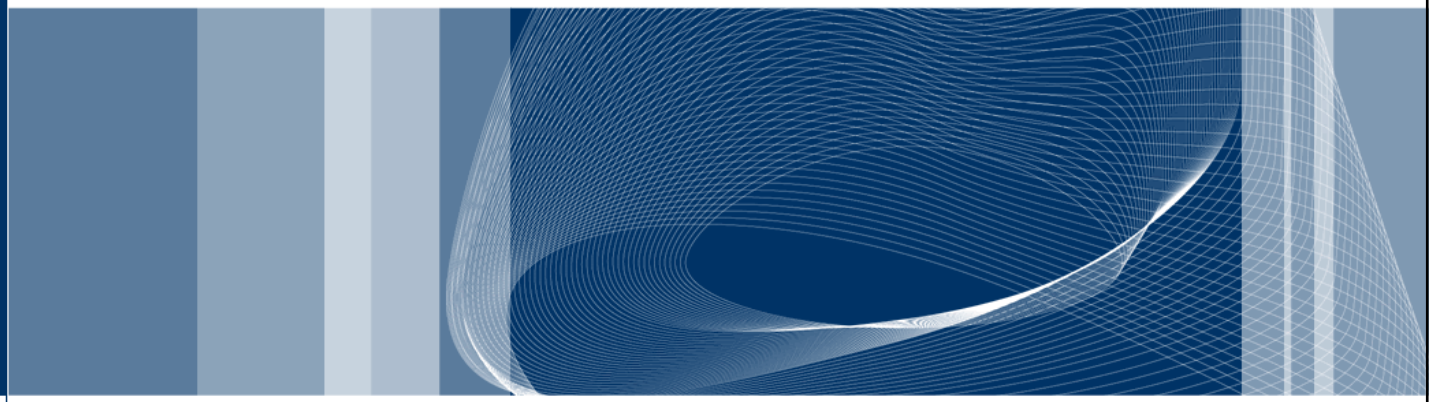
POLITECNICO DI MILANO



Text Mining

Data Science for Mobility

Prof. Pier Luca Lanzi

What is Text Mining?

- Text mining deals with the discovery of new, previously unknown information, by automatically extracting information from different unstructured textual documents

- The term identifies a family of problems and methods
  - Classification
  - Clustering
  - Sentiment Analysis
  - Summarization
  - Relations/Concepts/Events Extraction
  - Topic modeling
  - …

Text Mining

- Text mining is basically a synonyms of Text Analytics
- The goal is to turn text data into high-quality information or actionable knowledge
- Minimizes human effort (on consuming text data)
- Supplies knowledge for optimal decision making
- Text mining is strongly related to text retrieval, which is an essential component in any text mining system

Natural Language Processing (NLP)

Gov. Schwarzenegger helps inaugurate pricey new bridge approach

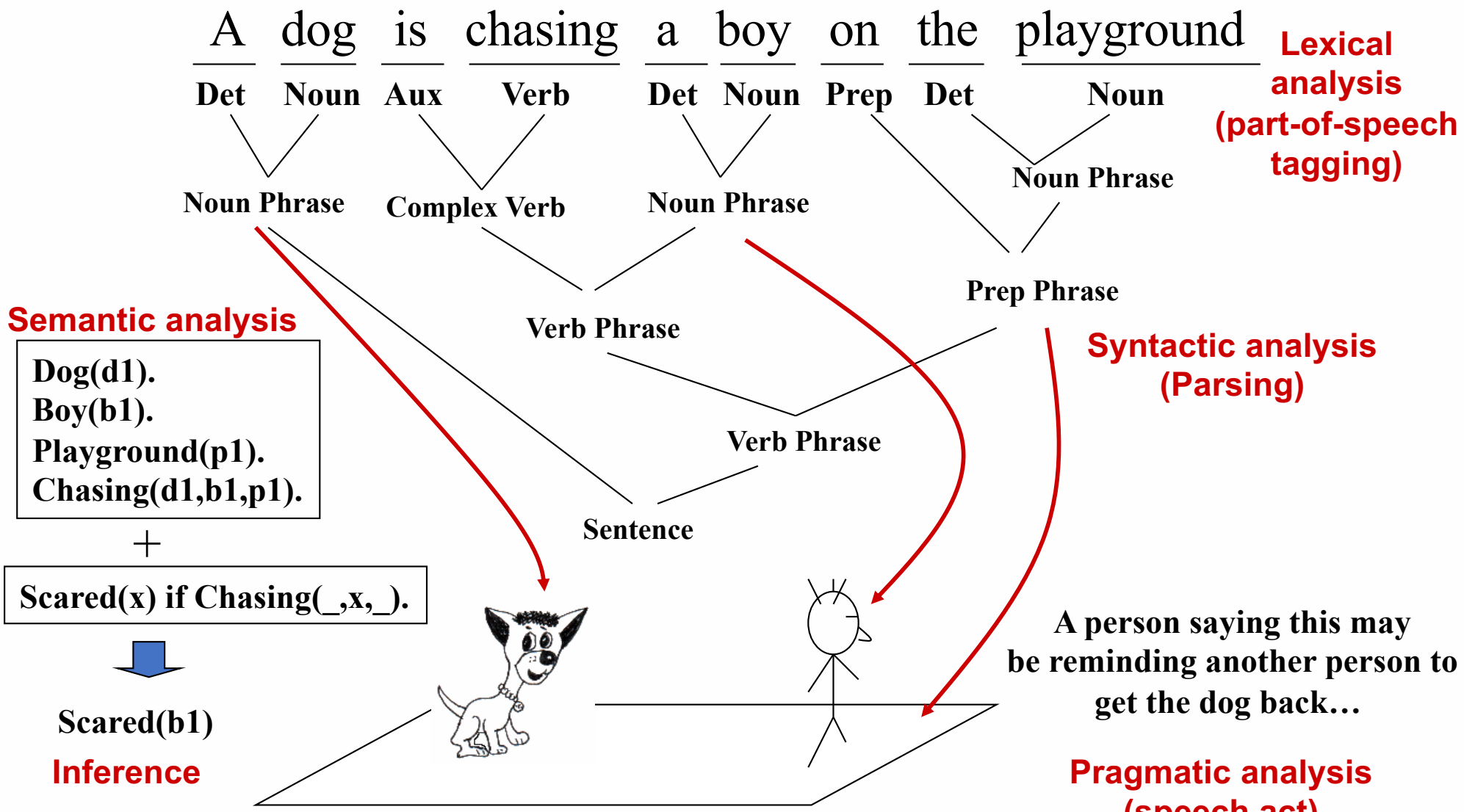
The Associated Press

Article Launched: 04/11/2008 01:40:31 PM PDT

SAN FRANCISCO—It briefly looked like a scene out of a "Terminator" movie, with Governor Arnold Schwarzenegger standing in the middle of San Francisco wielding a blow-torch in his hands. Actually, the governor was just helping to inaugurate a new approach to the San Francisco-Oakland Bay Bridge. Caltrans thinks the new approach will make it faster for commuters to get on the bridge from the San Francisco side.
The new section of the highway is scheduled to open tomorrow morning and cost 429 million dollars to construct.

- Is this article talks about entertainment? Or politics?
- Using just the words has severe limitations

- Schwarzenegger
- Bridge
- Caltrans
- Governor
- Scene
- Terminator



(Taken from ChengXiang Zhai, CS 397cxz – Fall 2003)

Natural Language Processing is Difficult!

- Natural language is designed for efficient human communication
- As a result,
  - We omit a lot of common sense knowledge, which we assume the hearer/reader possesses.
  - We keep a lot of ambiguities, which we assume the hearer/reader knows how to resolve.
- This makes every step of natural language processing very difficult
  - Ambiguity
  - Common sense reasoning

What the Difficulties?

- Word-level Ambiguity
  - "design" can be a verb or a noun
  - "root" has multiple meaning
- Syntactic Ambiguity
  - A man saw a boy with a telescope
- Presupposition
  - "He has quit smoking" implies he smoked
- Text Mining NLP Approach
  - Locate promising fragments using fast methods
  - Only apply slow NLP techniques to promising fragments

What the Open Problems?

- 100% POS tagging
  - "he turned off the highway" vs "he turned off the light"
- General complete parsing
  - "a man saw a boy with a telescope"
- Precise deep semantic analysis
- Robust and general NLP methods tend to be shallow while deep understanding does not scale up easily


JEOPARDY!
The IBM Challenge
JEOPARDY!

Information Retrieval

- Information retrieval deals with the problem of locating relevant documents with respect to the user input or preference

- Typical systems
  - Online library catalogs
  - Online document management systems

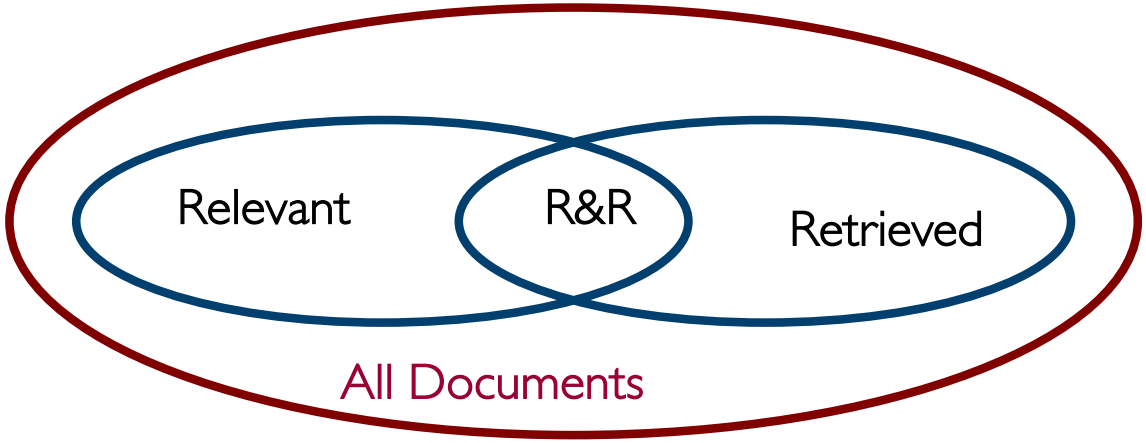
- Typical issues
  - Management of unstructured documents
  - Approximate search
  - Relevance

Two Modes of Text Access

- Pull Mode (search engines)
  - Users take initiative
  - Ad hoc information need
- Push Mode (recommender systems)
  - Systems take initiative
  - Stable information need or system has good knowledge about a user's need

Text Retrieval Methods

- Document Selection (keyword-based retrieval)
  - Query defines a set of requisites
  - Only the documents that satisfy the query are returned
  - A typical approach is the Boolean Retrieval Model
- Document Ranking (similarity-based retrieval)
  - Documents are ranked on the basis of their relevance with respect to the user query
  - For each document a "degree of relevance" is computed with respect to the query
  - A typical approach is the Vector Space Model



$$\text{precision} = \frac{|\{\text{Relevant}\} \cap \{\text{Retrieved}\}|}{\{\text{Retrieved}\}}$$

$$\text{recall} = \frac{|\{\text{Relevant}\} \cap \{\text{Retrieved}\}|}{\{\text{Relevant}\}}$$

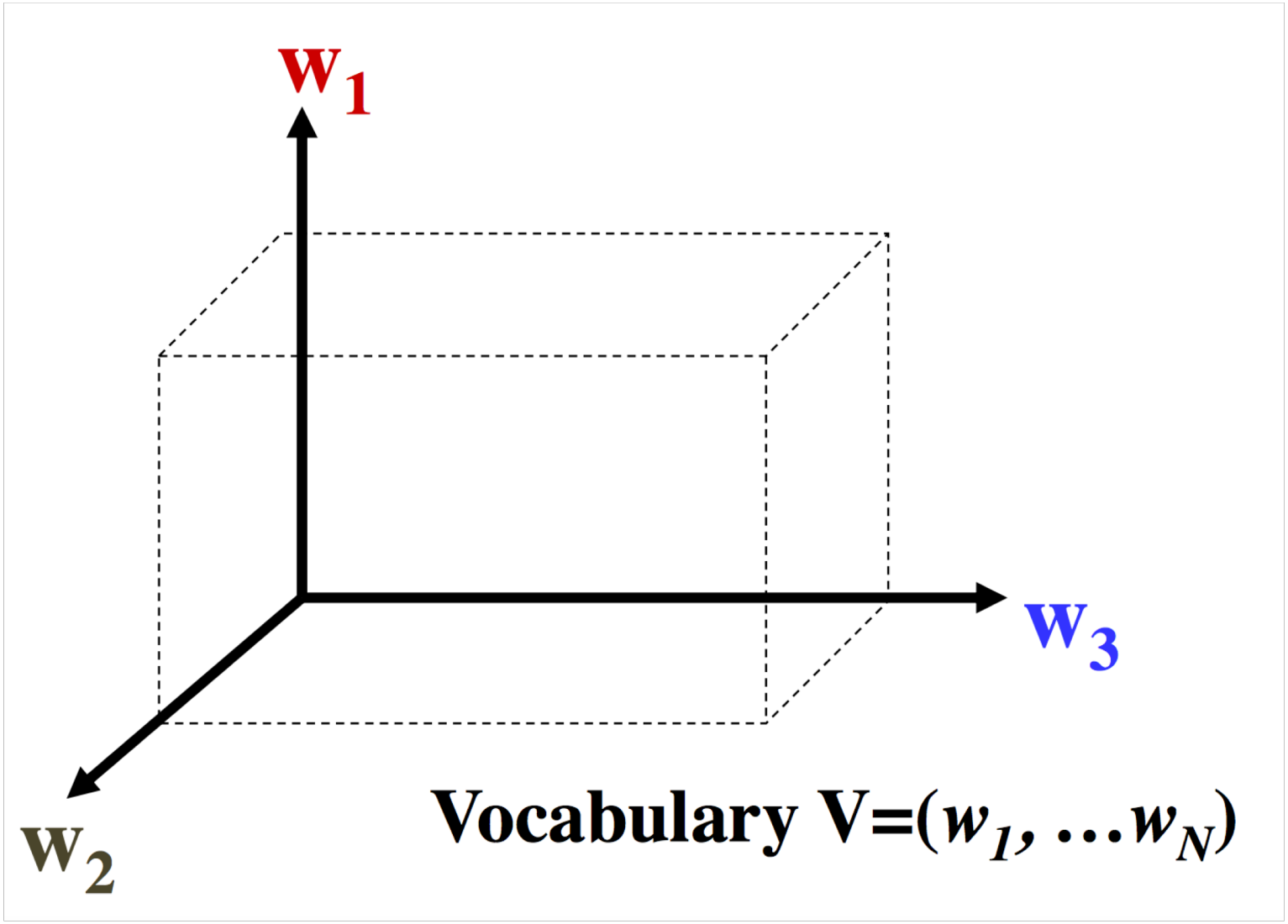
$$\text{F-score} = \frac{2 \times \text{precision} \times \text{recall}}{\text{precision} + \text{recall}}$$

Document Similarity

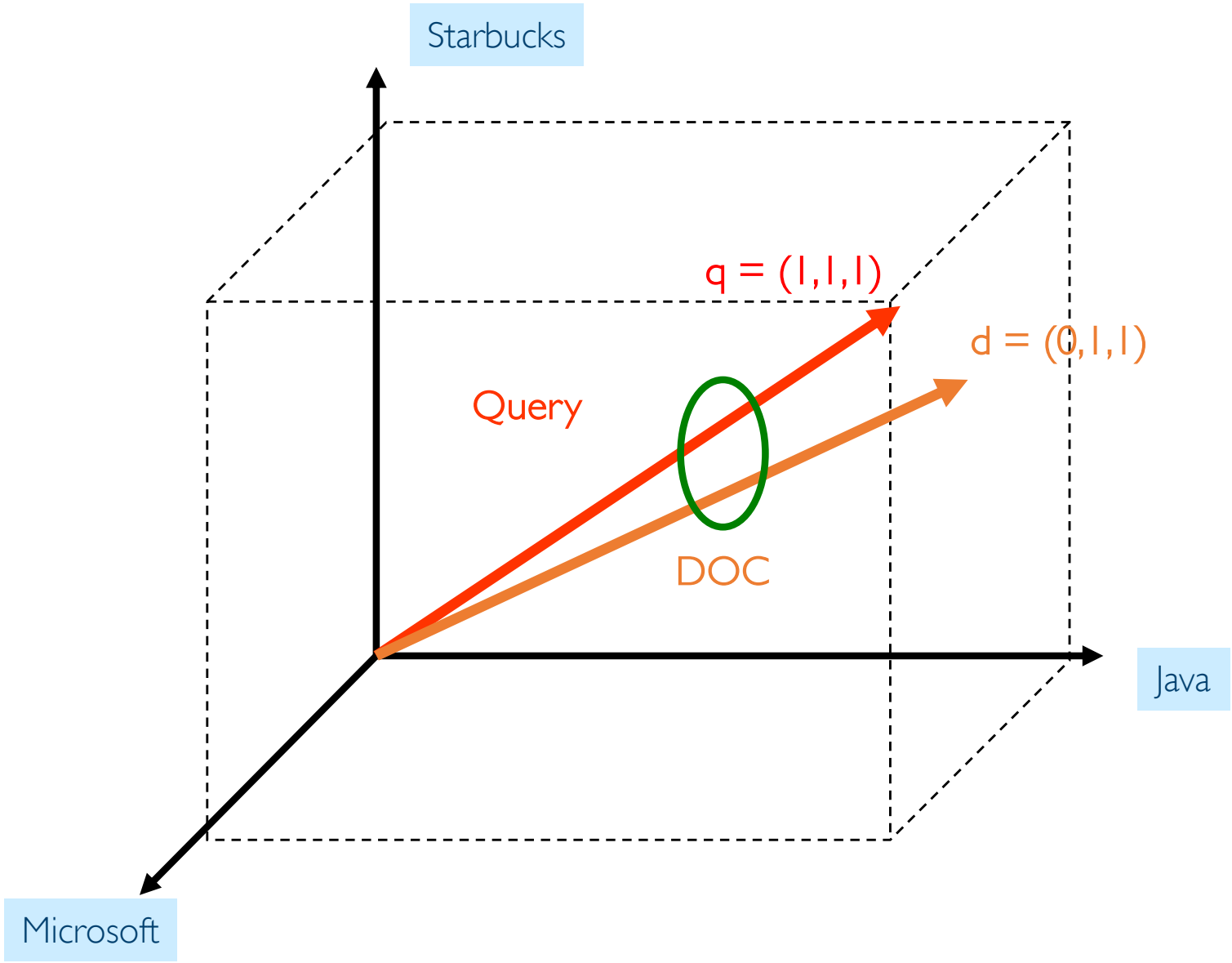
Vector Space Model

- A document and a query are represented as vectors in high-dimensional space corresponding to all the keywords
- Relevance is measured with an appropriate similarity measure defined over the vector space
- Issues
  - How to select keywords to capture "basic concepts" ?
  - How to assign weights to each term?
  - How to measure the similarity?

Bag of Words



Basic Vector Space Model



Document Ranking

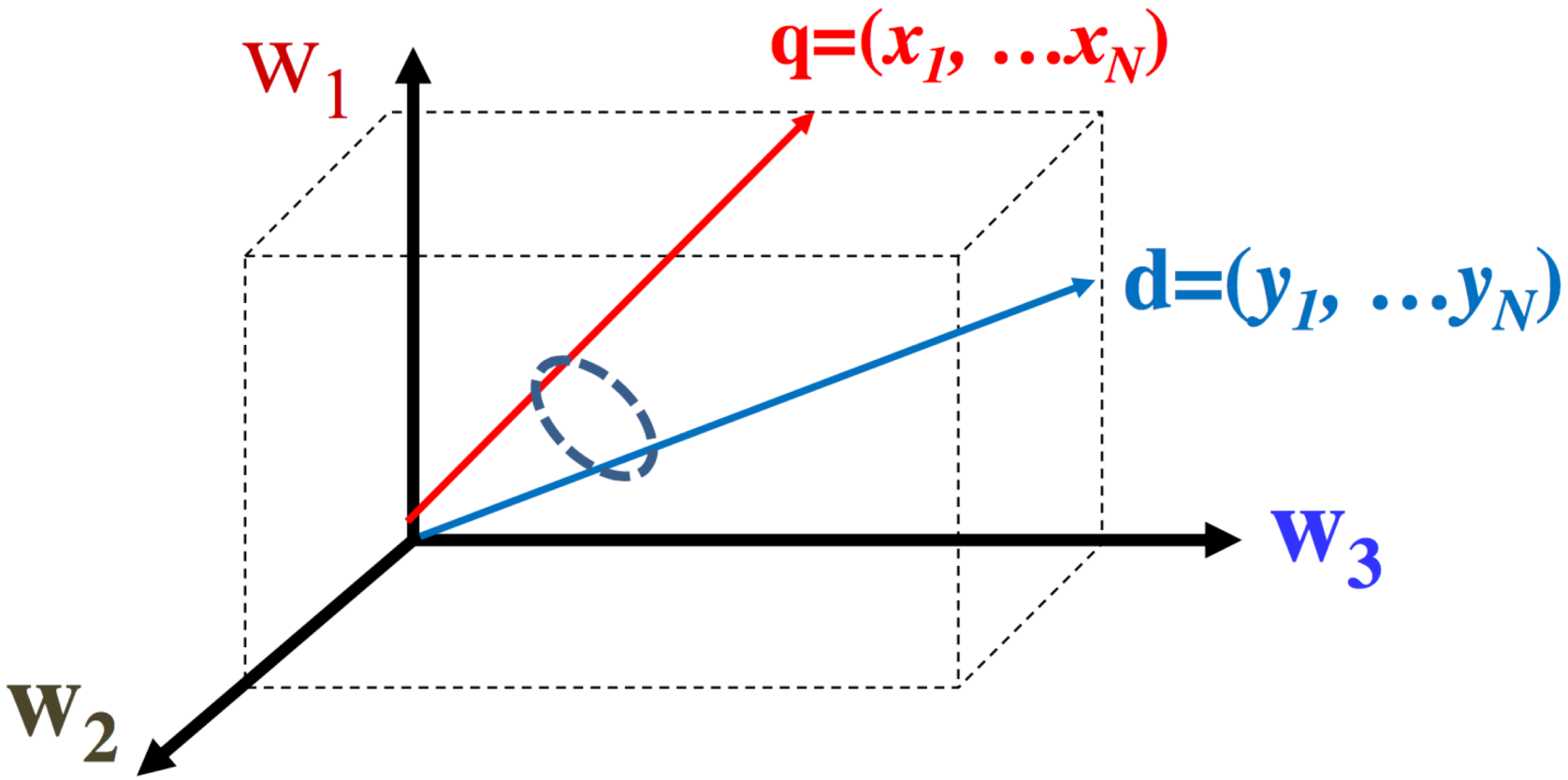
- Query $q = q_1, \ldots, q_m$ where q_i is a word
- Document $d = d_1, \ldots, d_n$ where d_i is a word (bag of words model)
- Ranking function f(q, d) which returns a real value
- A good ranking function should rank relevant documents on top of non-relevant ones
- The key challenge is how to measure the likelihood that document d is relevant to query q
- The retrieval model gives a formalization of relevance in computational terms

Retrieval Models

- Similarity-based models: f(q,d) = similarity(q,d)
  - Vector space model
- Probabilistic models: f(q,d) = p(R=1|d,q)
  - Classic probabilistic model
  - Language model
  - Divergence-from-randomness model
- Probabilistic inference model: f(q,d) = p(d->q)
- Axiomatic model: f(q,d) must satisfy a set of constraints

Basic Vector Space Model (VSM)

$$Sim(q,d) = q.d = x_1 y_1 + \ldots + x_N y_N = \sum_{i=1}^{N} x_i y_i$$



How Would You Rank These Docs?

Query = "news about presidential campaign"

		Ideal Ranking?
d1	… **news about** …	d4 +
d2	… **news about** organic food **campaign**…	d3 +
d3	… **news** of **presidential campaign** …	
d4	… **news** of **presidential campaign** … … **presidential** candidate …	d1 -
d5	… **news** of organic food **campaign**… **campaign**…**campaign**…**campaign**…	d2 - d5 -

Example with Basic VSM

Query = "news about presidential campaign"

d1 … **news about** …

d3 … **news** of **presidential campaign** …

V= {news, about, presidential, campaign, food …. }

q= (1, 1, 1, 1, 0, …)

d1= (1, 1, 0, 0, 0, …)

f(q,d1)= 1*1+1*1 +1* 0+1*0+0*0 + …= 2

d3= (1, 0, 1, 1, 0, …)

f(q,d3)= 1*1+1*0 +1*1 +1*1+0*0+ … = 3

Query = "news about presidential campaign"

d1	… **news about** …	f(q,d1)=2
d2	… **news about** organic food **campaign**…	f(q,d2)=3
d3	… **news** of **presidential campaign** …	f(q,d3)=3
d4	… **news** of **presidential campaign** … … **presidential** candidate …	f(q,d4)=3
d5	… **news** of organic food **campaign**… **campaign**…**campaign**…**campaign**…	f(q,d5)=2

Basic VSM returns the number of distinct query words matched in d.

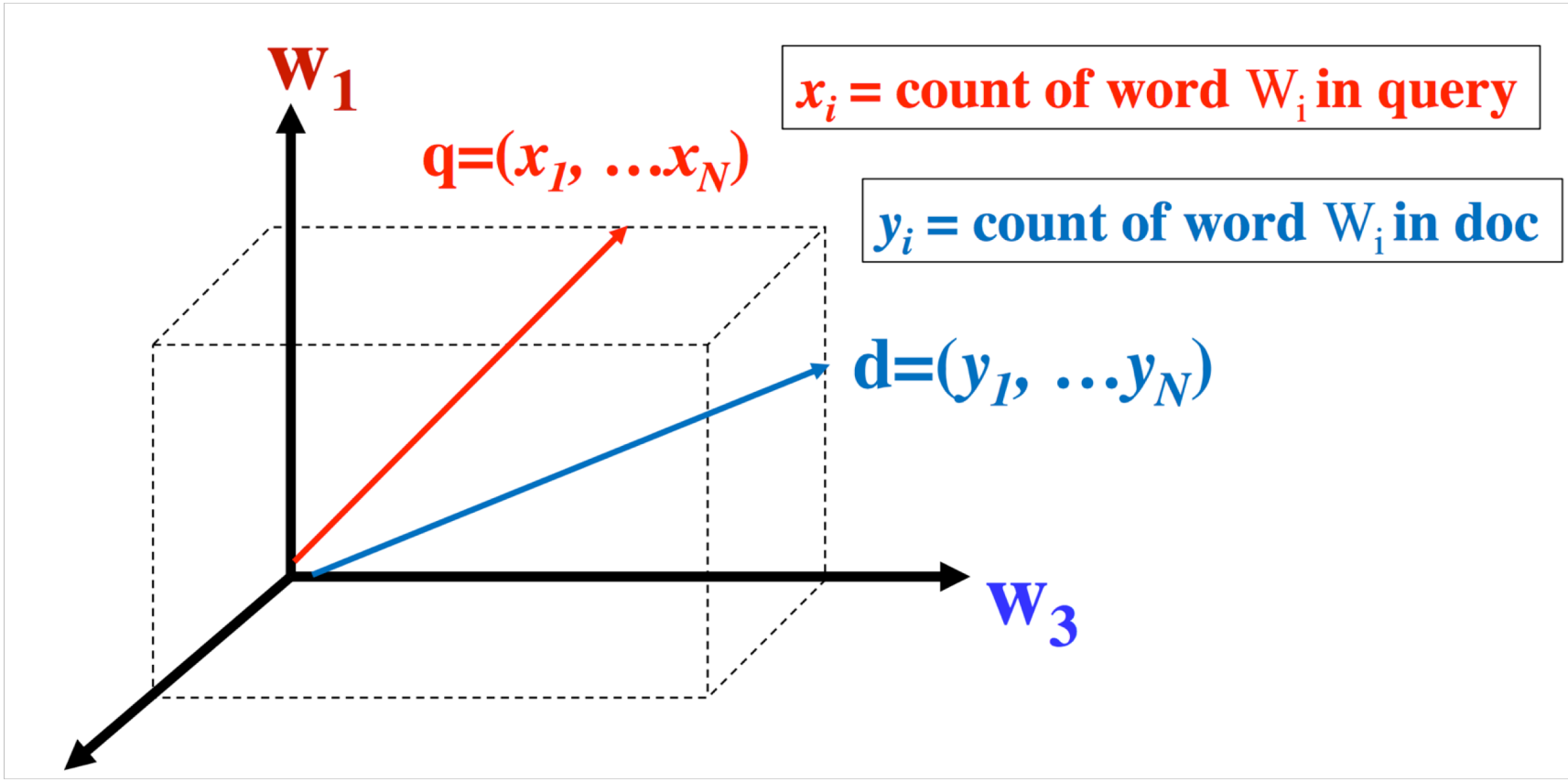
Two Problems of Basic VSM

Query = "news about presidential campaign"

d2	… **news about** organic food **campaign**…	**f(q,d2)=3**
d3	… **news** of **presidential campaign** …	**f(q,d3)=3**
d4	… **news** of **presidential campaign** … … **presidential** candidate …	**f(q,d4)=3**

1. Matching "presidential" more times deserves more credit
2. Matching "presidential" is more important than matching "about"

Term Frequency Weighting (TFW)



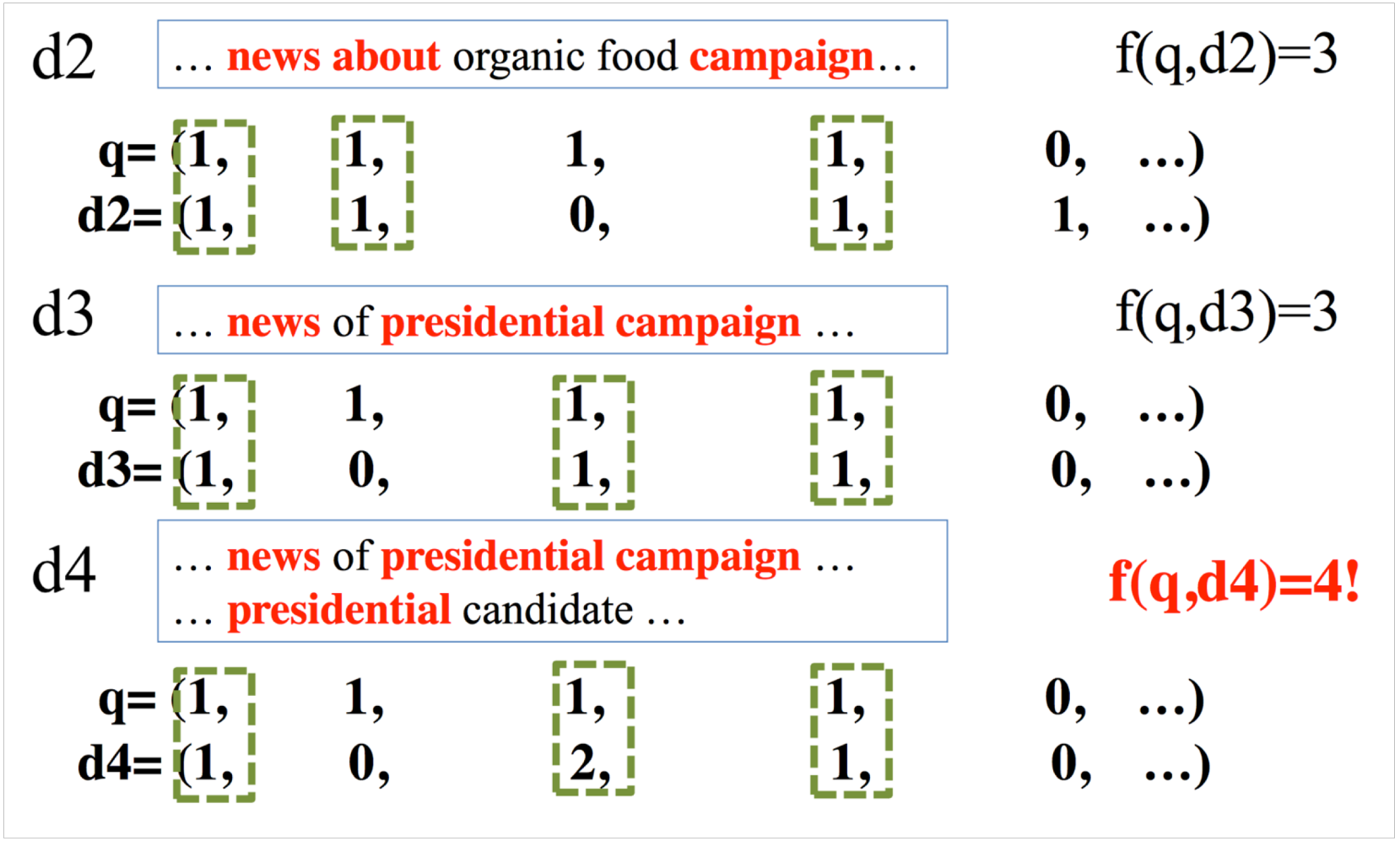
Term Frequency Weighting (TFW)

$q=(x_1, \ldots x_N)$ x_i = count of word W_i in query

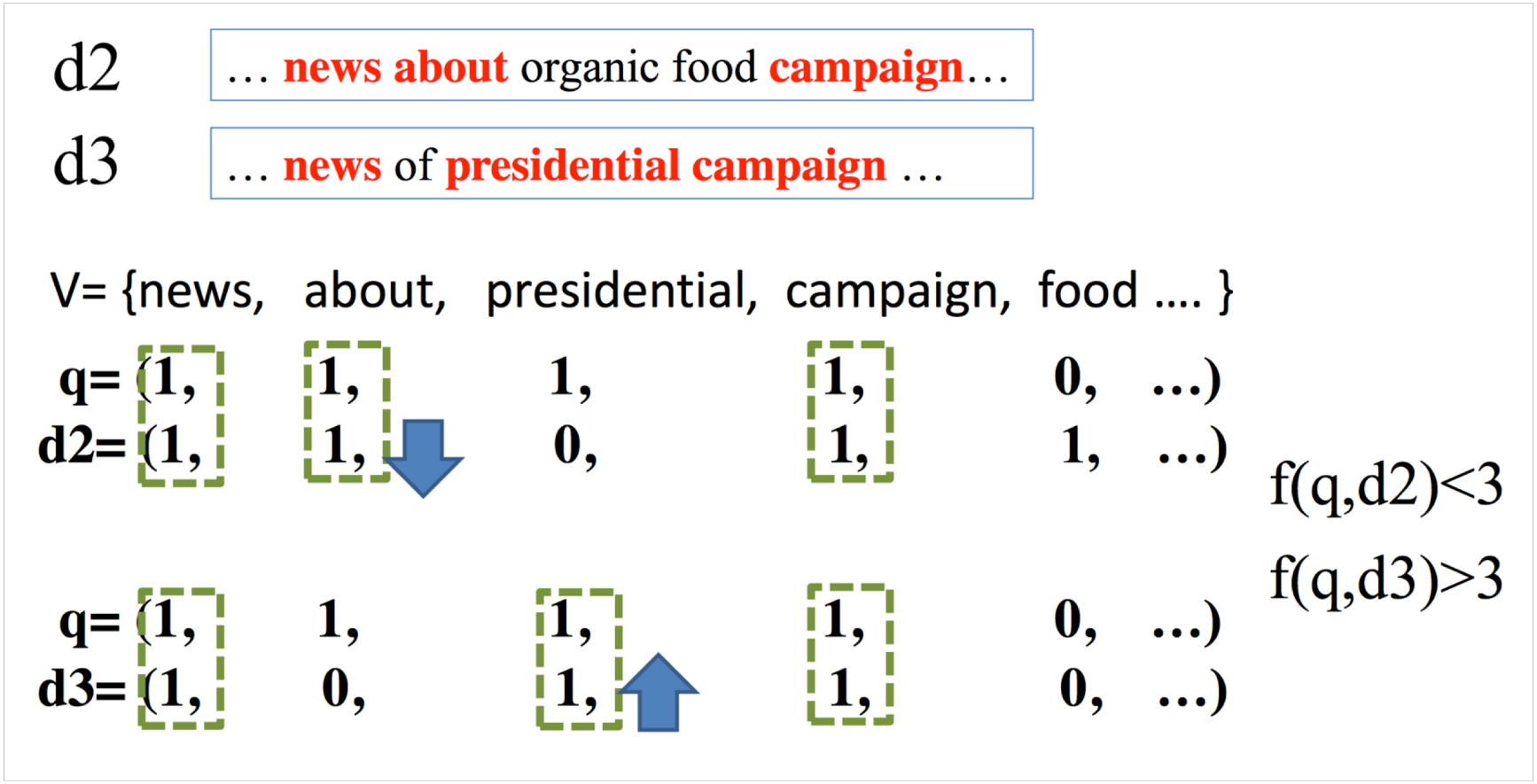
$d=(y_1, \ldots y_N)$ y_i = count of word W_i in doc

$$Sim(q,d)=q.d= x_1 y_1 + \ldots + x_N y_N = \sum_{i=1}^{N} x_i y_i$$

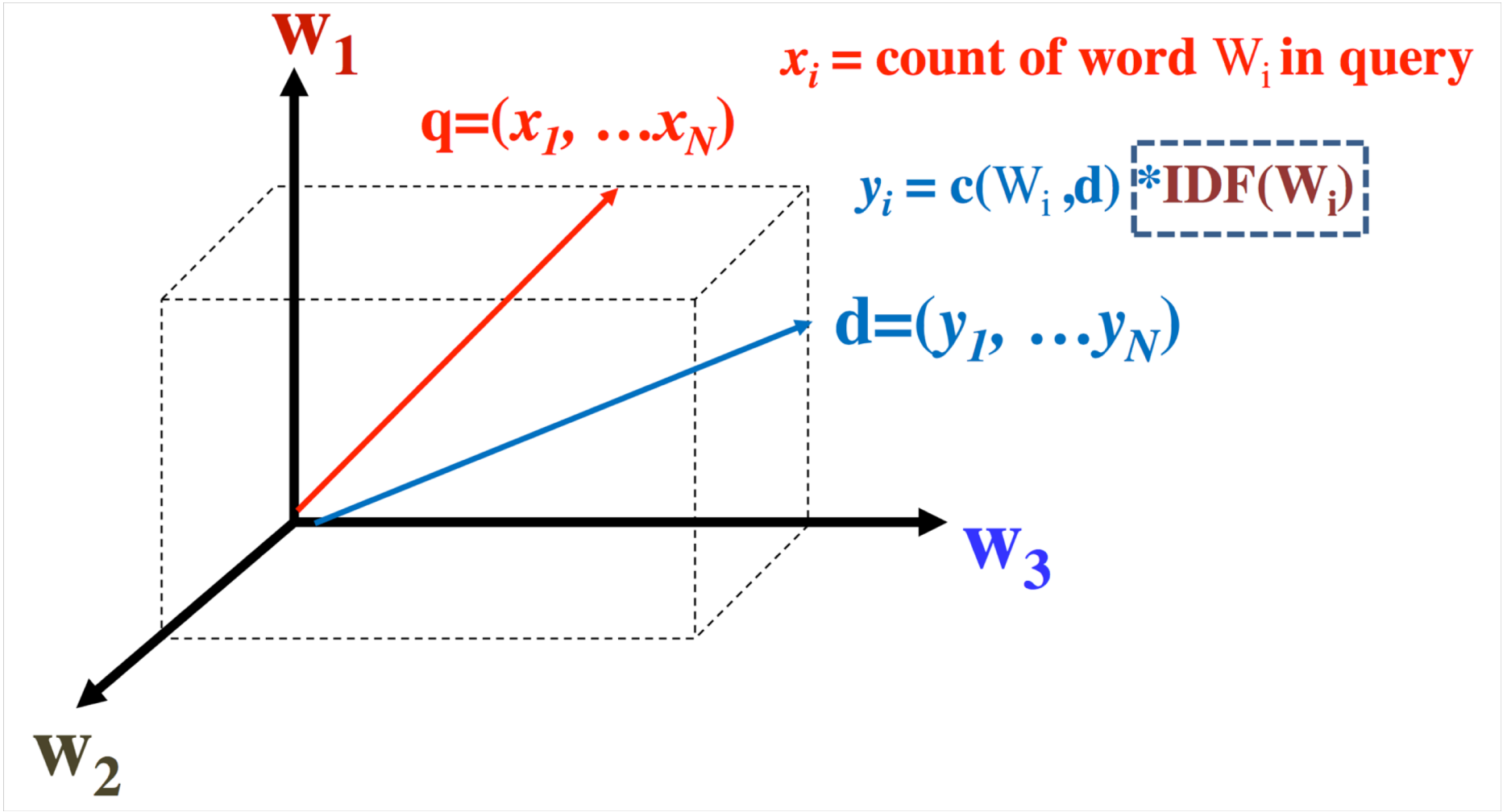
Ranking using TFW



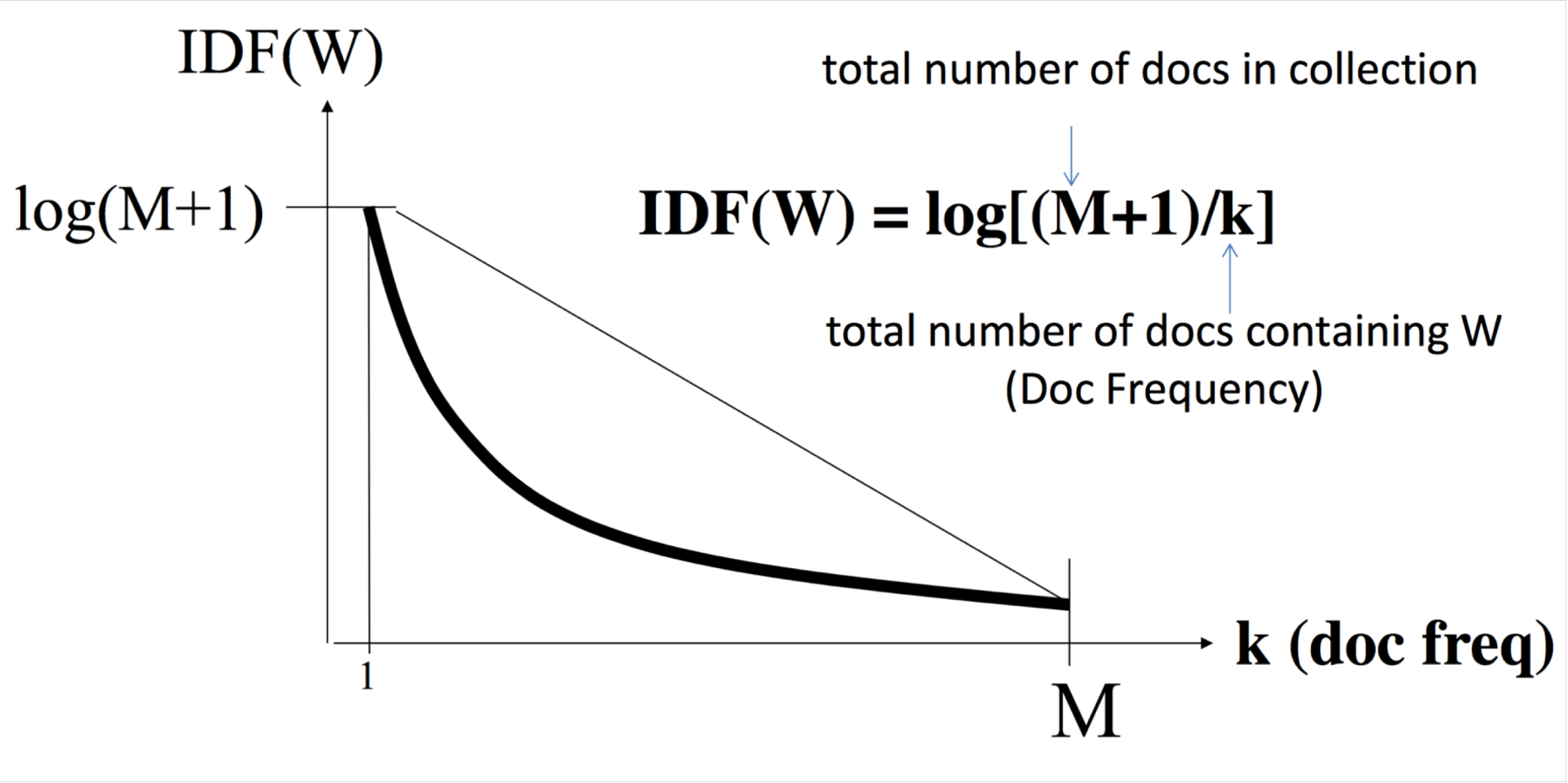
"presidential" vs "about"



Adding Inverse Document Frequency



Inverse Document Frequency



"presidential" vs "about"

d2 … **news about** organic food **campaign**…

d3 … **news** of **presidential campaign** …

V= {news, about, presidential, campaign, food …. }

IDF(W)= 1.5 1.0 2.5 3.1 1.8

q= (1, 1, 1, 1, 0, …)

d2= (1*1.5, 1*1.0, 0, 1*3.1, 0, …)

q= (1, 1, 1, 1, 0, …)

d3= (1*1.5, 0, 1*2.5, 1*3.1, 0, …)

f(q,d2) = 5.6 < f(q,d3)=7.1

Inverse Document Frequency Ranking

Query = "news about presidential campaign"

d1	… **news about** …	f(q,d1)=2.5
d2	… **news about** organic food **campaign**…	f(q,d2)=5.6
d3	… **news** of **presidential campaign** …	f(q,d3)=7.1
d4	… **news** of **presidential campaign** … … **presidential** candidate …	f(q,d4)=9.6
d5	… **news** of organic food **campaign**… **campaign**…**campaign**…**campaign**…	**f(q,d5)=13.9!**

Combining Term Frequency (TF) with Inverse Document Frequency Ranking

Total # of docs in collection

$$f(q,d) = \sum_{i=1}^{N} x_i y_i = \sum_{w \in q \cap d} c(w,q)\, c(w,d) \log \frac{M+1}{df(w)}$$

All matched query words in d

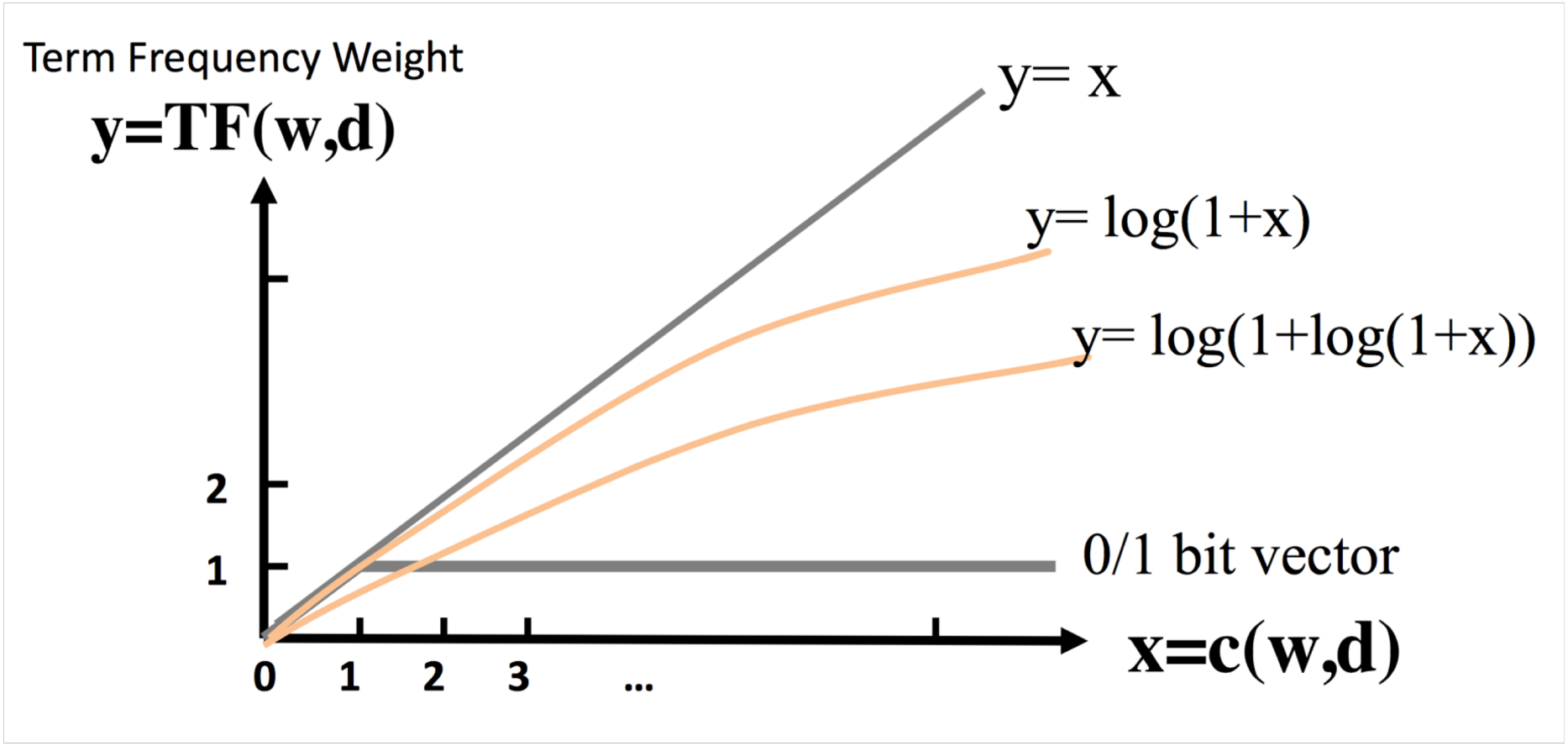
Doc Frequency

d5 … **news** of organic food **campaign**… **campaign**…**campaign**…**campaign**…

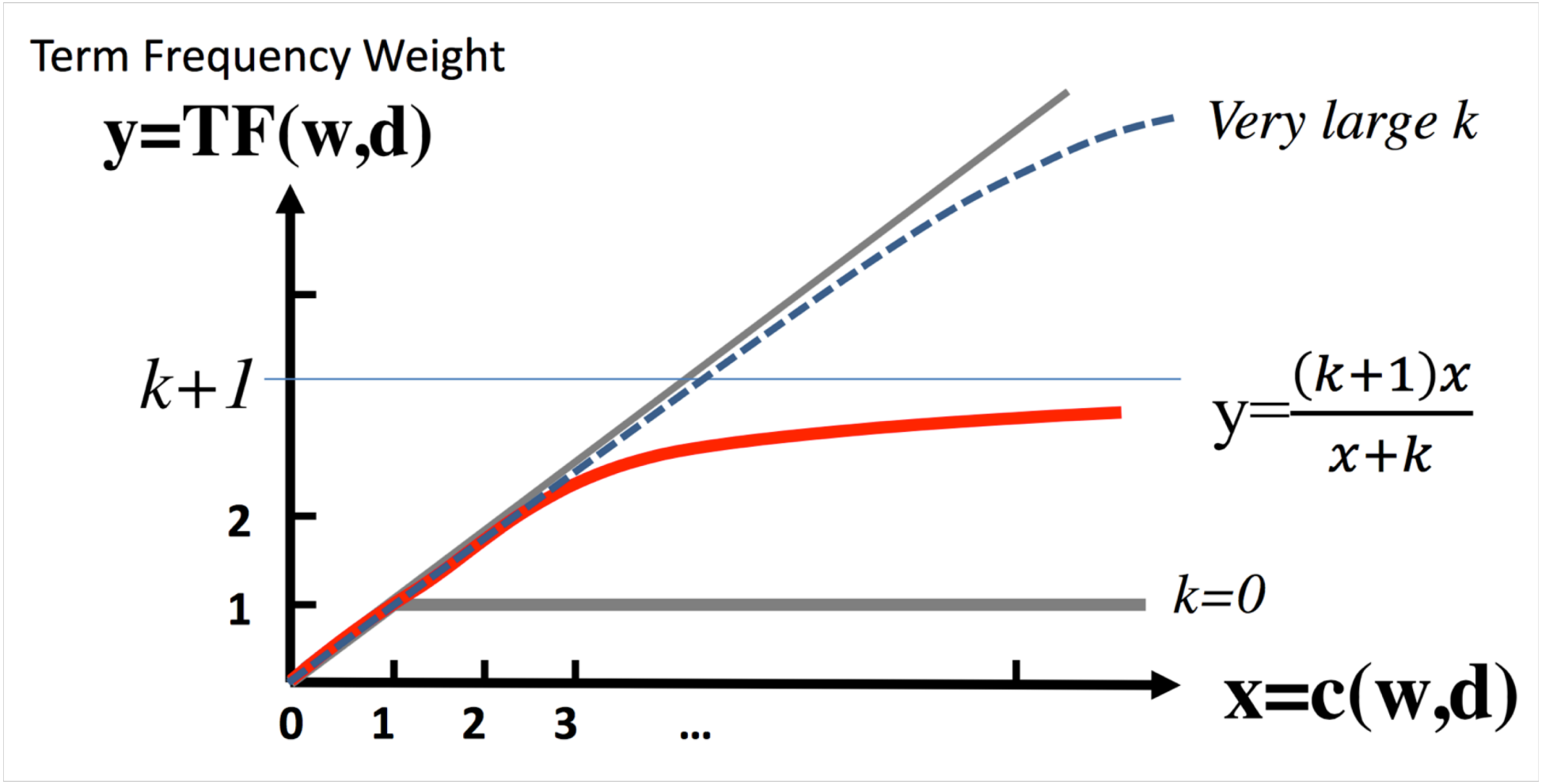
c("campaign",d5)=4

➔ f(q,d5)=13.9?

TF Transformation



BM25 Transformation



Ranking with BM25-TF

$$f(q,d) = \sum_{i=1}^{N} x_i y_i = \sum_{w \in q \cap d} c(w,q) \frac{(k+1)c(w,d)}{c(w,d)+k} \log \frac{M+1}{df(w)}$$

What about Document Length?

Query = "news about presidential campaign"

d4

… **news** of **presidential campaign** …
… **presidential** candidate …

100 words

d6 > d4?

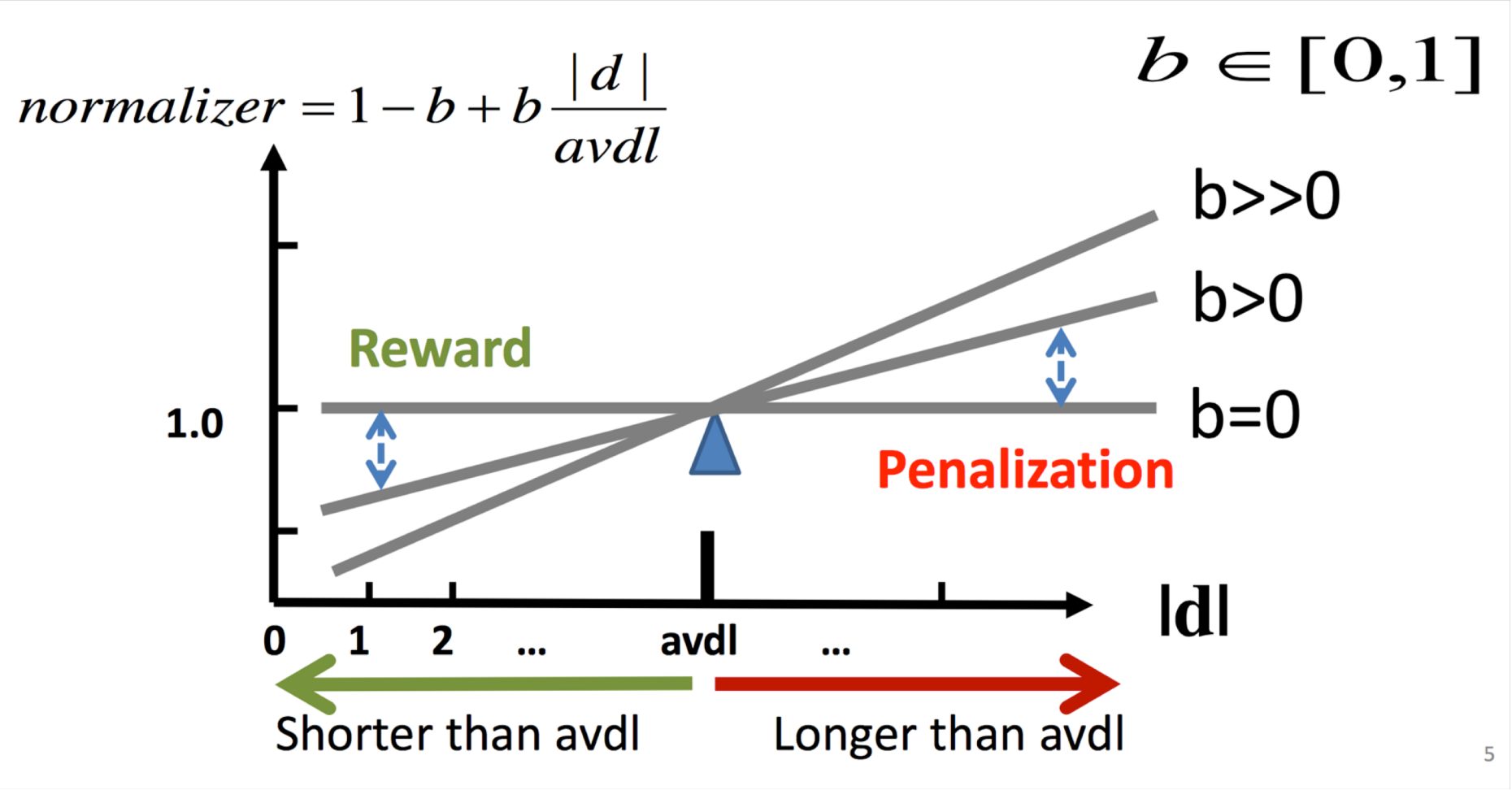
d6

… **campaign**…..... **campaign**..... **5000 words** .....
……
.....**news**.....
……
…… **news**…..
……
…… ……
…… **presidential** ……. **presidential**……

Document Length Normalization

- Penalize a long doc with a doc length normalizer
  - Long doc has a better chance to match any query
  - Need to avoid over-penalization
- A document is long because
  - it uses more words, then it should be more penalized
  - it has more contents, then it should be penalized less
- Pivoted length normalizer
  - It uses average doc length as "pivot"
  - The normalizer is 1 if the doc length (|d|) is equal to the average doc length (avdl)

Pivot Length Normalizer



State of the Art VSM Ranking Function

- Pivoted Length Normalization VSM [Singhal et al 96]

$$f(q,d) = \sum_{w \in q \cap d} c(w,q) \frac{\ln[1+\ln[1+c(w,d)]]}{1-b+b\frac{|d|}{avdl}} \log \frac{M+1}{df(w)}$$

- BM25/Okapi [Robertson & Walker 94]

$$f(q,d) = \sum_{w \in q \cap d} c(w,q) \frac{(k+1)c(w,d)}{c(w,d)+k(1-b+b\frac{|d|}{avdl})} \log \frac{M+1}{df(w)}$$

From Text to Numerical Vectors

Keywords Selection

- Text is preprocessed through tokenization
- Stop word list and word stemming are used to isolate and thus identify significant keywords
- Stop words elimination
  - Stop words are elements that are considered uninteresting with respect to the retrieval and thus are eliminated
  - For instance, "a", "the", "always", "along"
- Word stemming
  - Different words that share a common prefix are simplified and replaced by their common prefix
  - For instance, "computer", "computing", "computerize" are replaced by "comput"

Dimensionality Reduction

- Approaches presented so far involves high dimensional space (huge number of keywords)
  - Computationally expensive
  - Difficult to deal with **synonymy** and **polysemy** problems
  - "vehicle" is similar to "car"
  - "mining" has different meanings in different contexts
- Dimensionality reduction techniques
  - Latent Semantic Indexing (LSI)
  - Locality Preserving Indexing (LPI)
  - Probabilistic Semantic Indexing (PLSI)

Latent Semantic Indexing (LSI)

- Let x_i be vectors representing documents and X (the term frequency matrix) the all set of documents:

$$\vec{x}_1, \cdots, \vec{x}_n \in R^m \qquad X = [\vec{x_1}, \vec{x_2}, \cdots, \vec{x_n}]$$

- Let use the **singular value decomposition** (SVD) to reduce the size of frequency table:

$$X = U\Sigma V^T$$

- Approximate X with X_k that is obtained from the first k vectors of U
- It can be shown that such transformation minimizes the error for the reconstruction of X

Text Classification

Document classification

- Solve the problem of **labeling automatically text documents** on the basis of
  - Topic
  - Style
  - Purpose
- Usual classification techniques can be used to learn from a training set of **manually labeled documents**
- Which features? **Keywords** can be thousands…
- Major approaches
  - Similarity-based
  - Dimensionality reduction
  - Naïve Bayes text classifiers

Similarity-based Text Classifiers

- Exploits **Information Retrieval** and **k-nearest-neighbor** classifier
  - For a new document to classify, the **k** most similar documents in the training set are retrieved
  - Documents are classified on the basis of the class distribution among the k documents retrieved using the majority vote or a weighted vote
  - Tuning **k** is very important to achieve a good performance
- Limitations
  - **Space overhead** to store all the documents in training set
  - **Time overhead** to retrieve the similar documents

- As in the **Vector Space Model**, the goal is to reduce the number of features to represents text
- Usual dimensionality reduction approaches in Information Retrieval are based on the **distribution of keywords** among the **whole** documents database
- In text classification it is important to consider also the **correlation between keywords and classes**
  - Rare keywords have a high TF-IDF but might be uniformly distributed among classes
- Usual classification techniques can be then applied on reduced features space are SVMs and Naïve Bayes classifiers

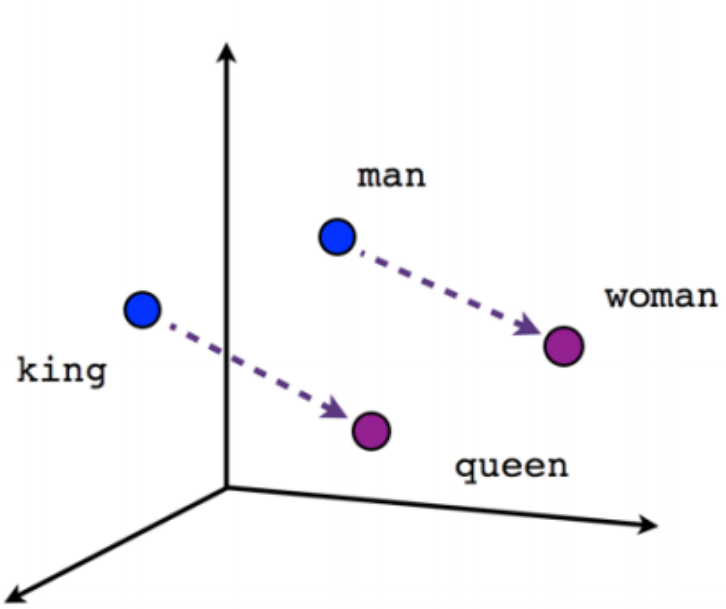
Word Embeddings

What Are Word Embeddings?

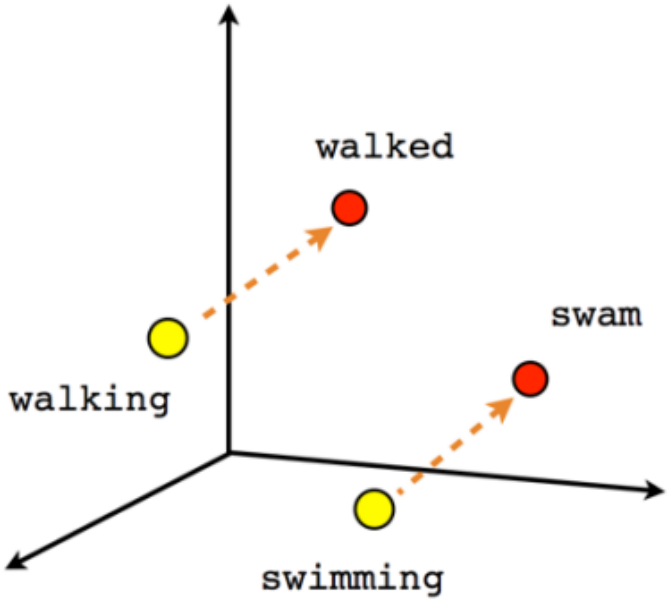
- Learned representation for text where words with similar meanings have similar representations
- Class of methods that represent individual words as real-valued vectors in a predefined vector space
- Each word is mapped to one vector and the vector values are learned in a way that resembles a neural network
- Each word is represented by a real-valued vector, often tens or hundreds of dimensions.

What Are Word Embeddings?

- Umbrella term for language modeling and feature learning techniques in natural language processing (NLP)
- Words or phrases from the vocabulary are mapped to vectors of real numbers
- Word embedding involves a mathematical embedding from a space with one dimension per word to a continuous vector space with a much lower dimension



Male-Female



Verbe Tense

vector[Queen] = vector[King] - vector[Man] + vector[Woman]

Word Representation

- Bag of Words Model (Traditional)
  - Uses one hot encoding
  - Words are represented by one bit position in a huge vector (representing the vocabulary of words)
  - Context information is not used
- Word Embeddings
  - Stores each word in as a point in continuous space
  - A word is represented by a vector of fixed number of dimensions (generally 300)
  - Generated from a huge corpus using unsupervised methods
  - Dimensions are basically projections along different axes, more of a mathematical concept

"A word is known by
the company it keeps"

Applications of Word Embeddings

- Word Similarity
  - Classic methods use Edit Distance, WordNet, Porter's Stemmer, Lemmatization using dictionaries
  - Word embeddings easily identifies similar words and synonyms since they occur in similar contexts
  - For example, (1) think, thought, ponder, pondering, (2) plane, aircraft, flight
- Machine Translation
- Part-of-Speech and Named Entity Recognition
- Relation Extraction (e.g., Paris-France, Rome-Italy)
- Sentiment Analysis
  - Classic methods are based on the classification of bag of word model vectors
  - Averaging the word embeddings possibly using TD/IDF approaches to weight the embeddings to classify sentences as positive and negative

Applications of Word Embeddings

- Co-reference Resolution
  - Chaining entity mentions across multiple documents - can we find and unify the multiple contexts in which mentions occurs?
- Clustering
  - Words in the same class naturally occur in similar contexts, and have similar embeddings
  - Embeddings can directly be used with any conventional clustering algorithms (K-Means, agglomerative, etc)
- Semantic Analysis of Documents
  - Build word distributions for various topics, etc.

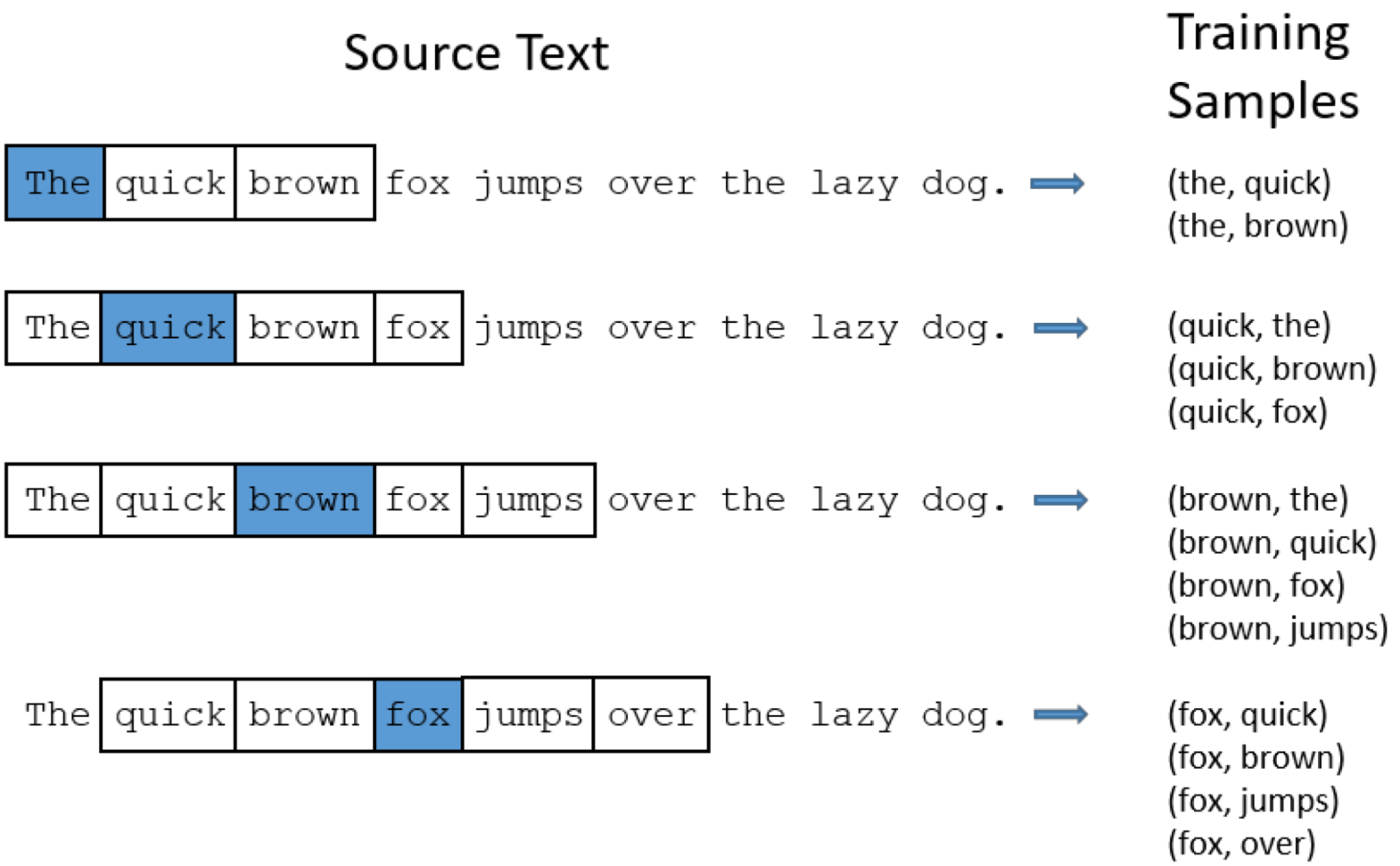
Word Embeddings Approaches

- Latent Semantic Indexing (LSI)
  - Co-occurrence Matrix with Singular Value Decomposition)
- Fastext - Facebook
- Word2vec (Google)
- Global Vector Representations (GloVe) (Stanford)

Word2Vec

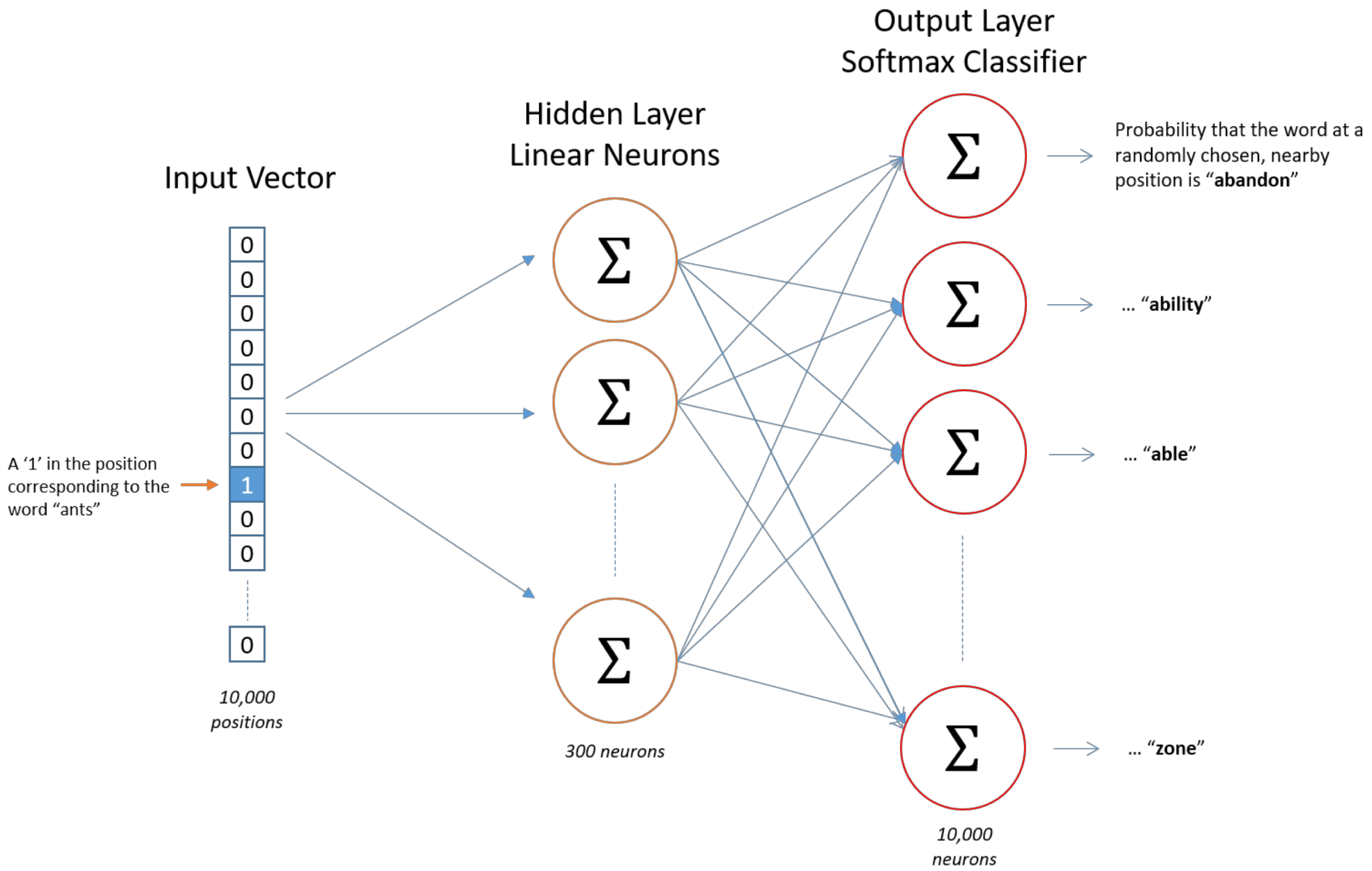
Word2Vec (Google)

- It employs a skip gram neural network architecture
- It trains a simple neural network with a single hidden layer to, given a specific word in the middle of a sentence (the input word), predict the probability for every word in our vocabulary of being the "nearby word" that we chose.
- Note that we are not interested in the entire model and we are not going to use it for prediction, instead we are going to use the hidden layer as a representation of the input word
- The output vector is a probability distribution



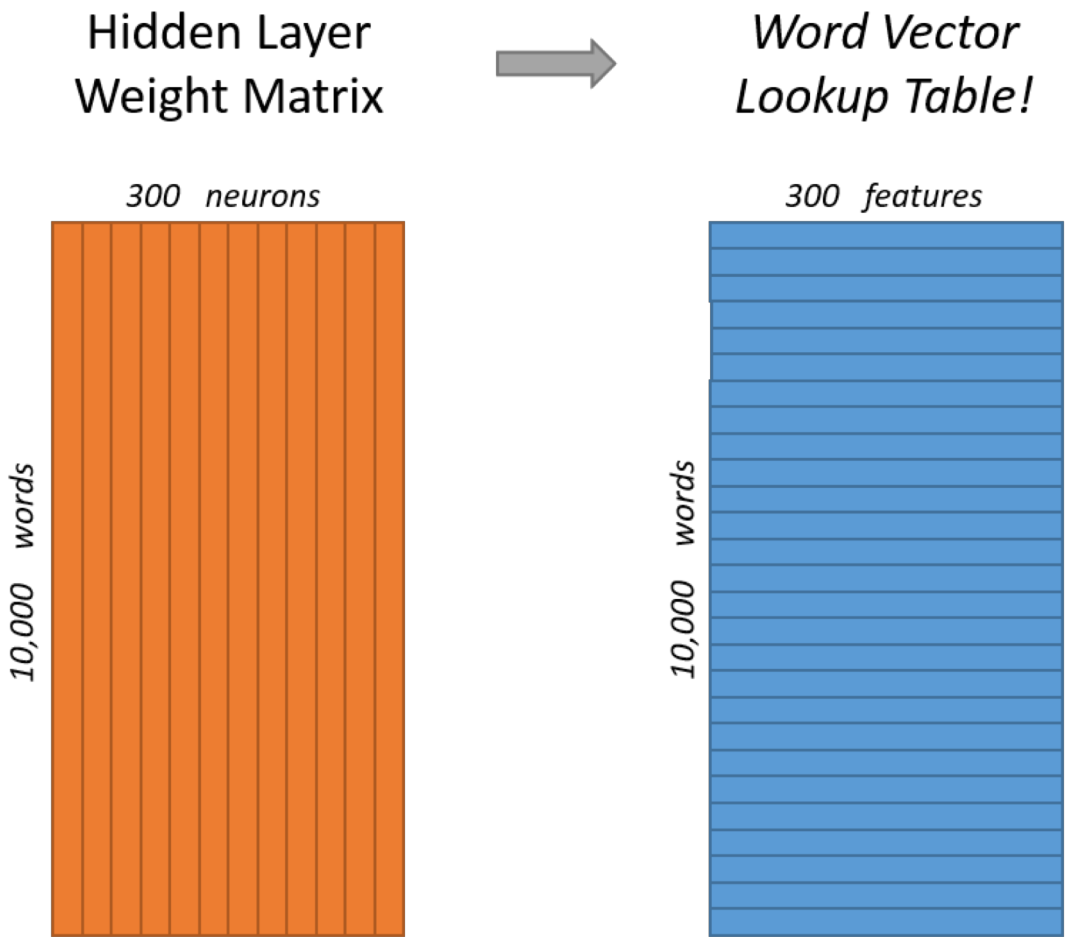
Training Examples for Word2Vec

http://mccormickml.com/2016/04/19/word2vec-tutorial-the-skip-gram-model/

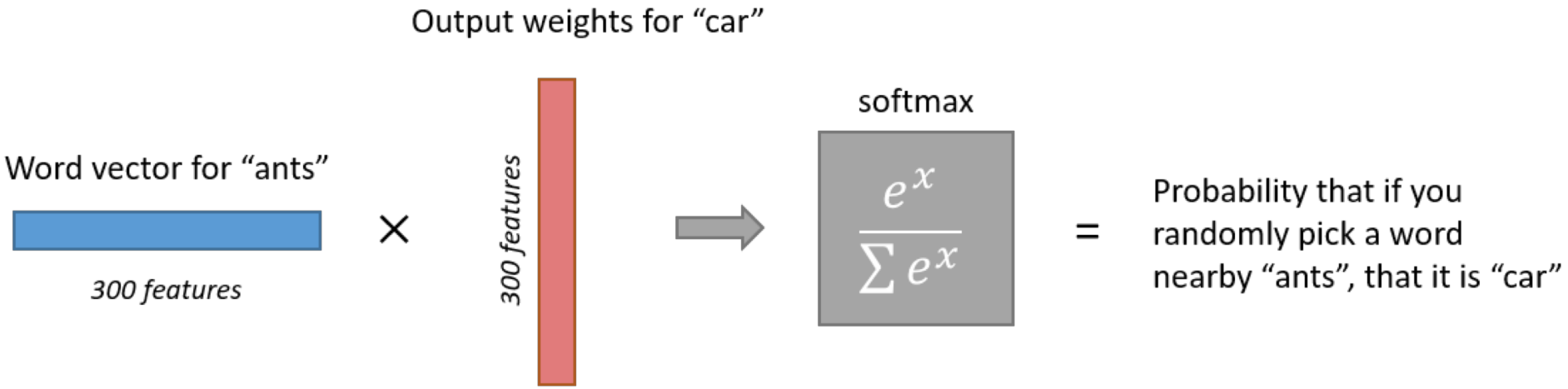


Word2Vec Skip Gram Architecture

http://mccormickml.com/2016/04/19/word2vec-tutorial-the-skip-gram-model/



Word2Vec representation of word embeddings
http://mccormickml.com/2016/04/19/word2vec-tutorial-the-skip-gram-model/



Word2Vec Skip Gram Architecture

http://mccormickml.com/2016/04/19/word2vec-tutorial-the-skip-gram-model/

Text Classification (Example)

Naïve Bayes for Text Classification

- Document categories $\{C_1, \ldots, C_n\}$
- Document to classify D
- Probabilistic model:

$$P(C_i \mid D) = \frac{P(D \mid C_i)P(C_i)}{P(D)}$$

- We chose the class C* such that

$$C^* = \arg\max_C P(C|D) = \arg\max_C P(D|C)P(C)$$

- Issues
  - Which features?
  - How to compute the probabilities?

Naïve Bayes for Text Classification

- Features can be simply defined as the **words in the document**
- Let a_i be a keyword in the doc, and w_j a word in the vocabulary, we get:

$$P(D|C) = P(a_1 = w_{j_1}, a_2 = w_{j_2}, \cdots, a_n = w_{j_n}|C)$$

Example

H={like,dislike}
D= "Our approach to representing arbitrary text documents is disturbingly simple"

$$P(D|Like) = P(a_1 = \text{our}, a_2 = \text{approach}, \cdots, a_10 = \text{simple}|Like)$$

Naïve Bayes for Text Classification

- Features can be simply defined as the **words in the document**
- Let a_i be a keyword in the doc, and w_j a word in the vocabulary,

$$P(D|C) = P(a_1 = w_{j_1}, a_2 = w_{j_2}, \cdots, a_n = w_{j_n}|C)$$

- Assumptions
  - Keywords distributions are inter-independent
  - Keywords distributions are order-independent

$$P(D|C) = \prod_{i=1}^{n} P(w_{j_i}|C)$$

$$P(D|Like) = P(\text{our}|Like)P(\text{approach}|Like)\cdots P(\text{simple}|Like)$$

Naïve Bayes for Text Classification

- How to compute probabilities?
  - Simply counting the occurrences may lead to wrong results when probabilities are small
- M-estimate approach adapted for text:

$$P(w_k|C) = \frac{N_{c,k} + 1}{N_c + |\text{Vocabulary}|}$$

  - N_c is the whole number of word positions in documents of class C
  - $N_{c,k}$ is the number of occurrences of w_k in documents of class C
  - |Vocabulary| is the number of distinct words in training set
  - Uniform priors are assumed

Naïve Bayes for Text Classification

- Final classification is performed as

$$C^* = \arg\max_C P(C) \prod_{i=1}^{n} P(w_{j_i}|C)$$

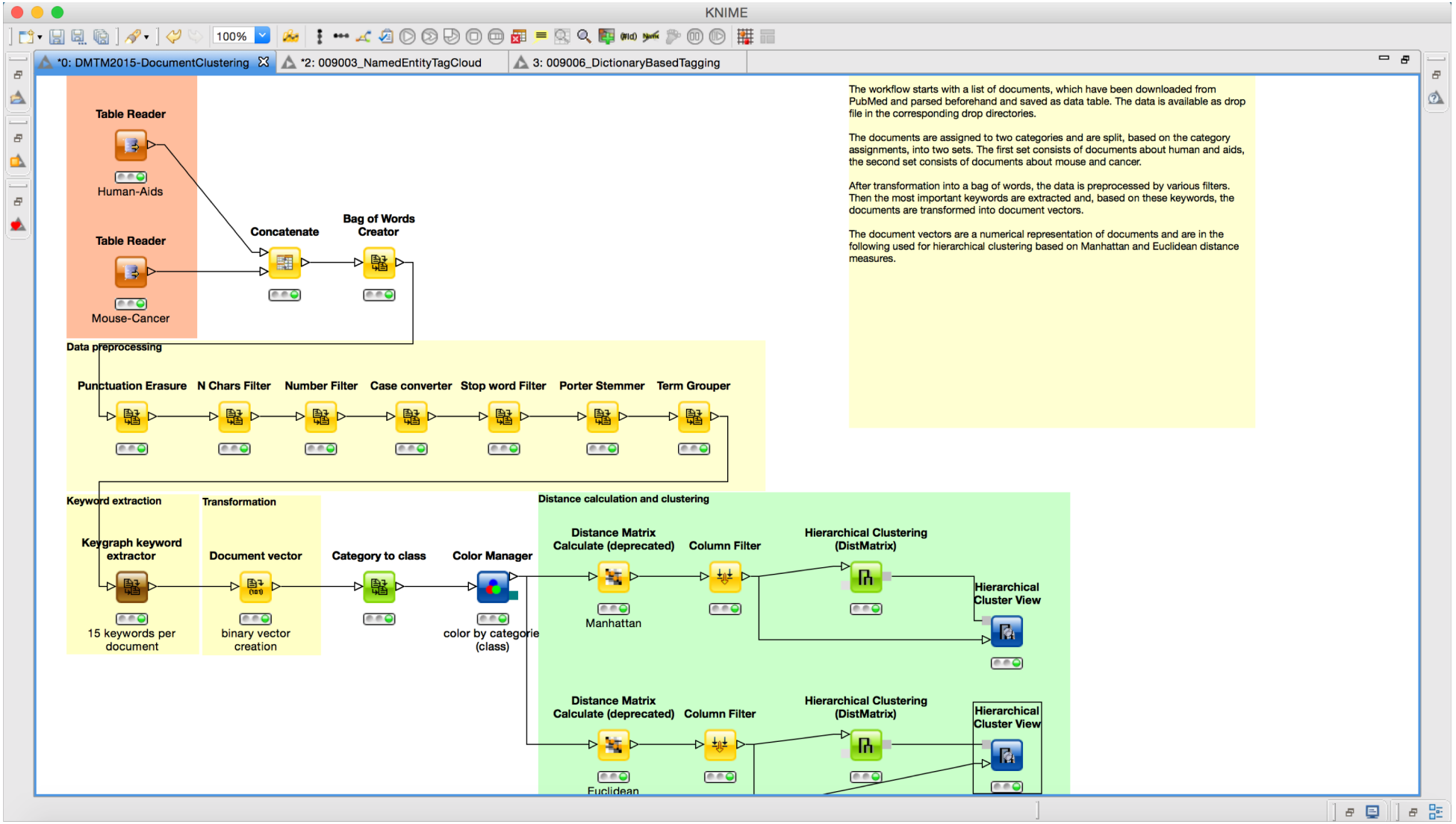
- Despite its simplicity Naïve Bayes classifiers works very well in practice

- Applications
  - Newsgroup post classification
  - NewsWeeder (news recommender)

Clustering Text (Example)

Text Clustering

- It involves the same steps as other text mining algorithms to preprocess the text data into an adequate representation
  - Tokenizing and stemming each synopsis
  - Transforming the corpus into vector space using TF-IDF
  - Calculating cosine distance between each document as a measure of similarity
  - Clustering the documents using the similarity measure
- Everything works as with the usual data except that text requires a rather long preprocessing.


KNIME
100%
*0: DMTM2015-DocumentClustering
*2: 009003_NamedEntityTagCloud
3: 009006_DictionaryBasedTagging
Table Reader
Human-Aids
Table Reader
Mouse-Cancer
Concatenate
Bag of Words Creator
The workflow starts with a list of documents, which have been downloaded from PubMed and parsed beforehand and saved as data table. The data is available as drop file in the corresponding drop directories.
The documents are assigned to two categories and are split, based on the category assignments, into two sets. The first set consists of documents about human and aids, the second set consists of documents about mouse and cancer.
After transformation into a bag of words, the data is preprocessed by various filters. Then the most important keywords are extracted and, based on these keywords, the documents are transformed into document vectors.
The document vectors are a numerical representation of documents and are in the following used for hierarchical clustering based on Manhattan and Euclidean distance measures.
Data preprocessing
Punctuation Erasure
N Chars Filter
Number Filter
Case converter
Stop word Filter
Porter Stemmer
Term Grouper
Keyword extraction
Keygraph keyword extractor
15 keywords per document
Transformation
Document vector
binary vector creation
Category to class
Color Manager
color by categorie (class)
Distance calculation and clustering
Distance Matrix Calculate (deprecated)
Manhattan
Column Filter
Hierarchical Clustering (DistMatrix)
Hierarchical Cluster View
Distance Matrix Calculate (deprecated)
Euclidean
Column Filter
Hierarchical Clustering (DistMatrix)
Hierarchical Cluster View

Run the KNIME workflow and Python notebook for the lecture

References

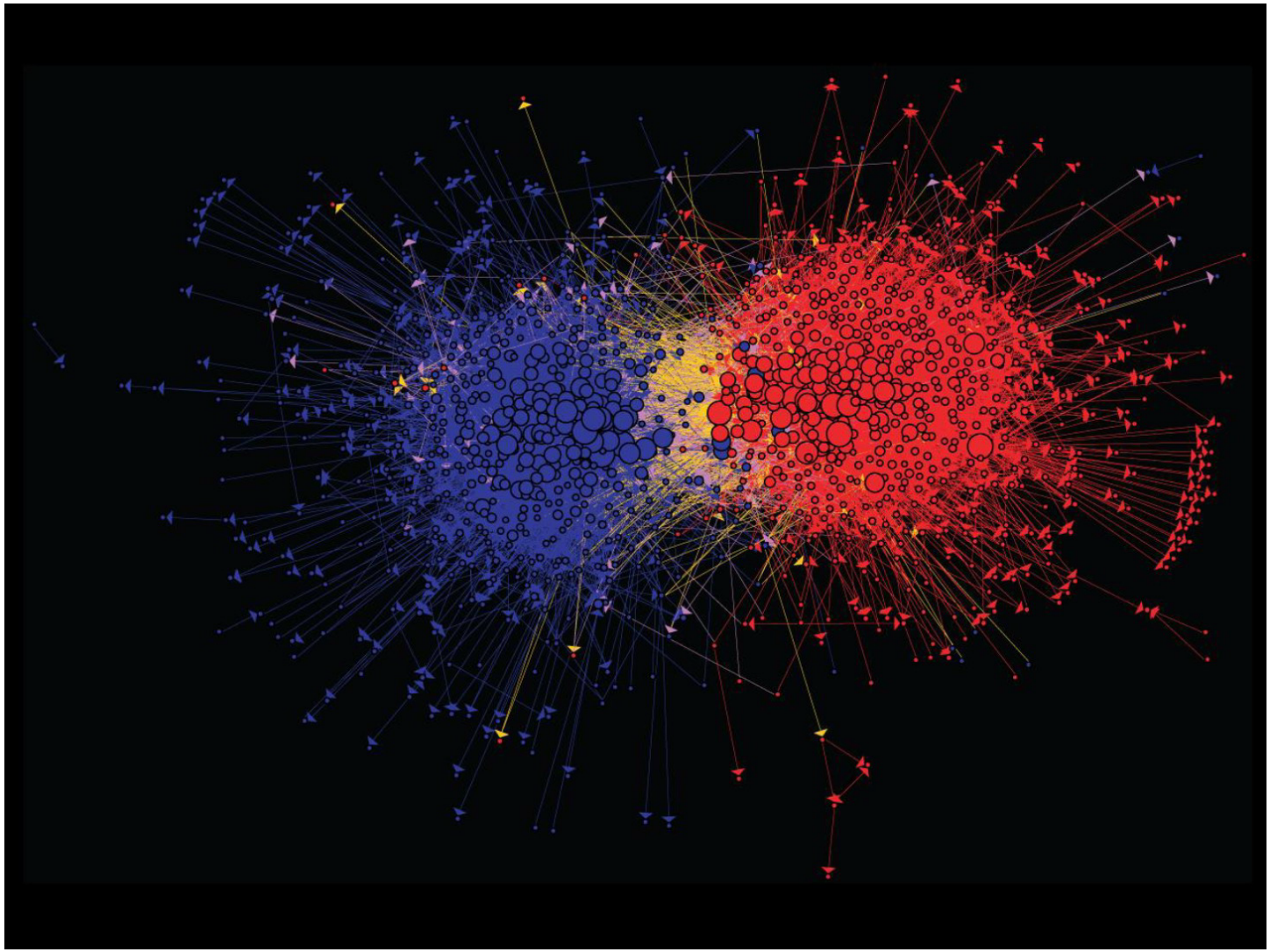
- ChengXiang Zhai, CS 397 – Fall 2003
- Word2Vec
  - http://mccormickml.com/2016/04/19/word2vec-tutorial-the-skip-gram-model/
  - http://mccormickml.com/2017/01/11/word2vec-tutorial-part-2-negative-sampling/
- Glove
  - https://cran.r-project.org/web/packages/text2vec/vignettes/glove.html
  - https://nlp.stanford.edu/projects/glove/
  - Glove implementation in C - https://github.com/stanfordnlp/GloVe
  - Glove paper - https://nlp.stanford.edu/pubs/glove.pdf

References

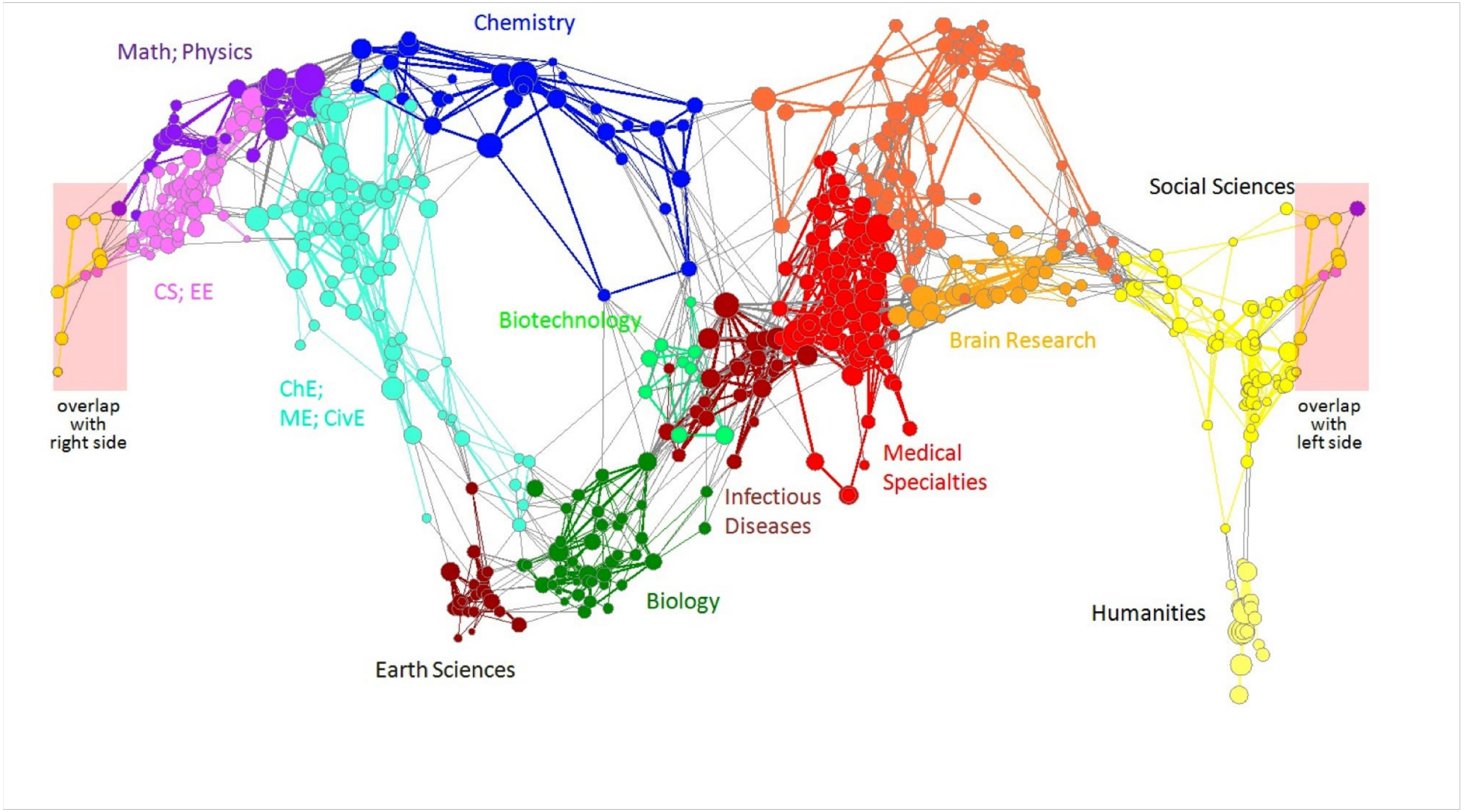
- Jure Leskovec, Anand Rajaraman, Jeff Ullman. Mining of Massive Datasets, Chapter 5 & Chapter 10

- Book and slides are available from http://www.mmds.org

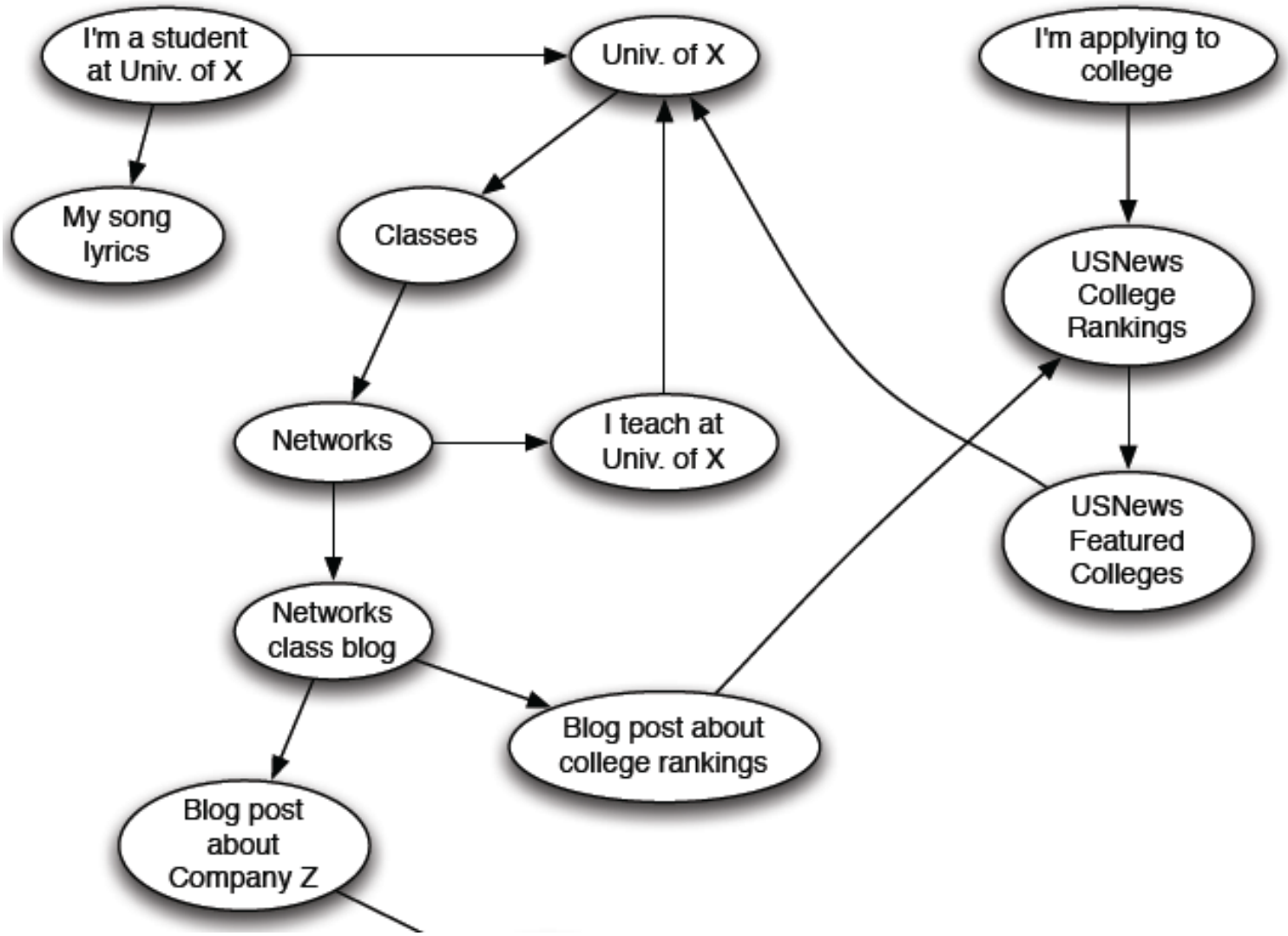
Facebook social graph
4-degrees of separation [Backstrom-Boldi-Rosa-Ugander-Vigna, 2011]



Connections between political blogs
Polarization of the network [Adamic-Glance, 2005]



Citation networks and Maps of science
[Börner et al., 2012]



Web as a graph: pages are nodes, edges are links

How is the Web Organized?

- Initial approaches
  - Human curated Web directories
  - Yahoo, DMOZ, LookSmart

- Then, Web search
  - Information Retrieval investigates: Find relevant docs in a small and trusted set
  - Newspaper articles, Patents, etc.

Web is huge, full of untrusted documents, random things, web spam, etc.

Web Search Challenges

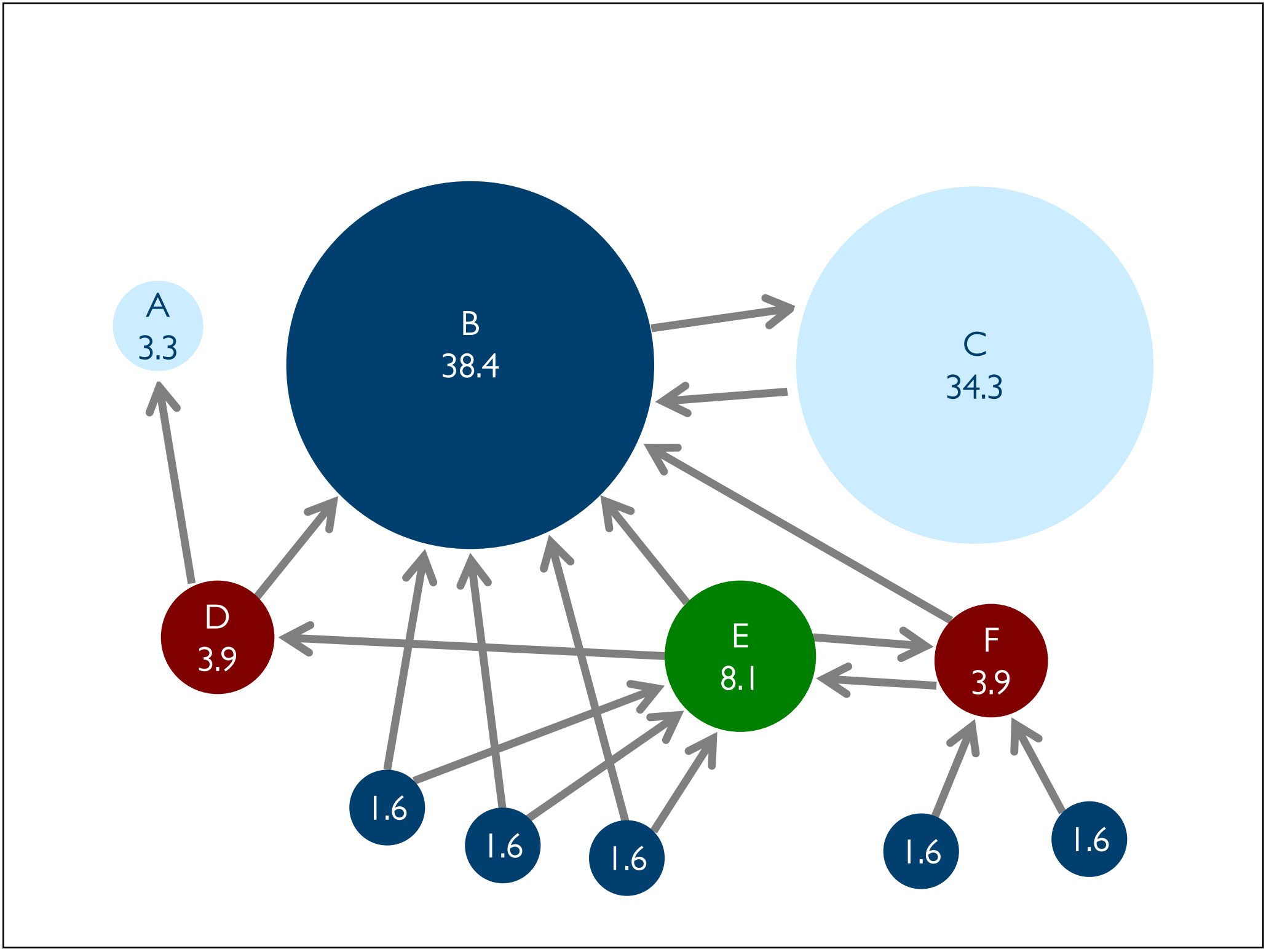
- Web contains many sources of information
  - Who should we "trust"?
  - Trick: Trustworthy pages may point to each other!
- What is the "best" answer to query "newspaper"?
  - No single right answer
  - Trick: Pages that actually know about newspapers might all be pointing to many newspapers

Page Rank

https://www.youtube.com/watch?v=wPMZr9RDmVk

Page Rank Algorithm

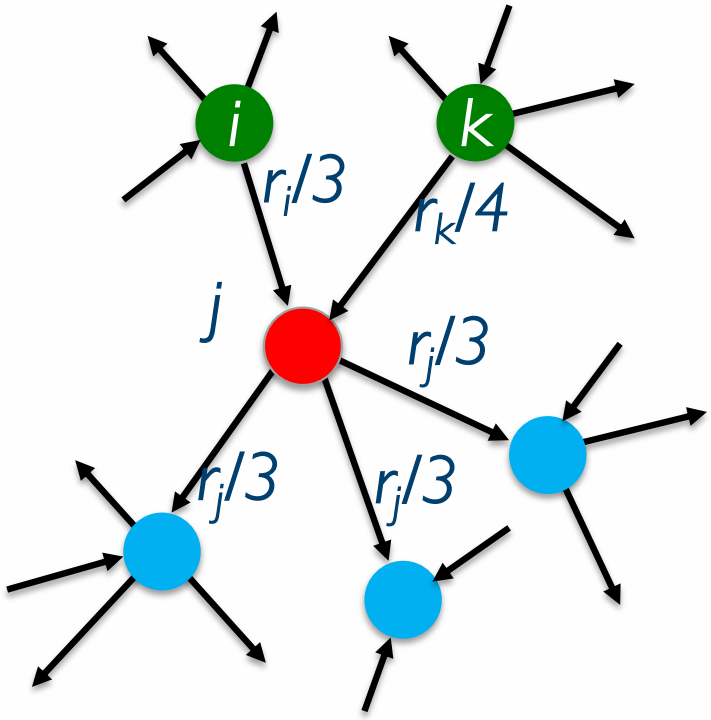
- The underlying idea is to look at links as votes
- A page is more important if it has more links
  - In-coming links? Out-going links?
- Intuition
  - www.stanford.edu has 23,400 in-links
  - www.joe-schmoe.com has one in-link
- Are all in-links are equal?
  - Links from important pages count more
  - Recursive question!


A
3.3
B
38.4
C
34.3
D
3.9
E
8.1
F
3.9
1.6
1.6
1.6
1.6
1.6

Simple Recursive Formulation

- Each link's vote is proportional to the importance of its source page
- If page j with importance r_j has n out-links, each link gets r_j/n votes
- Page j's own importance is the sum of the votes on its in-links

$$r_j = r_i/3 + r_k/4$$

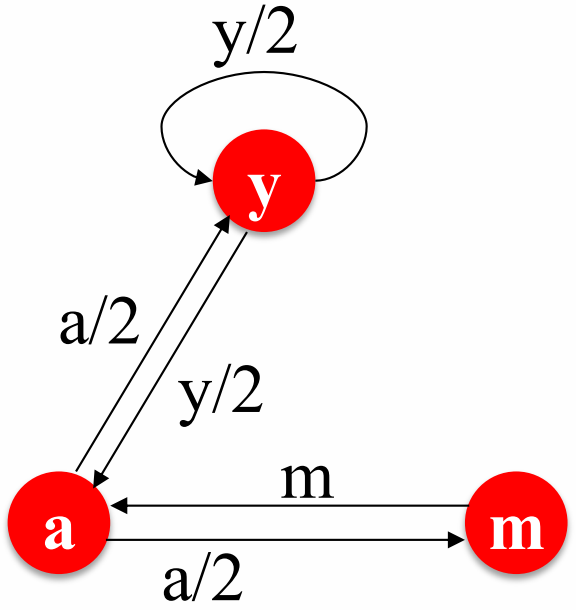


The "Flow" Model

- A "vote" from an important page is worth more
- A page is important if it is pointed to by other important pages
- Define a "rank" r_j for page j

$$r_j = \sum_{i \to j} \frac{r_i}{d_i}$$

where d_i is the out-degree of node i



- "Flow" equations

$r_y = r_y/2 + r_a/2$

$r_a = r_y/2 + r_m$

$r_m = r_a/2$

Solving the Flow Equations

- The equations, three unknowns variables, no constant
  - No unique solution
  - All solutions equivalent modulo the scale factor
- An additional constraint ($r_y+r_a+r_m=1$) forces uniqueness
- Gaussian elimination method works for small examples, but we need a better method for large web-size graphs

We need a different formulation that scales up!

The Matrix Formulation

- Represent the graph as a transition matrix M
  - Suppose page i has d_i out-links
  - If page i is linked to page j M_{ji} is set to 1/di else $M_{ji}=0$
  - M is a "column stochastic matrix" since the columns sum up to 1

- Given the rank vector r with an entry per page, where r_i is the importance of page i and the r_i sum up to one

$$r_j = \sum_{i \to j} \frac{r_i}{\mathrm{d_i}}$$

The flow equation can be written as r = Mr

The Eigenvector Formulation

- Since the flow equation can be written as $r = Mr$, the rank vector r is also an eigenvector of M
- Thus, we can solve for r using a simple iterative scheme ("power iteration")
- **Power iteration:** a simple iterative scheme
  - Suppose there are N web pages
  - Initialize: $\mathbf{r}^{(0)} = [1/N,\ldots,1/N]^T$
  - Iterate: $\mathbf{r}^{(t+1)} = \mathbf{M} \bullet \mathbf{r}^{(t)}$
  - Stop when $|\mathbf{r}^{(t+1)} - \mathbf{r}^{(t)}|_1 < \varepsilon$

The Random Walk Formulation

- Suppose that a random surfer that at time t is on page i and will continue it navigation by following one of the out-link at random
- At time t+1, will end up on page j and from there it will continue the random surfing indefinitely
- Let p(t) the vector of probabilities $p_i(t)$ that the surfer is on page i at time t (p(t) is the probability distribution over pages)
- Then, p(t+1) = Mp(t) so that

p(t) is the stationary distribution for the random walk

Existence and Uniqueness

For graphs that satisfy certain conditions, the stationary distribution is unique and eventually will be reached no matter what the initial probability distribution is

Hubs and Authorities (HITS)

Hubs and Authorities

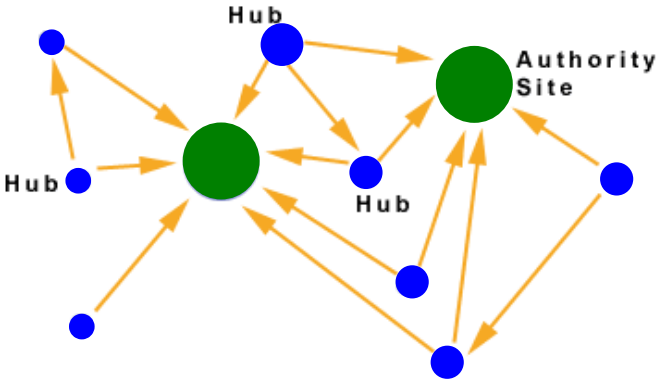
- HITS (Hypertext-Induced Topic Selection)
  - Is a measure of importance of pages and documents, similar to PageRank
  - Proposed at around same time as PageRank (1998)
- Goal: Say we want to find good newspapers
  - Don't just find newspapers. Find "experts", that is, people who link in a coordinated way to good newspapers
- The idea is similar, links are viewed as votes
  - Page is more important if it has more links
  - In-coming links? Out-going links?

Hubs and Authorities

- Each page has 2 scores
- Quality as an expert (hub)
  - Total sum of votes of authorities pointed to
- Quality as a content (authority)
  - Total sum of votes coming from experts
- Principle of repeated improvement

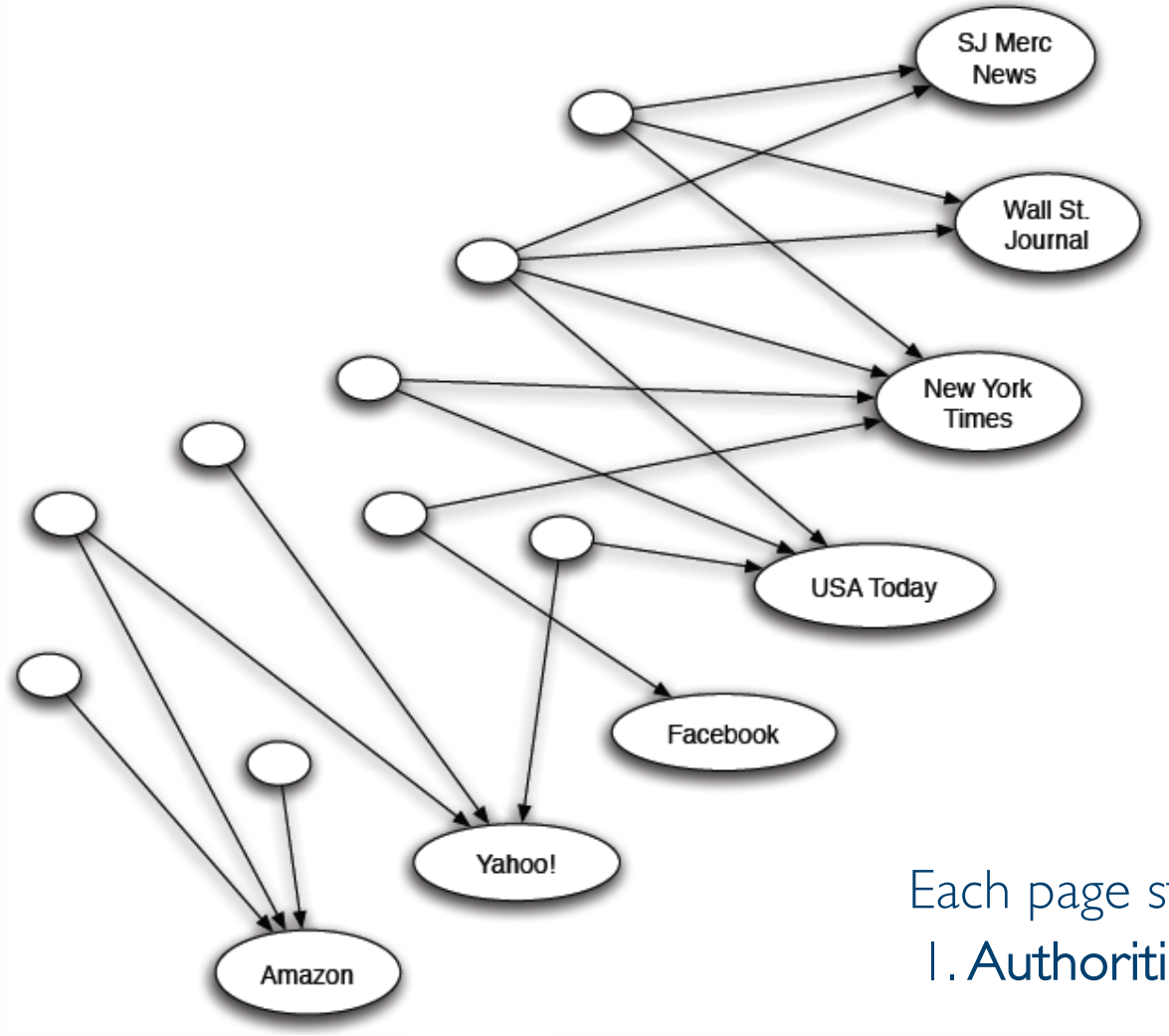
Hubs and Authorities

- Authorities are pages containing useful information
  - Newspaper home pages
  - Course home pages
  - Home pages of auto manufacturers



- Hubs are pages that link to authorities
  - List of newspapers
  - Course bulletin
  - List of US auto manufacturers

Counting in-links: Authority

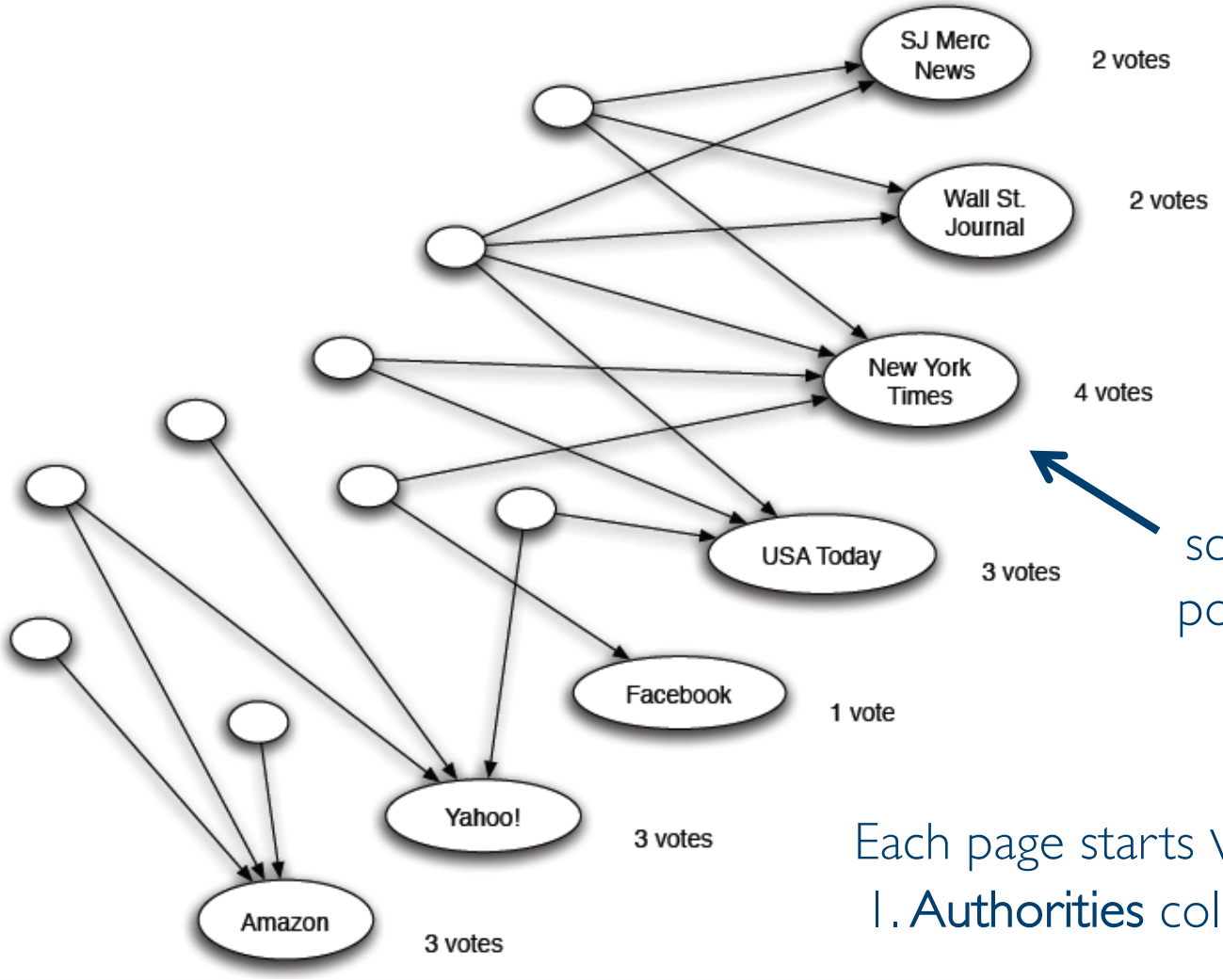


Each page starts with **hub** score

1. **Authorities** collect their votes

(Note this is idealized example. In reality graph is not bipartite and each page has both the hub and authority score)

Counting in-links: Authority

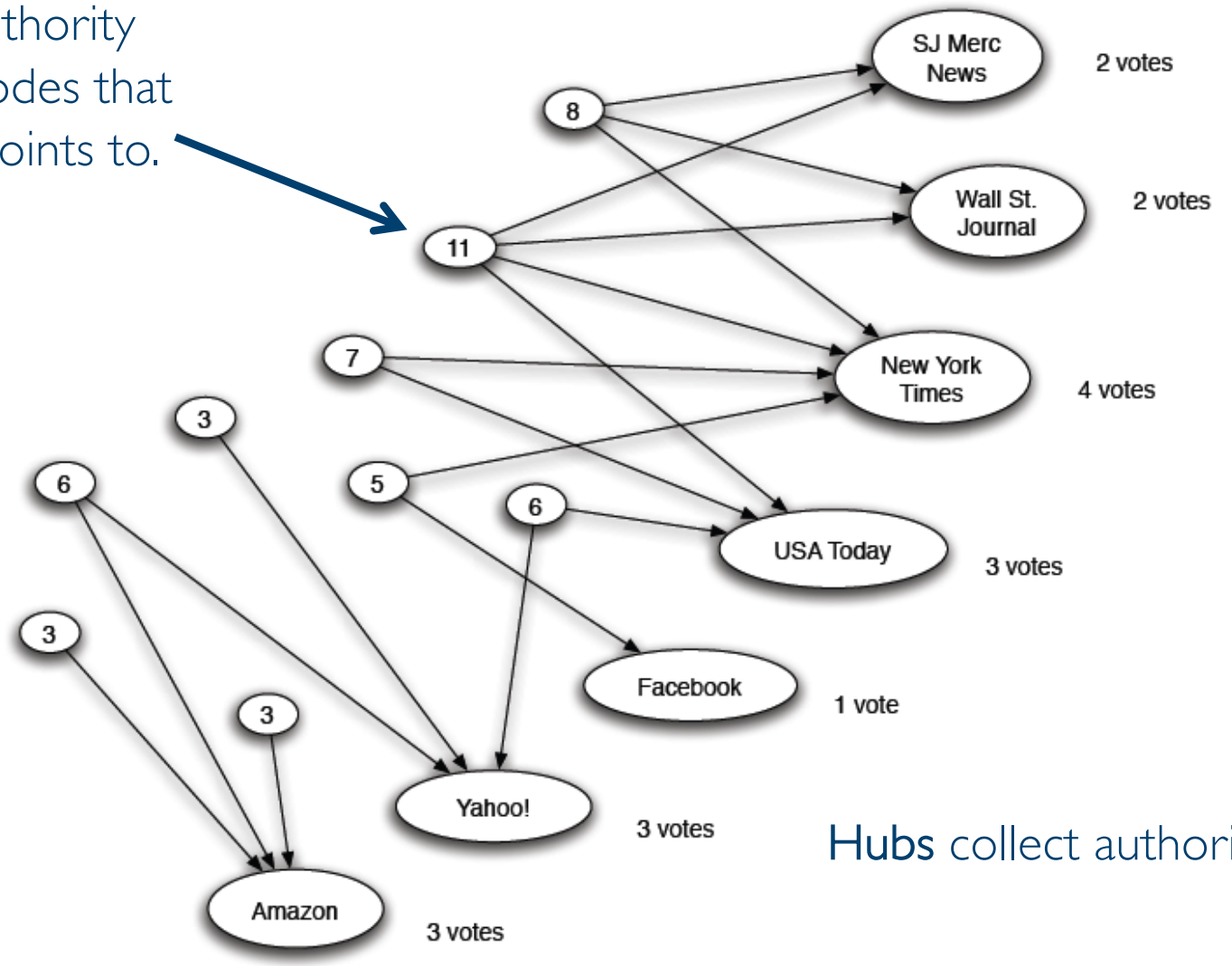


Sum of **hub** scores of nodes pointing to NYT.

Each page starts with **hub** score 1. **Authorities** collect their votes

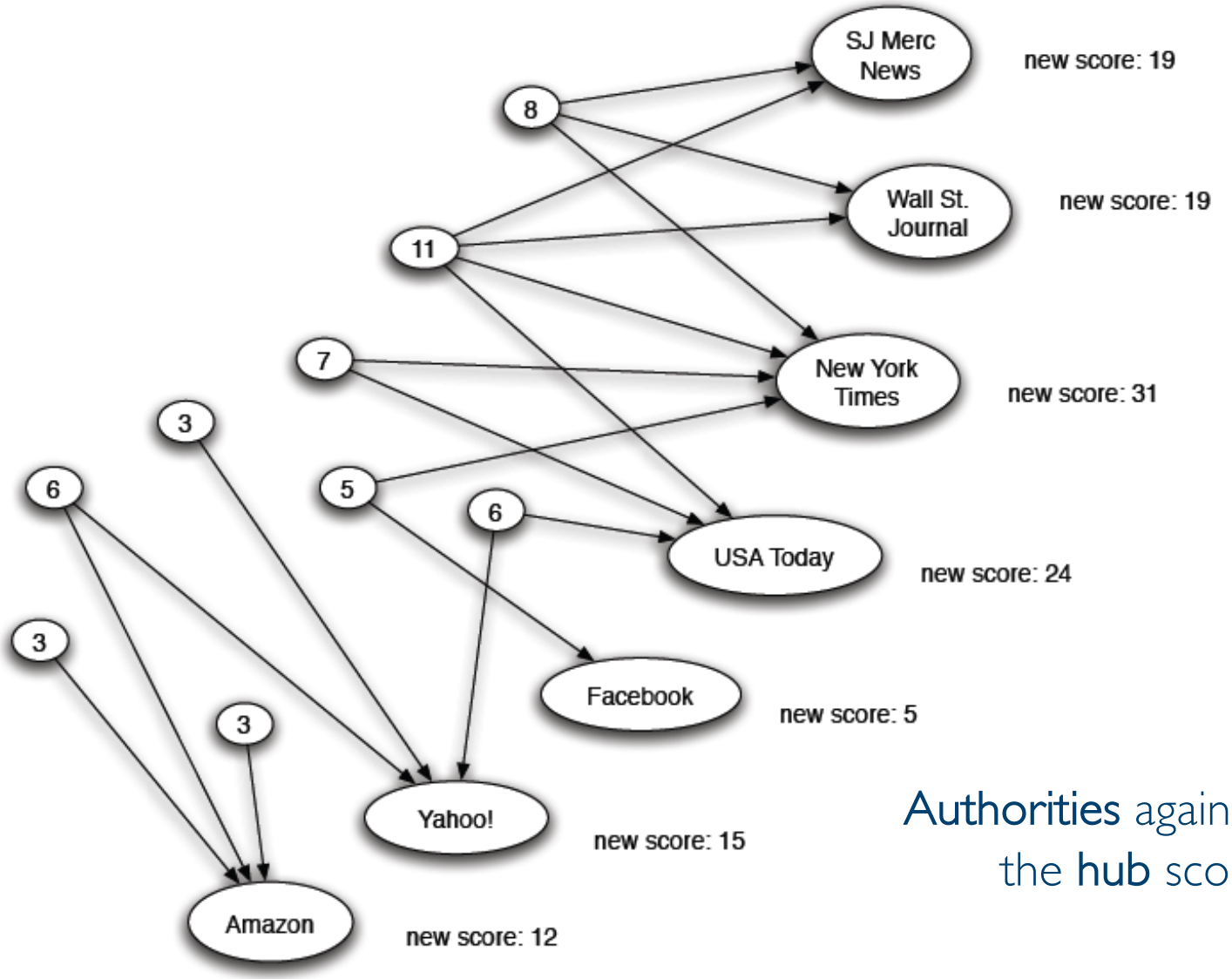
Expert Quality: Hub

Sum of authority scores of nodes that the node points to.



Hubs collect authority scores

Reweighting



Authorities again collect the hub scores

Mutually Recursive Definition

- A good hub links to many good authorities
- A good authority is linked from many good hubs
- Model using two scores for each node:
  - Hub score and Authority score
  - Represented as vectors and

The HITS Algorithm

- Initialize scores
- Iterate until convergence:
  - Update authority scores
  - Update hub scores
  - Normalize

- Two vectors a = (a_1, …, a_n) and h=(h_1, …, h_n) and the adjacency matrix A, with Aij=1 is 1 if i connects to j are connected, 0 otherwise

The HITS Algorithm (vector notation)

- Set $a_i = h_i = 1/\sqrt{n}$
- Repeat until convergence
  - $h = Aa$
  - $a = A^T h$
- Convergence criteria

$$\sum_i (h_i(t) - h_i(t-1))^2 < \varepsilon$$

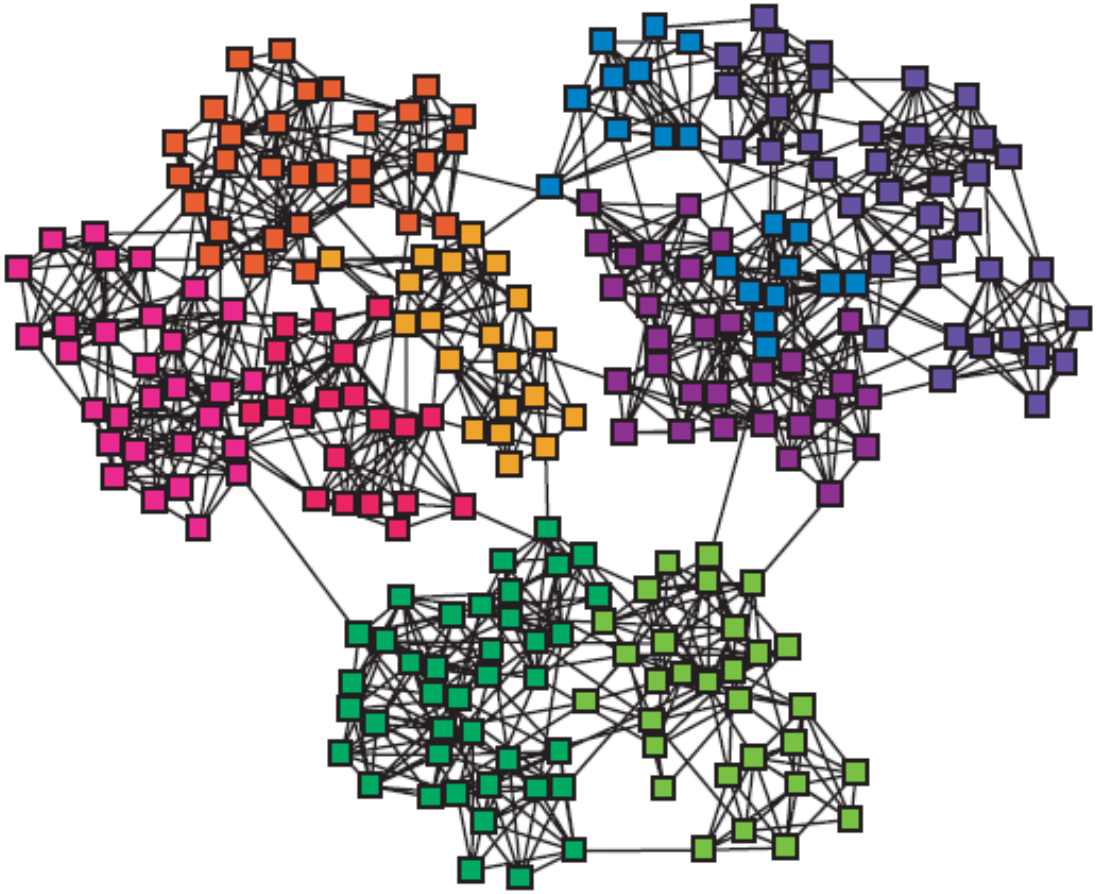
$$\sum_i (a_i(t) - a_i(t-1))^2 < \varepsilon$$

- Under reasonable assumptions about A, HITS converges to vectors h^* and a^* where
  - h^* is the principal eigenvector of matrix $A\,A^T$
  - a^* is the principal eigenvector of matrix $A^T A$

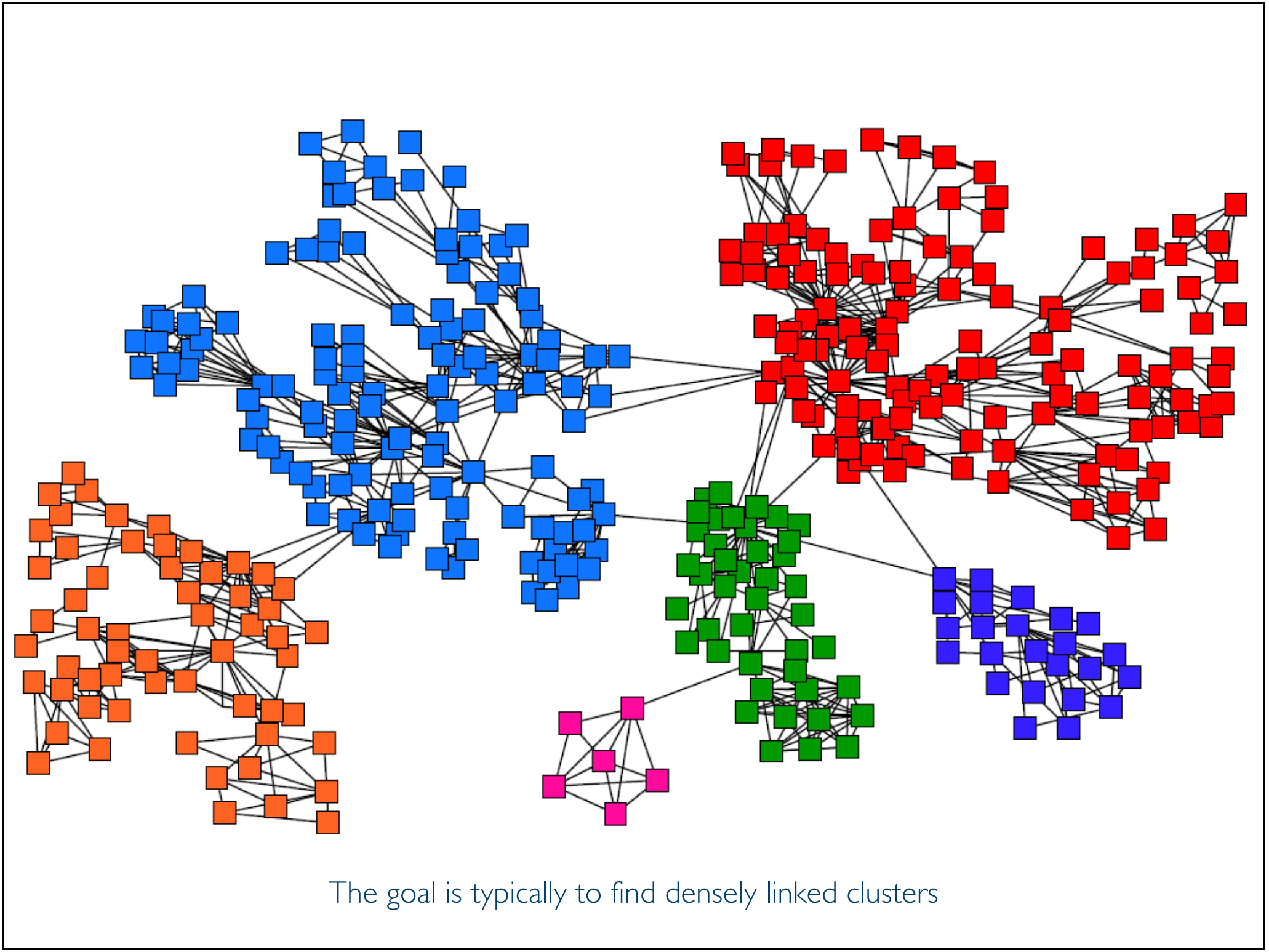
PageRank vs HITS

- PageRank and HITS are two solutions to the same problem
  - What is the value of an in-link from u to v?
  - In the PageRank model, the value of the link depends on the links into u
  - In the HITS model, it depends on the value of the other links out of u
- The destinies of PageRank and HITS after 1998 were very different

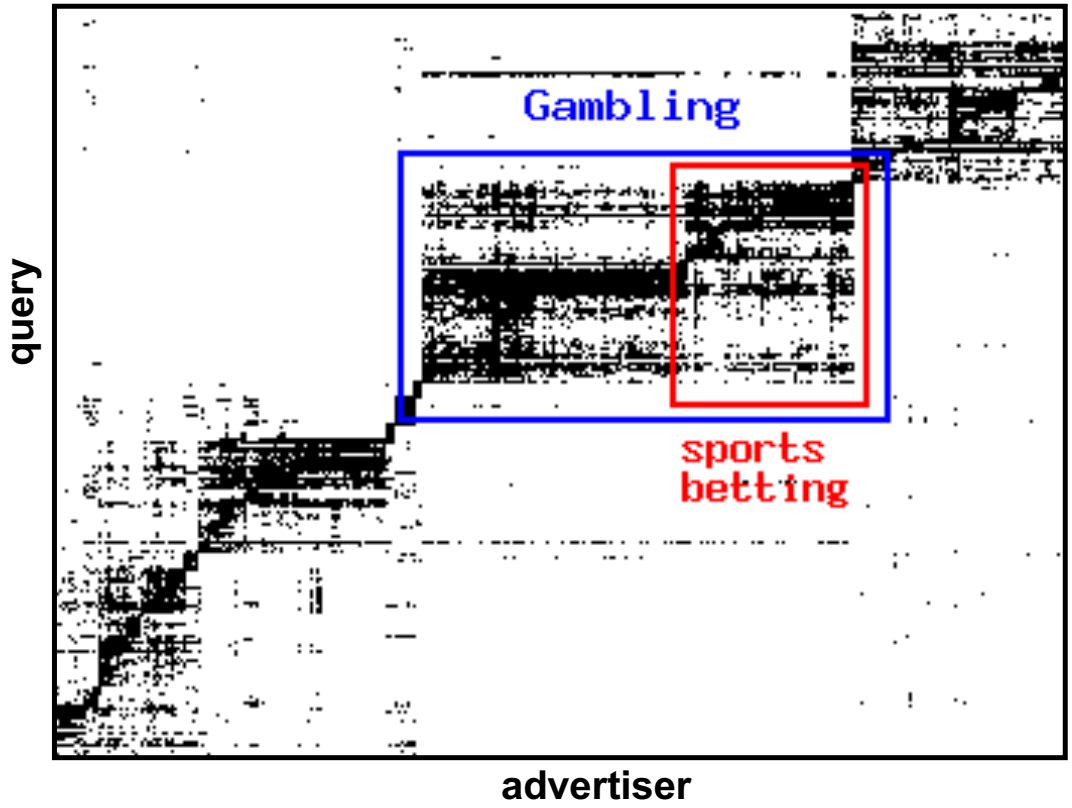
Community Detection



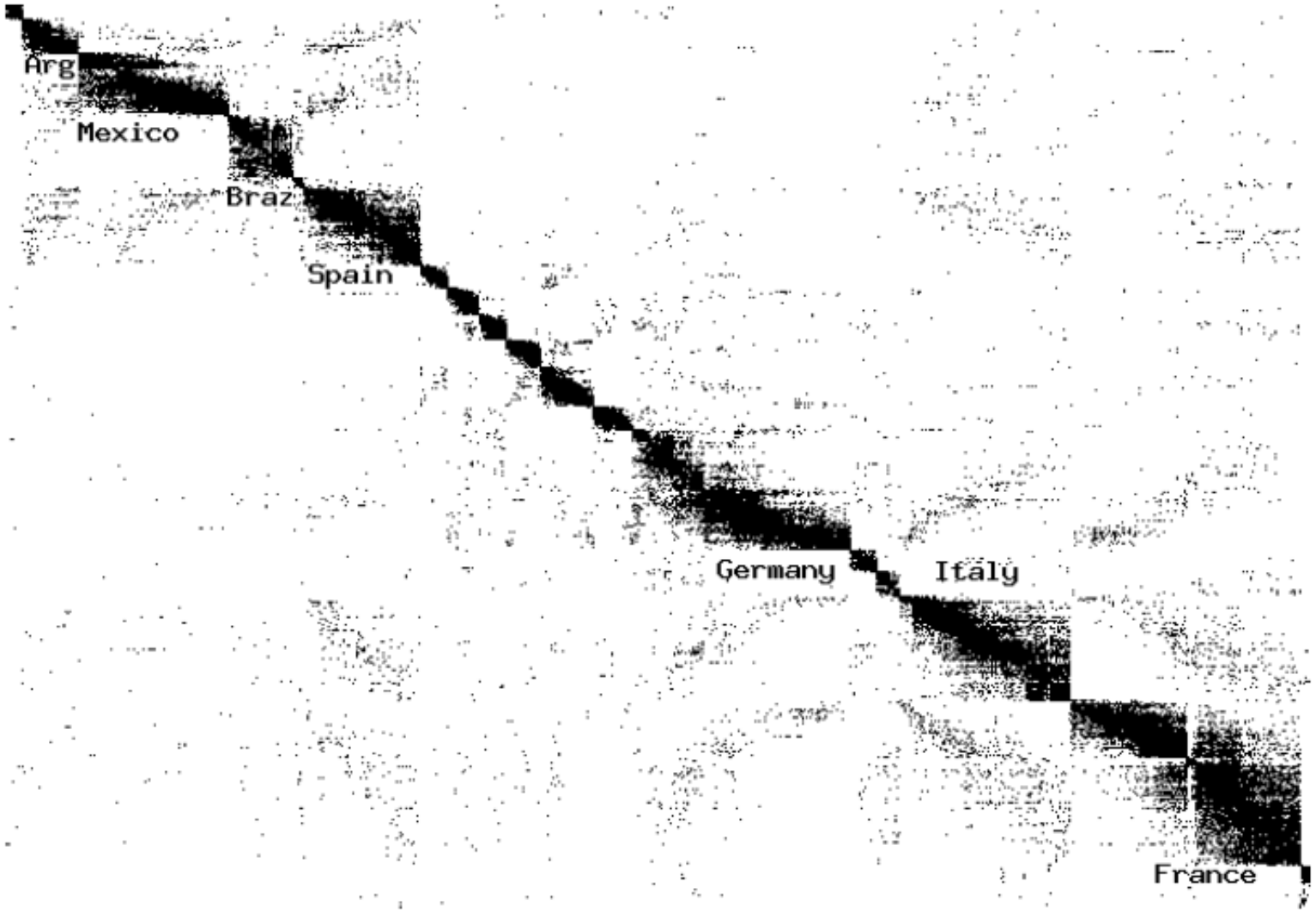
We often think of networks being organized into modules, cluster, communities:



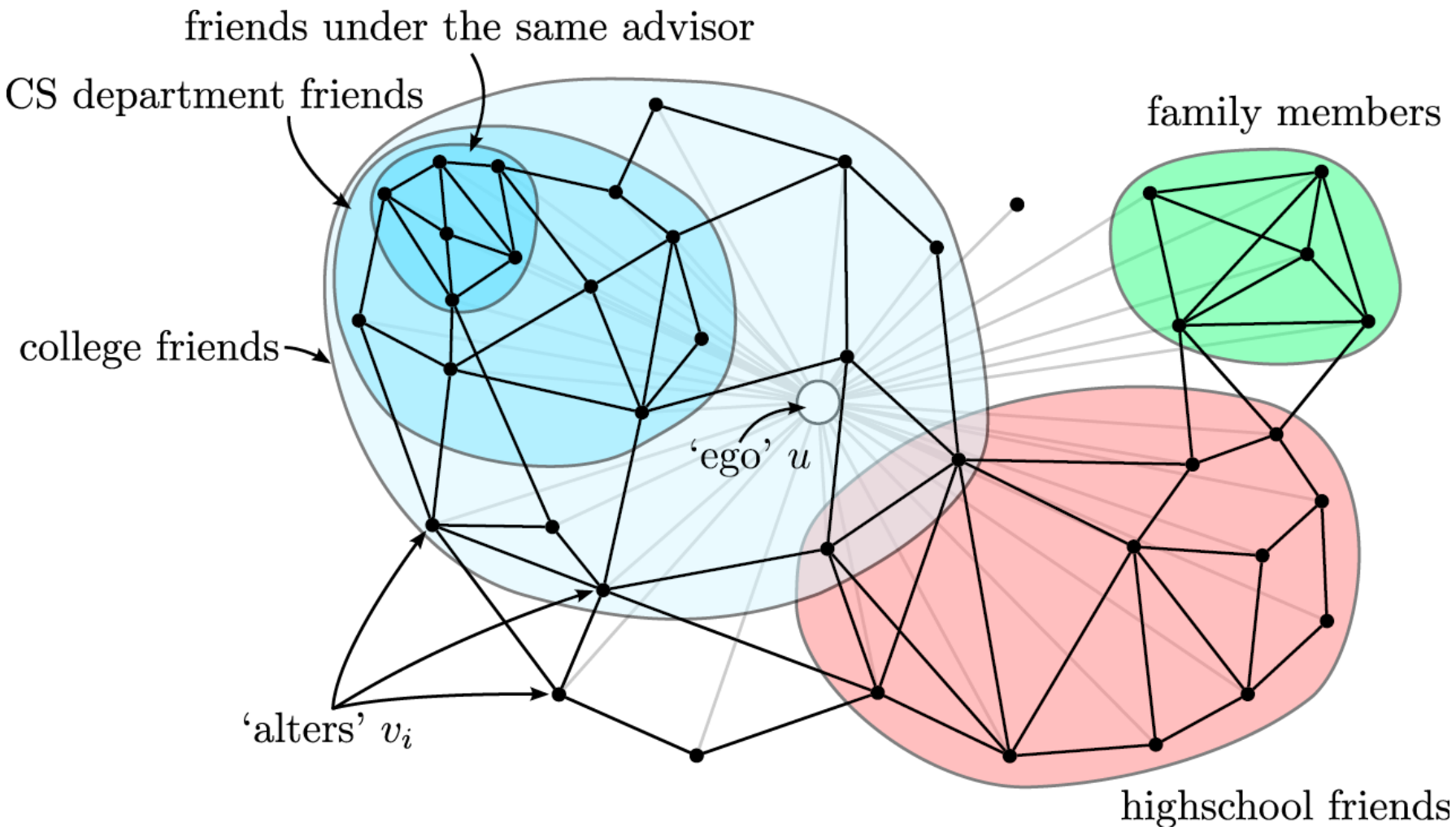
The goal is typically to find densely linked clusters



Micro-Markets in Sponsored Search: find micro-markets by partitioning the query-to-advertiser graph (Andersen, Lang: Communities from seed sets, 2006)



Clusters in Movies-to-Actors graph
(Andersen, Lang: Communities from seed sets, 2006)

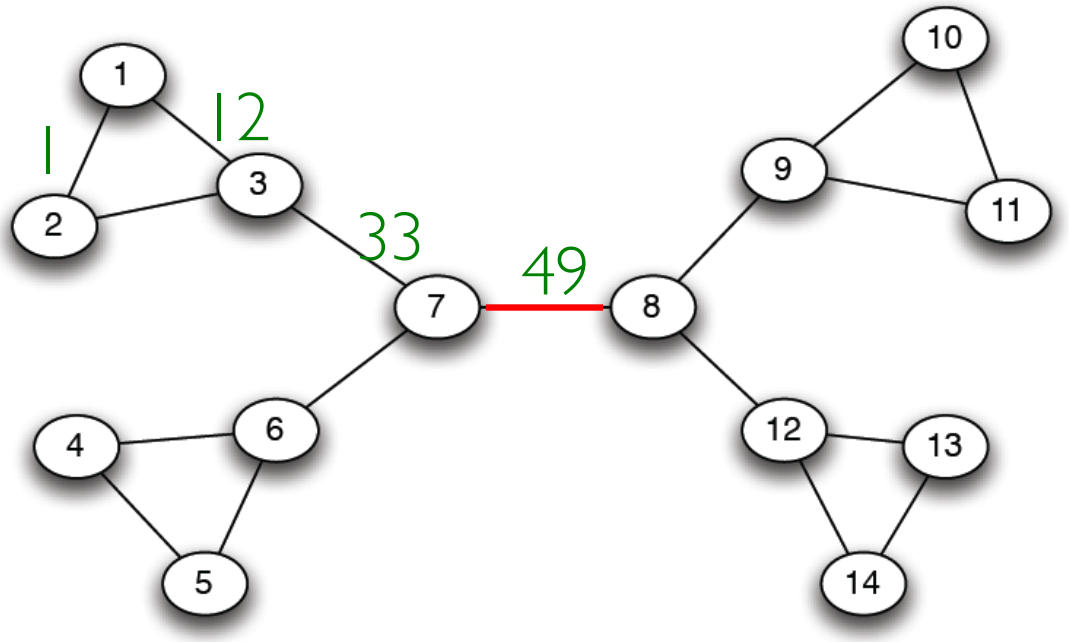


Discovering social circles, circles of trust
(McAuley, Leskovec: Discovering social circles in ego networks, 2012)

how can we identify communities?

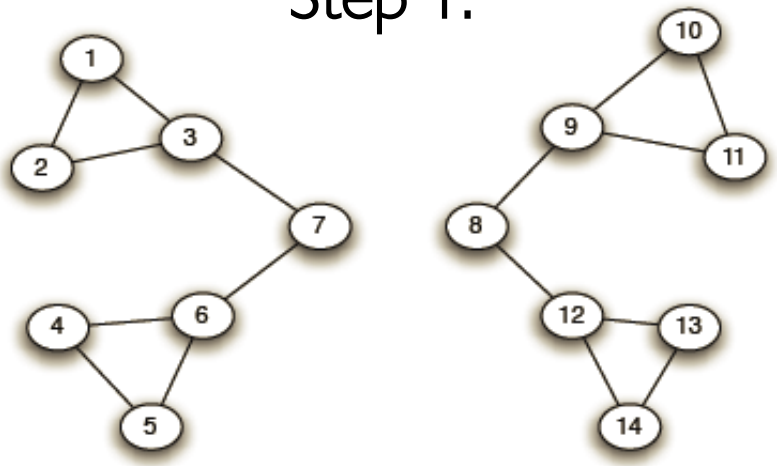
Girvan-Newman Method

- Define edge betweenness as the number of shortest paths passing over the edge
- Divisive hierarchical clustering based on the notion of edge betweenness
- The Algorithm
  - Start with an undirected graph
  - Repeat until no edges are left
    - Calculate betweenness of edges
    - Remove edges with highest betweenness
- Connected components are communities
- Gives a hierarchical decomposition of the network

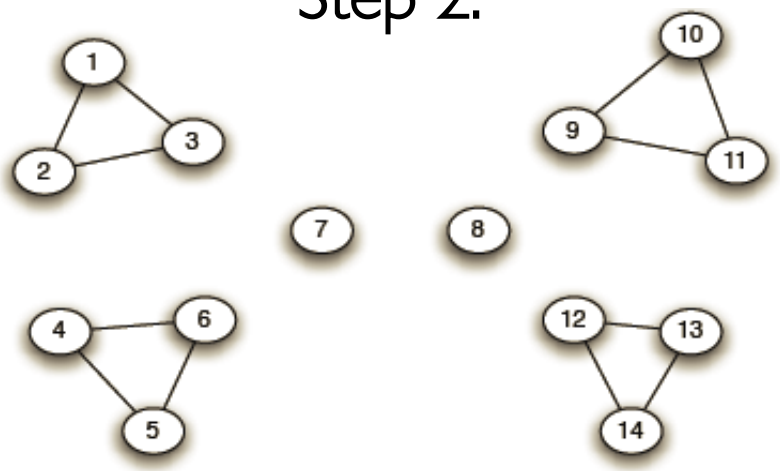


Need to re-compute
betweenness at every step

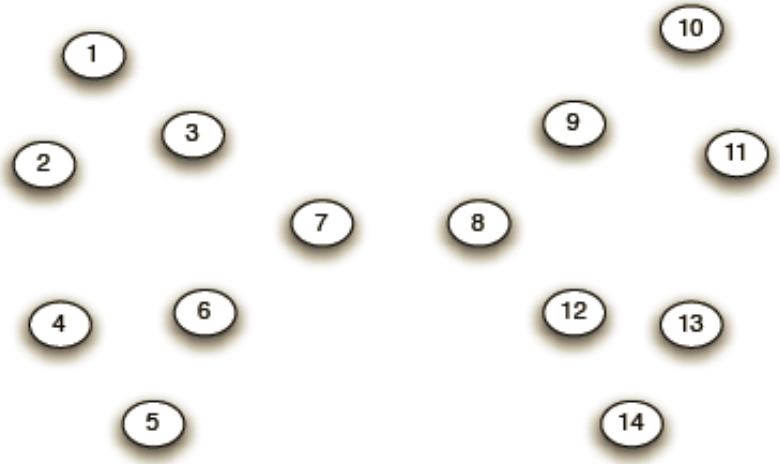
Step 1:



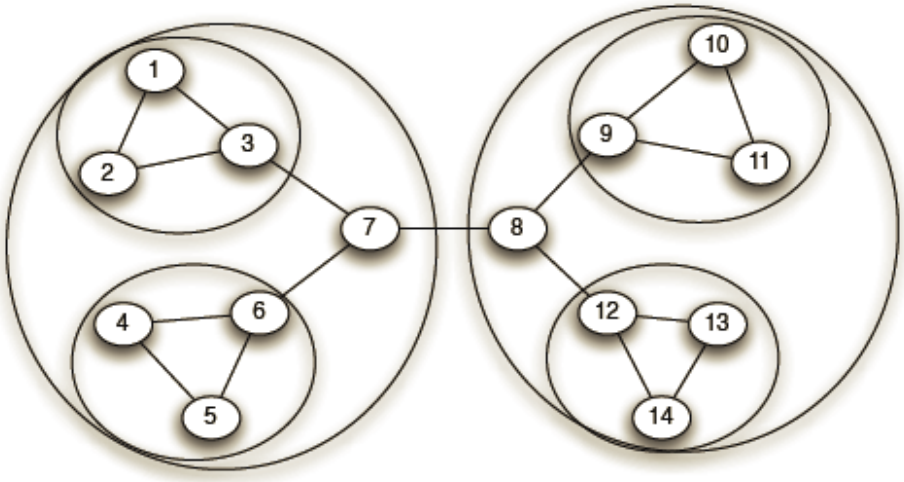
Step 2:

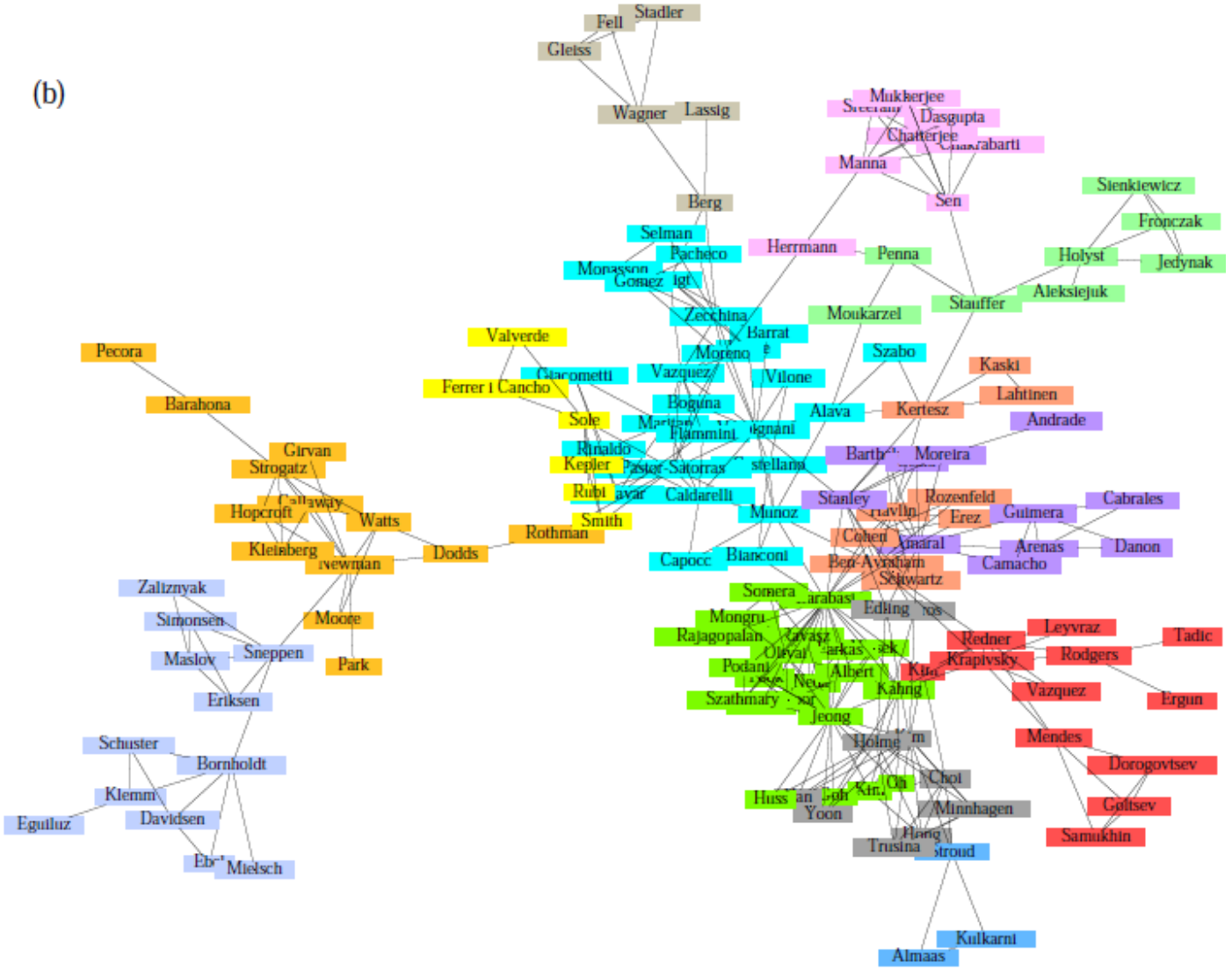


Step 3:



Hierarchical network decomposition



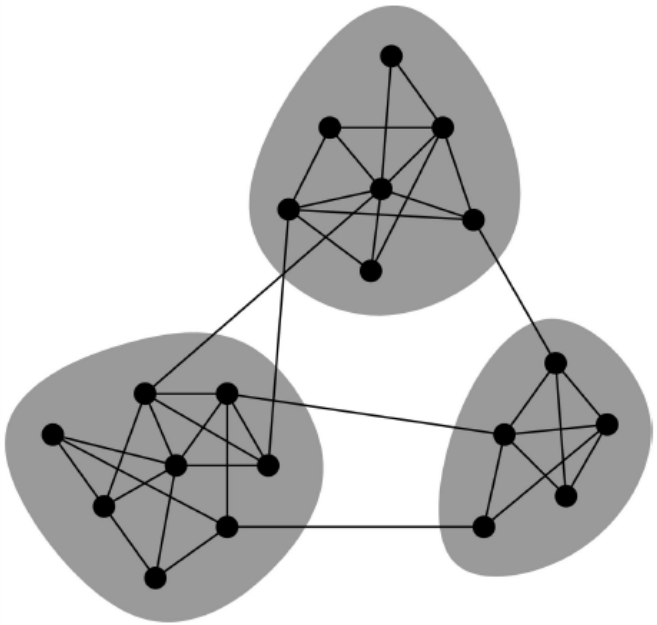


Communities in physics collaborations

how to select the number of clusters?

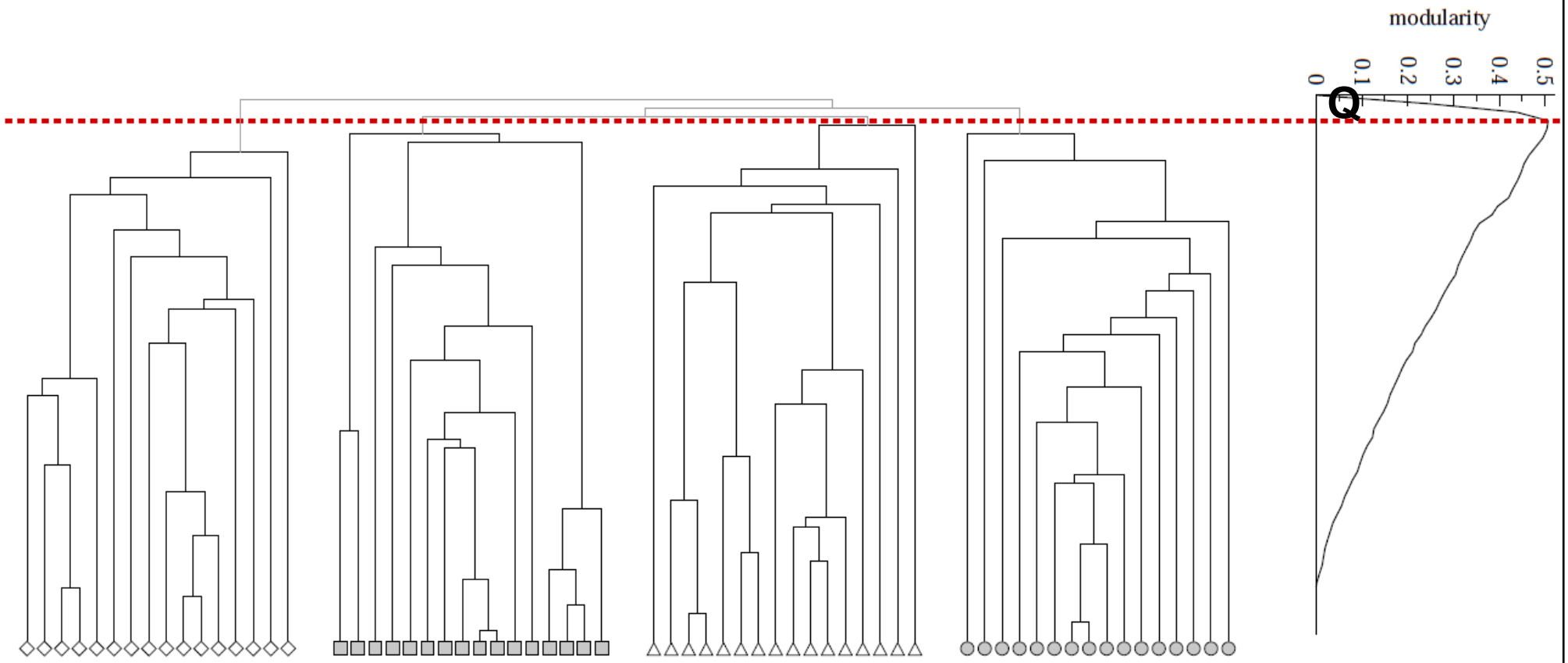
Network Communities

- Communities are viewed as sets of tightly connected nodes
- We define modularity as a measure of how well a network is partitioned into communities
- Given a partitioning of the network into a set of groups S we define the modularity Q as



$$Q \propto \sum_{s \in S} [(\#\text{ edges within group s}) - (\text{expected }\#\text{ edges within group s})]$$

Need a null model!



Modularity is useful for selecting the number of clusters:

Example

Example #1 – Compute betweenness

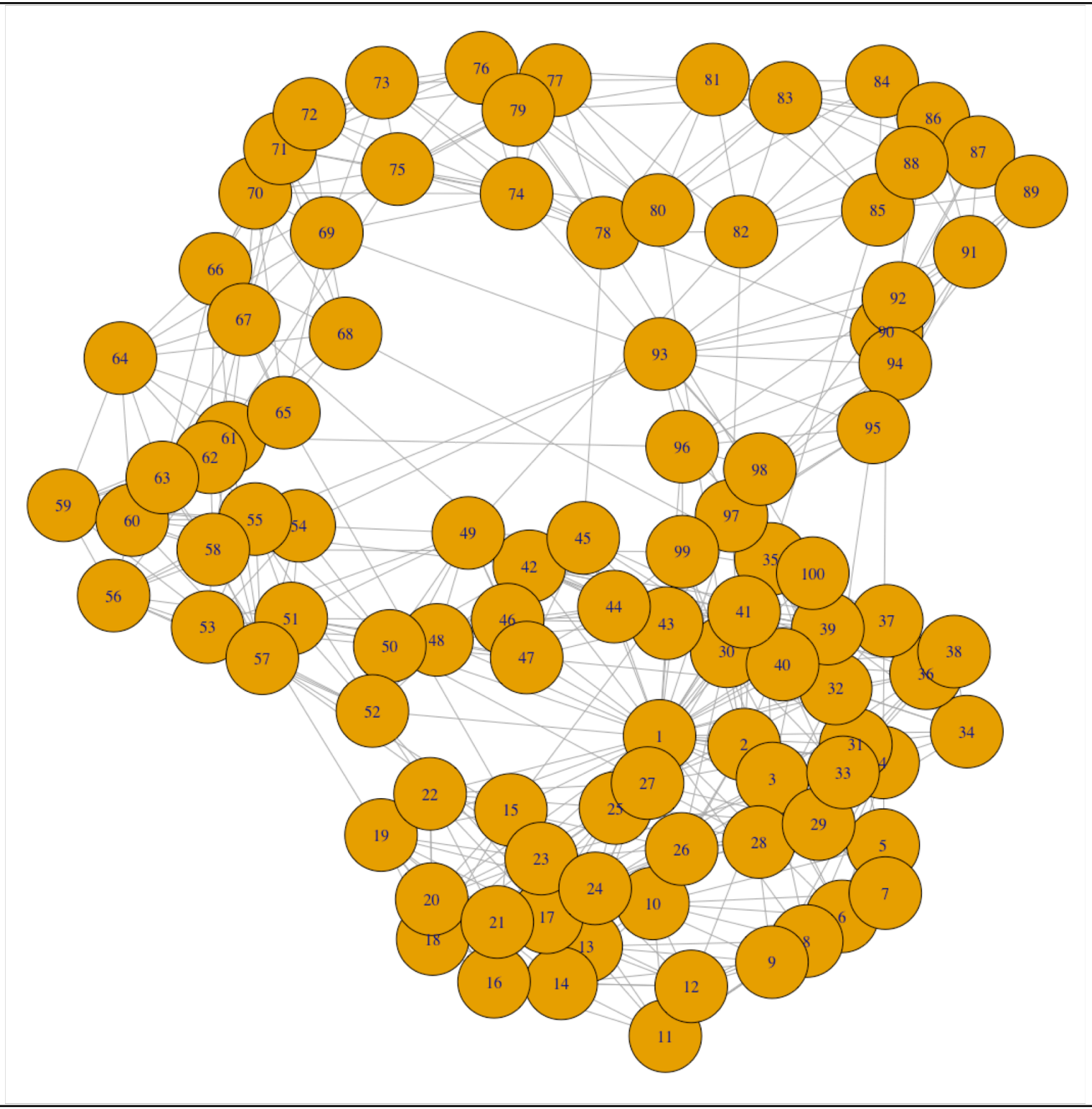

```
# First we load the ipgrah package
library(igraph)

# let's generate two networks and merge them into one graph.
g2 <- barabasi.game(50, p=2, directed=F)
g1 <- watts.strogatz.game(1, size=100, nei=5, p=0.05)
g <- graph.union(g1,g2)

# let's remove multi-edges and loops
g <- simplify(g)

plot(g)

# compute betweenness
ebc <- edge.betweenness.community(g, directed=F)
```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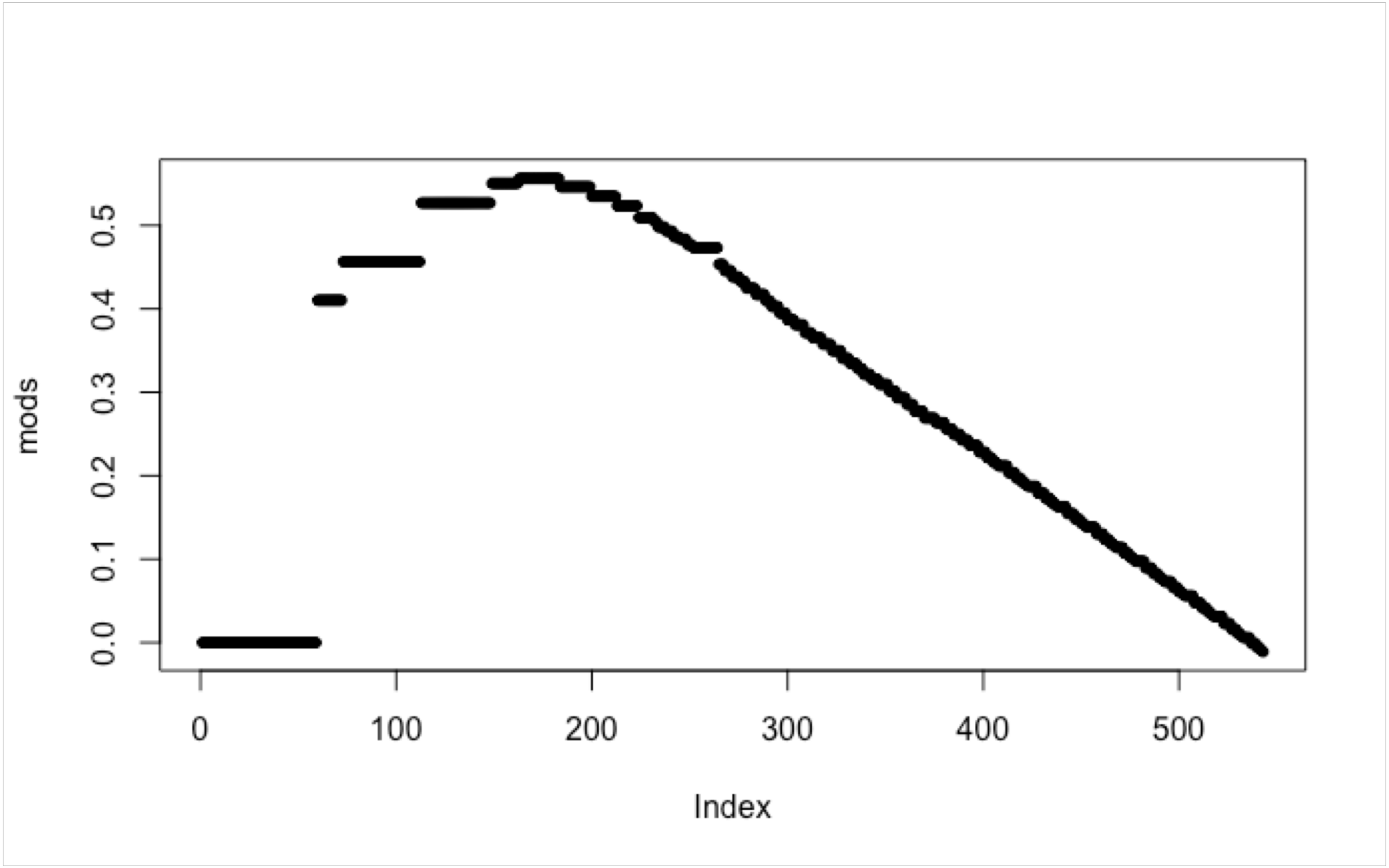
100

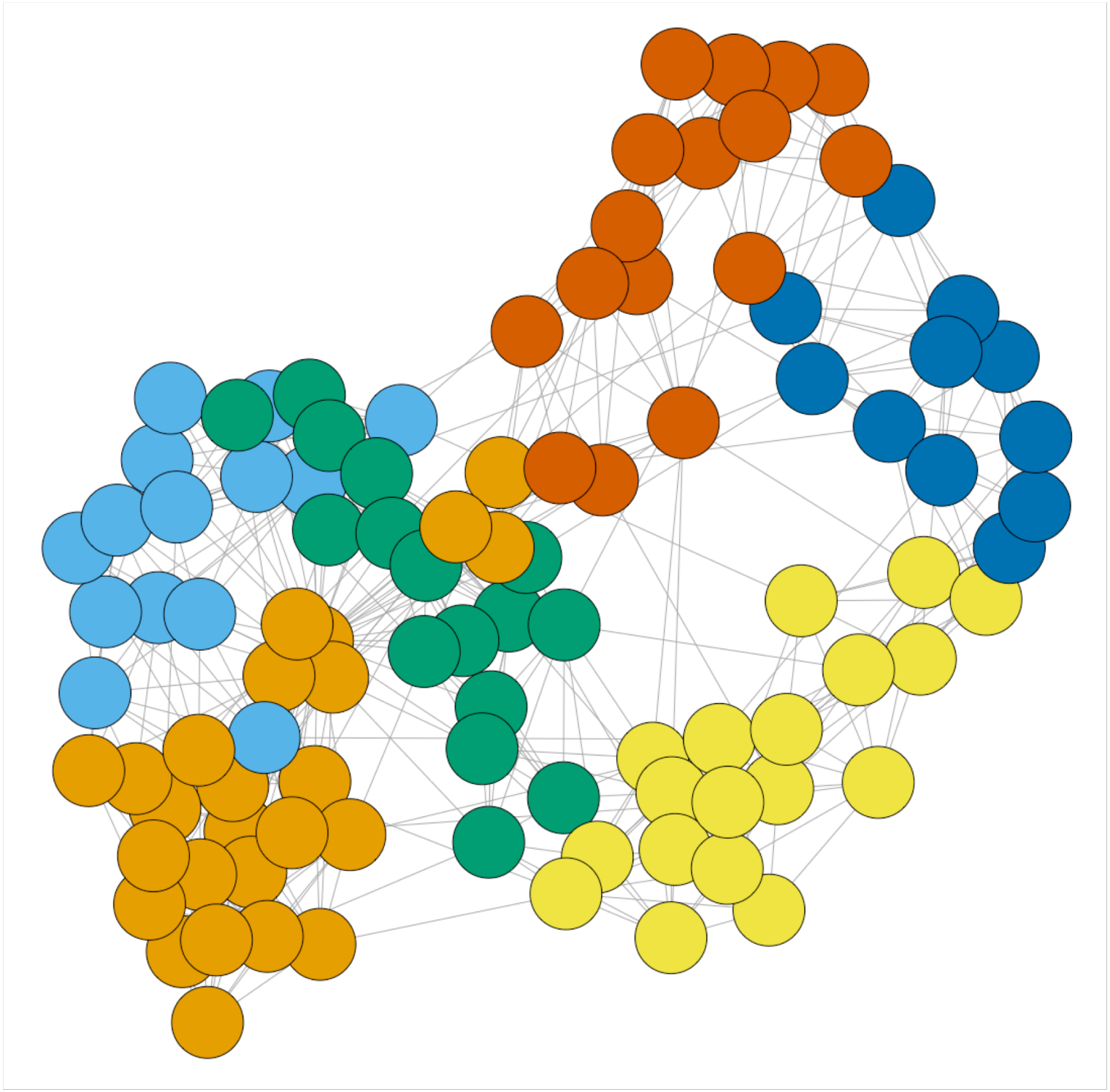
Example #1 – Build Dendrogram and Compute Modularity


```
mods <- sapply(0:ecount(g), function(i){
  g2 <- delete.edges(g, ebc$removed.edges[seq(length=i)])
  cl <- clusters(g2)$membership
  # March 13, 2014 - compute modularity on the original graph g
  # (Thank you to Augustin Luna for detecting this typo) and not on the
induced one g2.
  modularity(g,cl)
})

# we can now plot all modularities
plot(mods, pch=20)
```


mods
0.0
0.1
0.2
0.3
0.4
0.5
0
100
200
300
400
500
Index

Example #1 – Select the cut

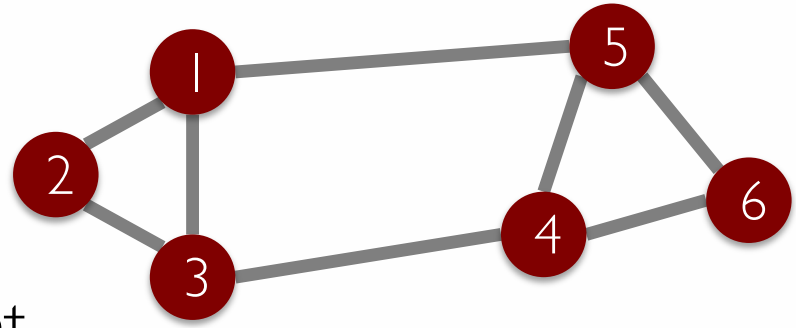

```
# Now, let's color the nodes according to their membership
g2<-delete.edges(g, ebc$removed.edges[seq(length=which.max(mods)-1)])
V(g)$color=clusters(g2)$membership

# Let's choose a layout for the graph
g$layout <- layout.fruchterman.reingold

# plot it
plot(g, vertex.label=NA)
```



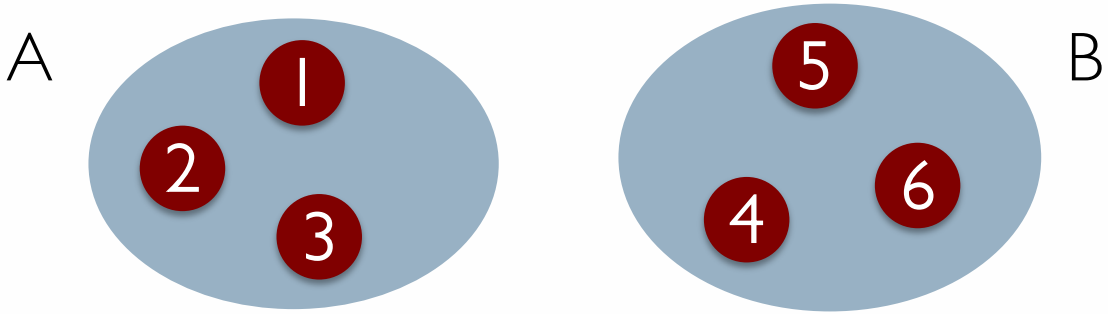
Spectral Clustering

What Makes a Good Cluster?

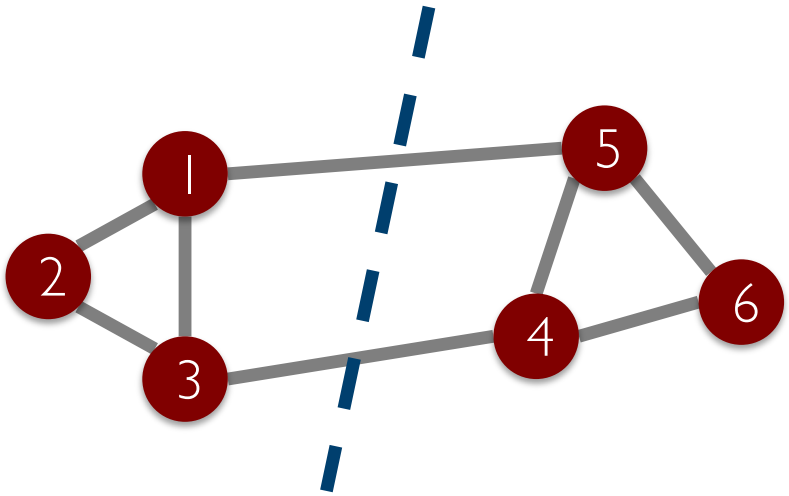
- Undirected graph G(V,E)



- Partitioning task
  - Divide the vertices into two disjoint groups A, B=V\A



- Questions
  - How can we define a "good partition" of G?
  - How can we efficiently identify such a partition?

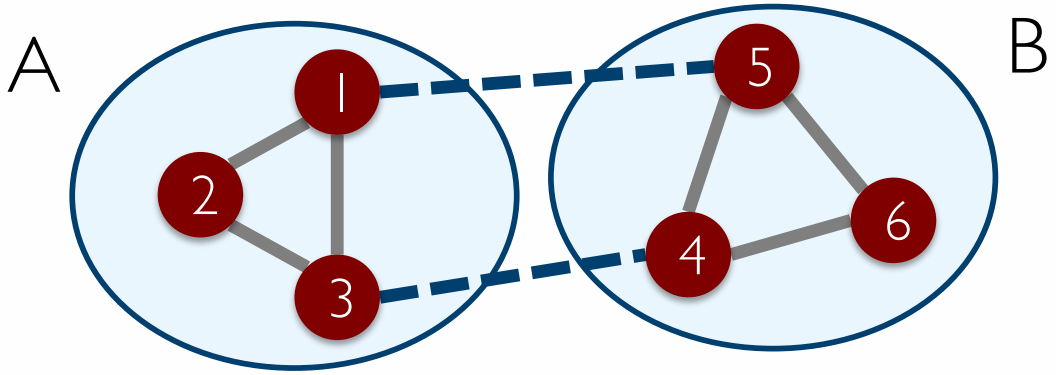


What makes a good partition?

Maximize the number of within-group connections

Minimize the number of between-group connections

- Express partitioning objectives as a function of the "edge cut" of the partition
- Cut is defined as the set of edges with only one vertex in a group

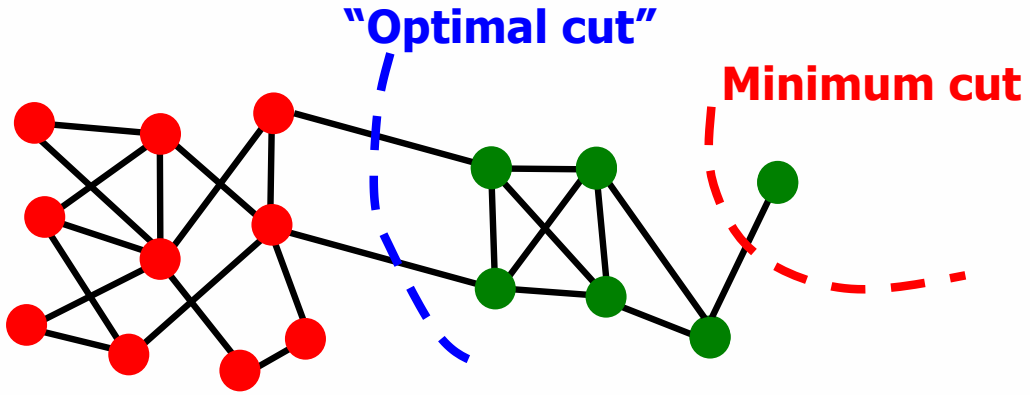


- The cut of the set A, B is cut(A,B) = 2 or in more general

$$\text{cut}(\text{A},\text{B}) = \sum_{i \in A, j \notin A} w_{ij}$$

Graph Cut Criterion

- Partition quality
  - Minimize weight of connections between groups, i.e., arg $\min_{A,B}$ cut(A,B)
- Degenerate case:



- Problems
  - Only considers external cluster connections
  - Does not consider internal cluster connectivity

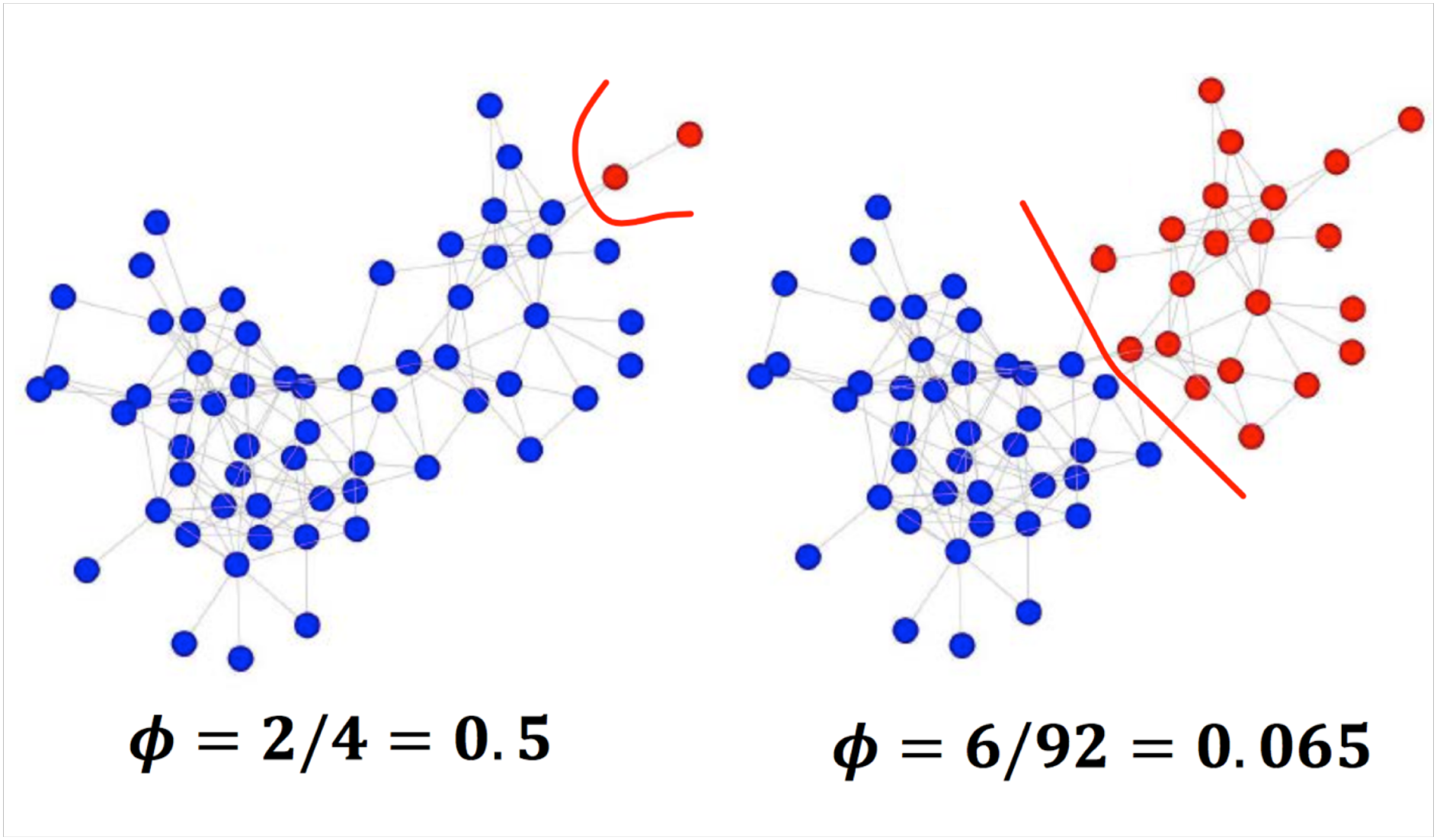
Graph Partitioning Criteria: Normalized cut (Conductance)

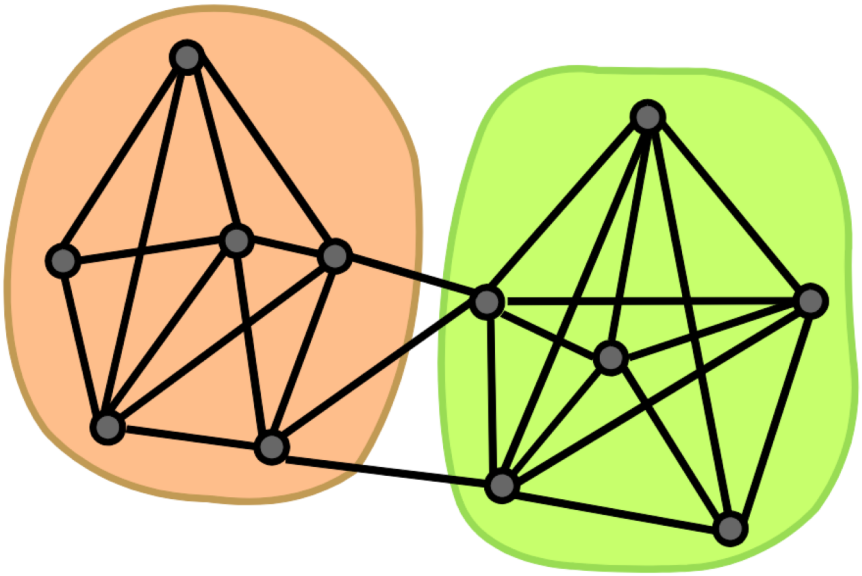
- Connectivity of the group to the rest of the network should be relative to the density of the group

$$\text{ncut}(\text{A},\text{B}) = \frac{\text{cut}(\text{A},\text{B})}{\text{vol}(\text{A})} + \frac{\text{cut}(\text{A},\text{B})}{\text{vol}(\text{B})}$$

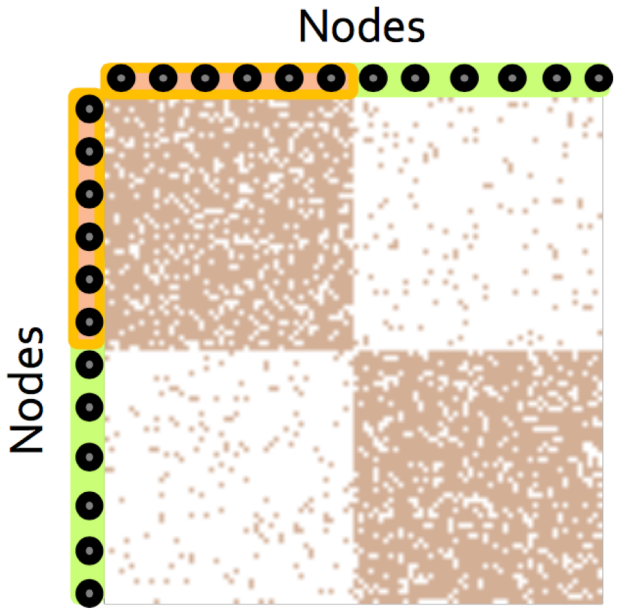
$$\phi(A) = \frac{\text{cut}(\text{A})}{\text{vol}(\text{A})}$$

- Where vol(A) is the total weight of the edges that have at least one endpoint in A


$\phi = 2/4 = 0.5$
$\phi = 6/92 = 0.065$



Network



Adjacency matrix

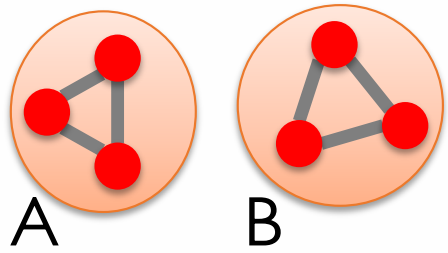
Spectral Graph Partitioning

- Let A be the adjacent matrix of the graph G with n nodes
  - A_{ij} is 1 if there is an edge between i and j, 0 otherwise
  - x a vector of n components $(x_1, \ldots, x_n)$ that represents labels/values assigned to each node of G
  - Ax returns a vector in which each component j is the sum of the labels of the neighbors of node j

- Spectral Graph Theory
  - Analyze the spectrum of G, that is, the eigenvectors x_i of the graph corresponding to the eigenvalues Λ of G sorted in increasing order
  - $\Lambda = \{ \lambda_1, \ldots, \lambda_n \}$ such that $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$

Example: d-regular Graph

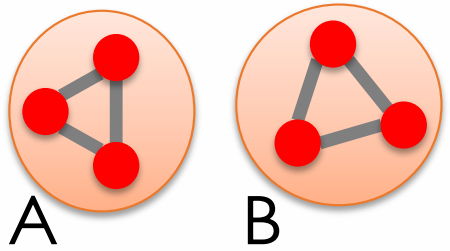
- Suppose that all the nodes in G have degree d and G is connected
- What are the eigenvalues/eigenvectors of G? $Ax=\lambda x$
  - Ax returns the sum of the labels of each node's neighbors and since each node has exactly d neighbors, x = (1, …, 1) is an eigenvector and d is an eigenvalue
- What if G is not connected but still d-regular



- A vector with all the ones is A and all the zeros in B (or viceversa) is still an eigenvector of A with eigenvalue d

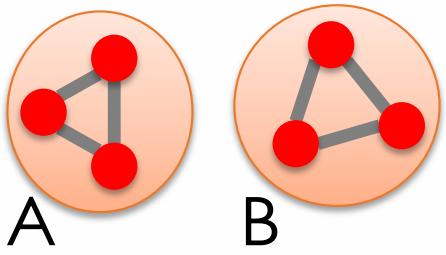
Example: d-regular Graph (not connected)

- What if G has two separate components but it is still d-regular

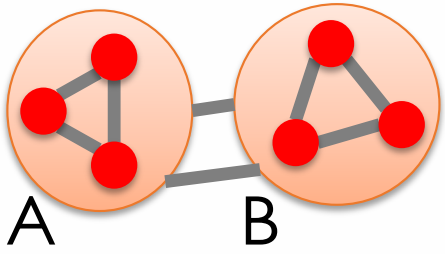


- A vector with all the ones is A and all the zeros in B (or viceversa) is still an eigenvector of A with eigenvalue d

- Underlying intuition



$\lambda_1 = \lambda_2$



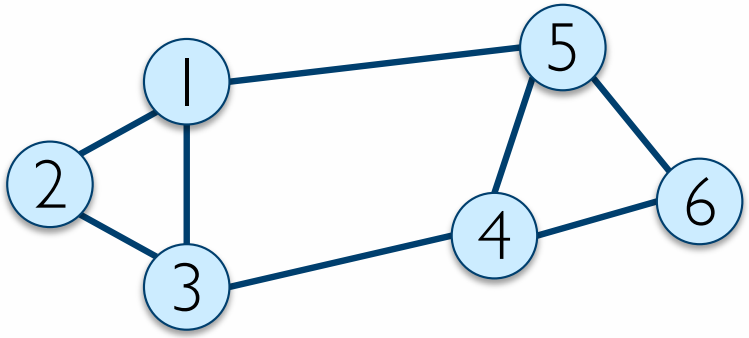
$\lambda_1 \approx \lambda_2$

Spectral Graph Partitioning

- Adjacency matrix A (nxn)
  - Symmetric
  - Real and orthogonal eigenvectors
- Degree Matrix
  - nxn diagonal matrix
  - D_{ii} = degree of node i

	1	2	3	4	5	6
1	0	1	1	0	1	0
2	1	0	1	0	0	0
3	1	1	0	1	0	0
4	0	0	1	0	1	1
5	1	0	0	1	0	1
6	0	0	0	1	1	0

	1	2	3	4	5	6
1	3	0	0	0	0	0
2	0	2	0	0	0	0
3	0	0	3	0	0	0
4	0	0	0	3	0	0
5	0	0	0	0	3	0
6	0	0	0	0	0	2



Graph Laplacian Matrix

- Computed as L = D-A
  - nxn symmetric matrix
  - x=(1,…,1) is a trivial eigenvector since Lx=0 so λ_1=0

- Important properties of L
  - Eigenvalues are non-negative real numbers
  - Eigenvectors are real and orthogonal

	1	2	3	4	5	6
1	3	-1	-1	0	-1	0
2	-1	2	-1	0	0	0
3	-1	-1	3	-1	0	0
4	0	0	-1	3	-1	-1
5	-1	0	0	-1	3	-1
6	0	0	0	-1	-1	2

λ_2 as optimization problem

- For symmetric matrix M,

$$\lambda_2 = \min_x \frac{x^T M x}{x^T x}$$

- What is the meaning of $x^T L x$ on G? We can show that,

$$x^T L x = \sum_{(i,j) \in E} (x_i - x_j)^2$$

- So that, considering that the second eigenvector x is the unit vector, and x is orthogonal to the unit vector (1, …, 1)

$$\lambda_2 = \min_x \frac{\sum_{(i,j) \in E} (x_i - x_j)^2}{\sum_i x_i^2}$$

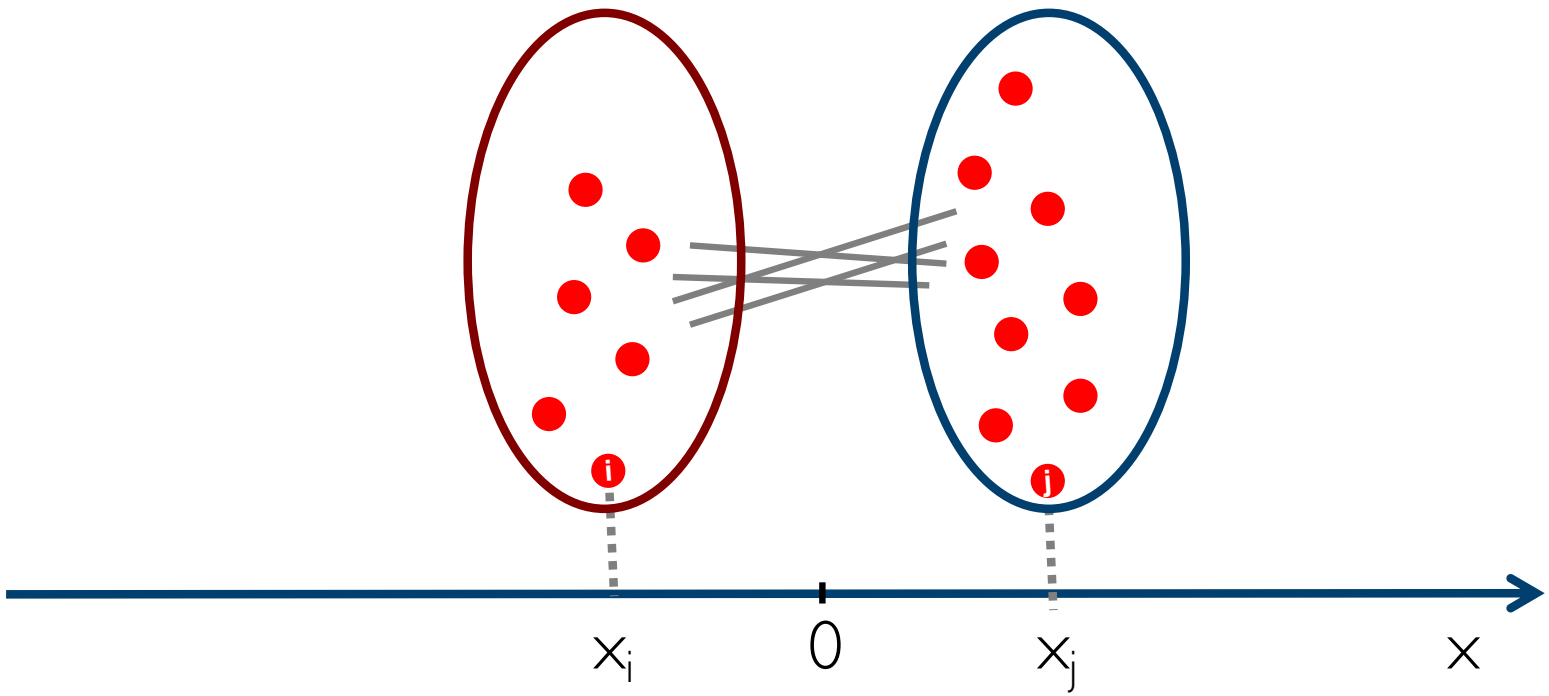
λ_2 as optimization problem

- So that, considering that the second eigenvector x is the unit vector, and x is orthogonal to the unit vector (1, …, 1)

$$\lambda_2 = \min_x \frac{\sum_{(i,j)\in E}(x_i - x_j)^2}{\sum_i x_i^2}$$

- Such that,

$$\sum_i x_i = 0$$



λ_2 and its eigenvector x balance to minimize

Finding the Optimal Cut

- Express the partition (A,B) as a vector y where,
  - $y_i = +1$ if node i belongs to A
  - $y_i = -1$ if node i belongs to B

- We can minimize the cut of the partition by finding a non-trivial vector that minimizes

$$\arg \min_{y \in [-1,+1]^n} f(y) = \sum_{(i,j) \in E} (y_i - y_j)^2$$

Can't solve exactly! Let's relax y and allow y to take any real value.

Rayleigh Theorem

$$\arg\min_{y \in R^n} f(y) = \sum_{(i,j) \in E} (y_i - y_j)^2 = y^T L y$$

- We know that,

$$\lambda_2 = \min_y f(y)$$

- The minimum value of f(y) is given by the second smallest eigenvalue $\boldsymbol{\lambda}_2$ of the Laplacian matrix L

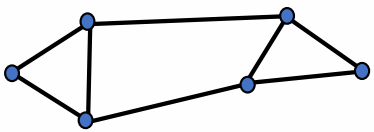
- Thus, the optimal solution for y is given by the corresponding eigenvector x, referred as the Fiedler vector

Spectral Clustering Algorithms

1. Pre-processing
   - Construct a matrix representation of the graph
2. Decomposition
   - Compute eigenvalues and eigenvectors of the matrix
   - Map each point to a lower-dimensional representation based on one or more eigenvectors
3. Grouping
   - Assign points to two or more clusters, based on the new representation

Spectral Partitioning Algorithm

- Pre-processing:
  - Build Laplacian matrix L of the graph



	1	2	3	4	5	6
1	3	-1	-1	0	-1	0
2	-1	2	-1	0	0	0
3	-1	-1	3	-1	0	0
4	0	0	-1	3	-1	-1
5	-1	0	0	-1	3	-1
6	0	0	0	-1	-1	2

- Decomposition:
  - Find eigenvalues λ and eigenvectors x of the matrix L
  - Map vertices to corresponding components of λ_2

$\lambda =$

0.0
1.0
3.0
3.0
4.0
5.0

$X =$

0.4	0.3	-0.5	-0.2	-0.4	-0.5
0.4	0.6	0.4	-0.4	0.4	0.0
0.4	0.3	0.1	0.6	-0.4	0.5
0.4	-0.3	0.1	0.6	0.4	-0.5
0.4	-0.3	-0.5	-0.2	0.4	0.5
0.4	-0.6	0.4	-0.4	-0.4	0.0

1	0.3
2	0.6
3	0.3
4	-0.3
5	-0.3
6	-0.6

Spectral Partitioning Algorithm

- Grouping:
  - Sort components of reduced 1-dimensional vector
  - Identify clusters by splitting the sorted vector in two
- How to choose a splitting point?
  - Naïve approaches: split at 0 or median value
  - More expensive approaches: Attempt to minimize normalized cut in 1-dimension (sweep over ordering of nodes induced by the eigenvector)

1	0.3
2	0.6
3	0.3
4	-0.3
5	-0.3
6	-0.6

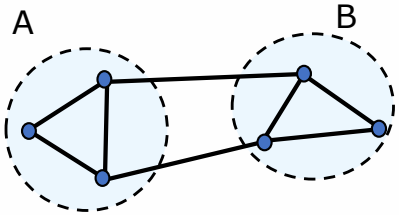
Split at 0:

Cluster A: Positive points

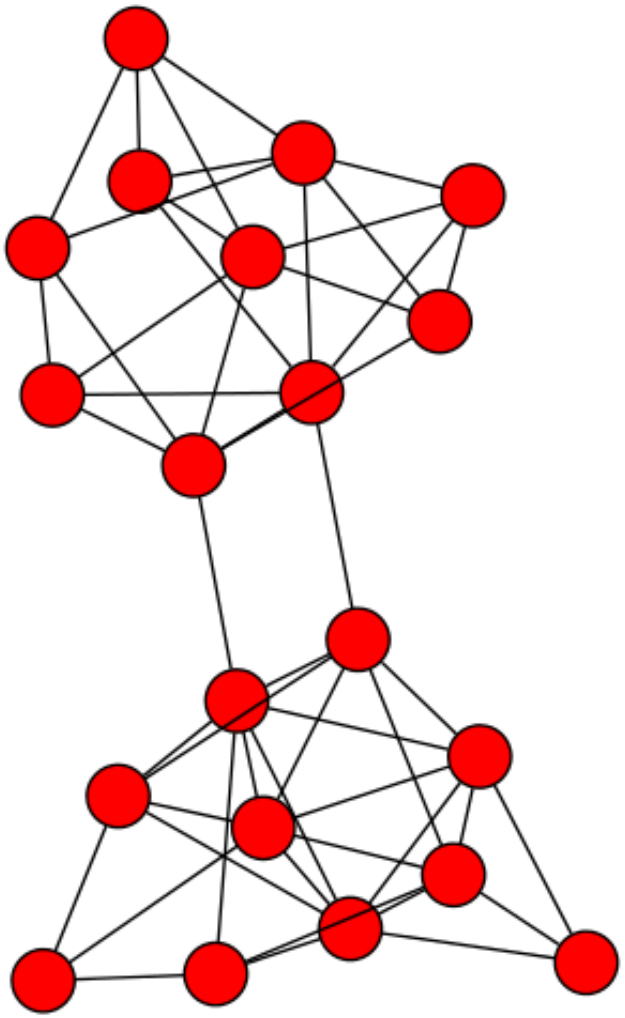
Cluster B: Negative points

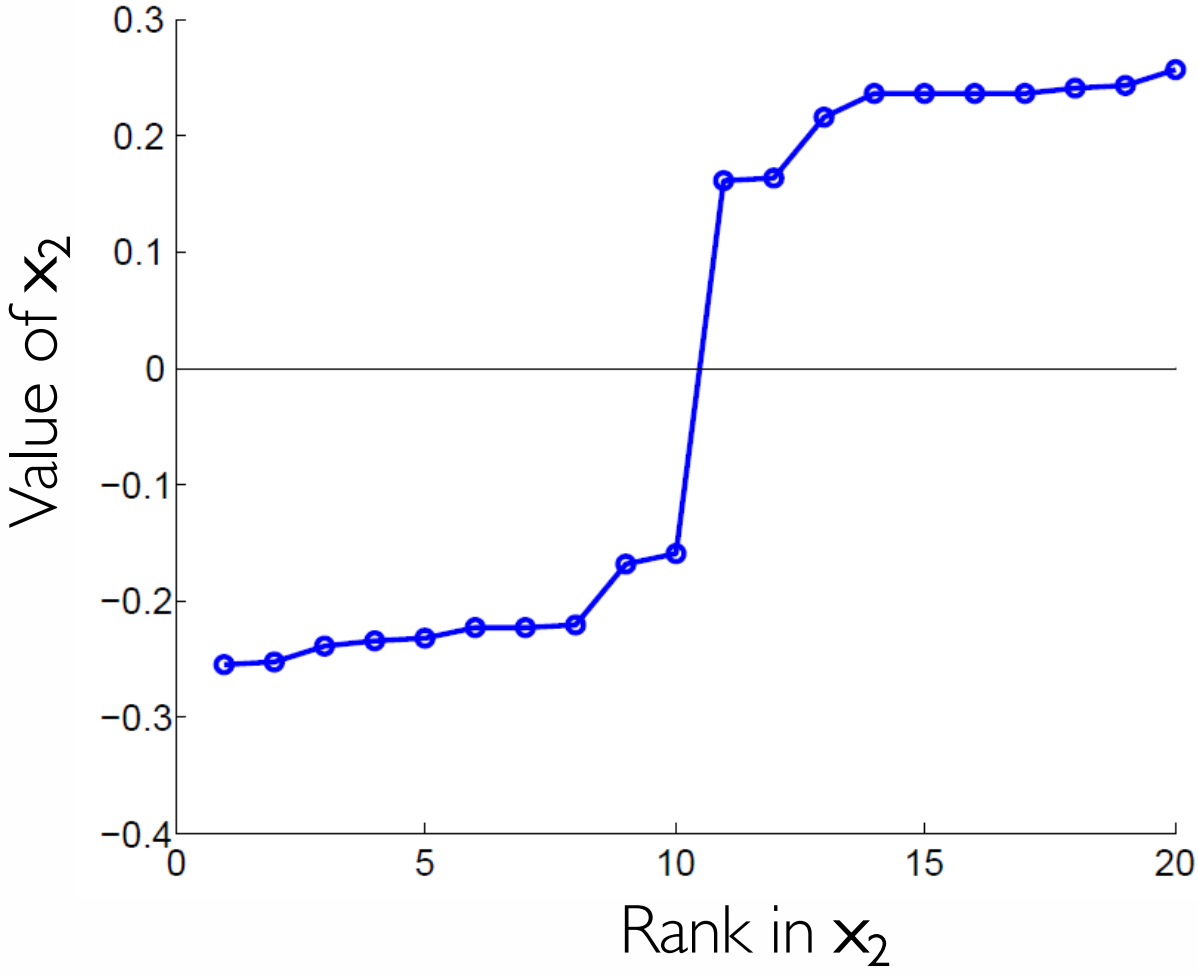
1	0.3
2	0.6
3	0.3

4	**-0.3**
5	-0.3
6	-0.6

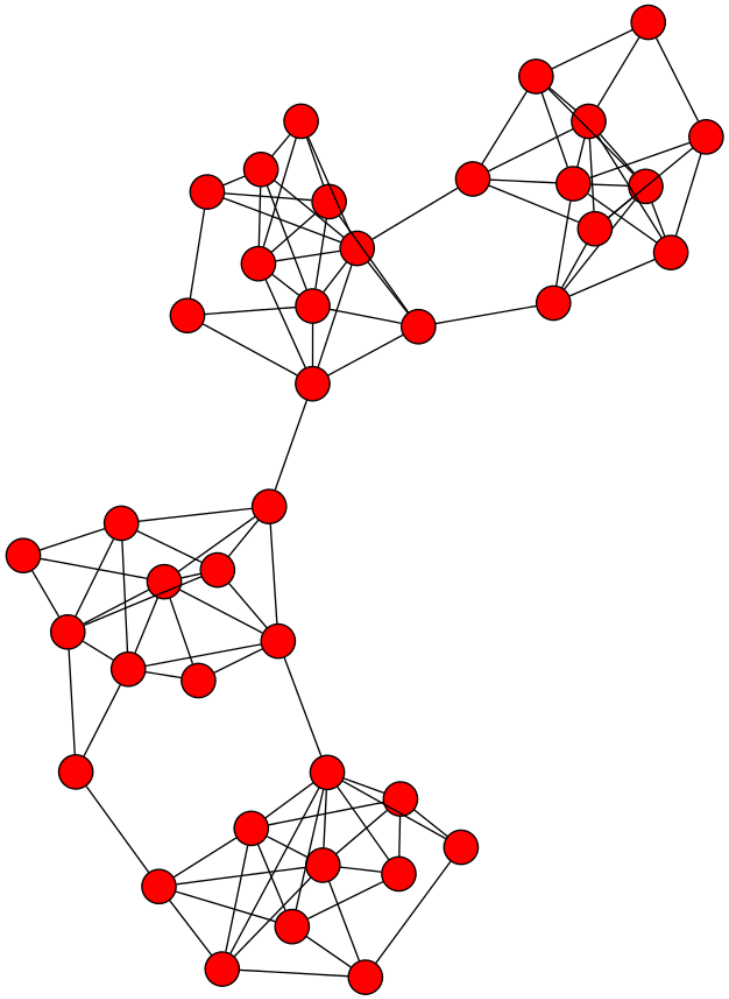


Example: Spectral Partitioning

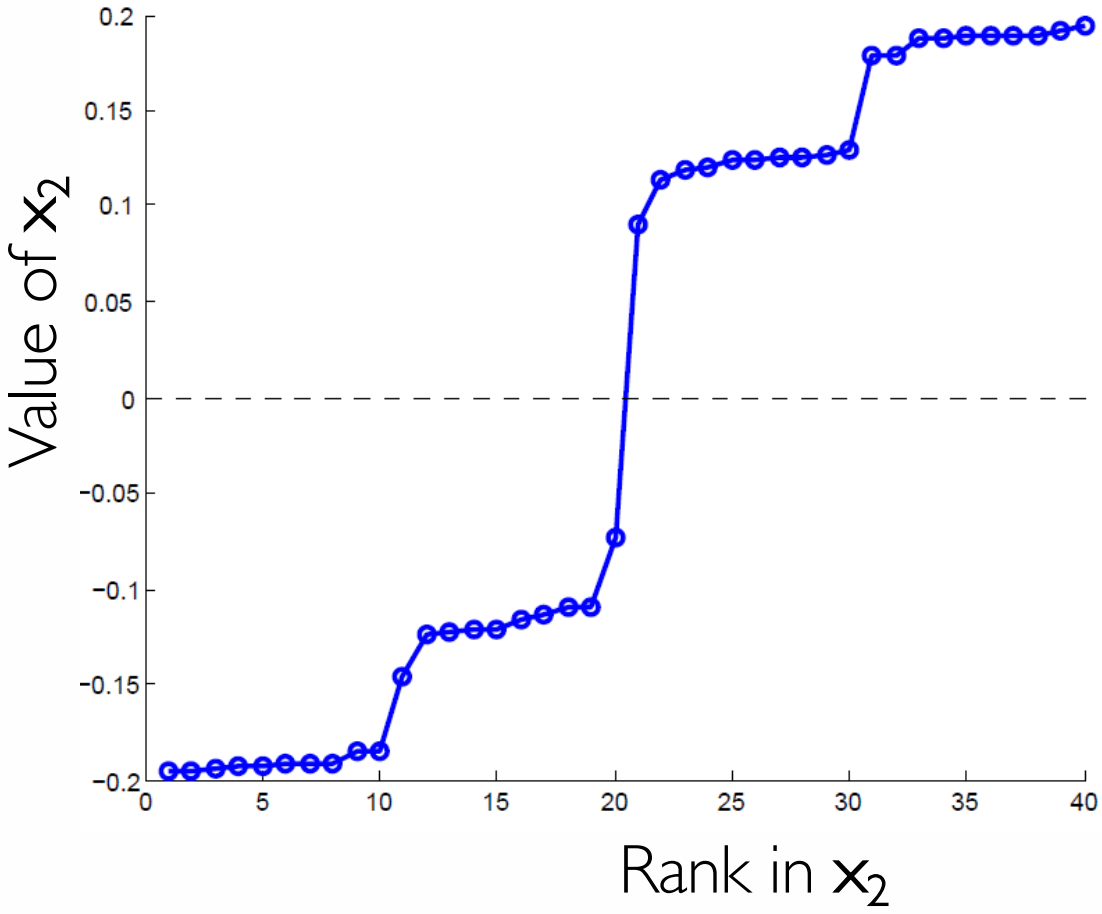




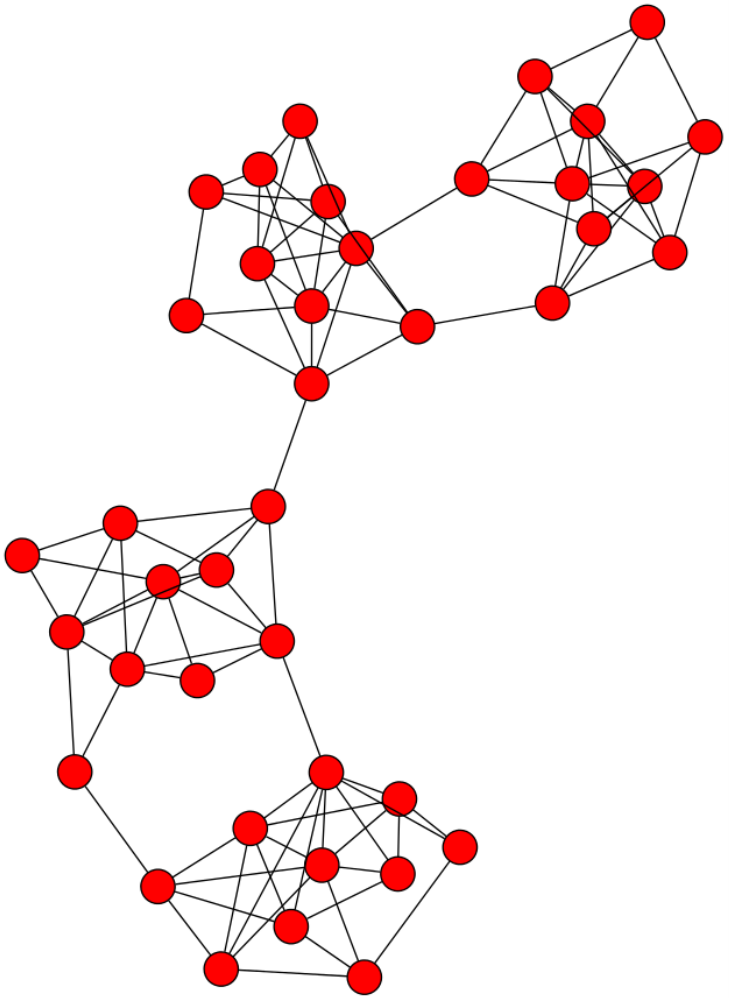
Example: Spectral Partitioning

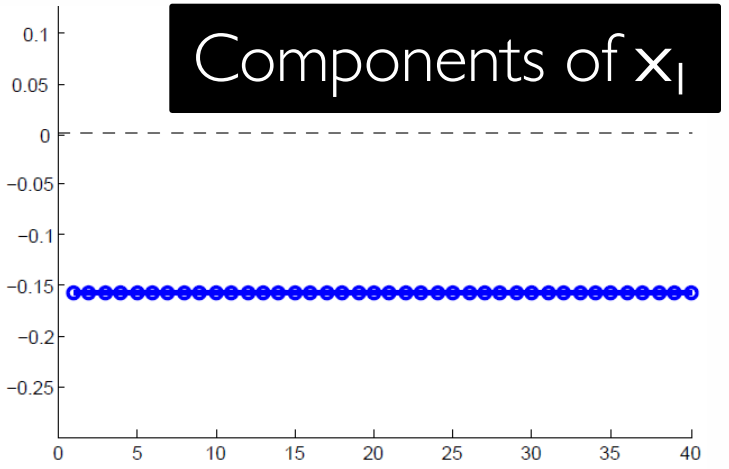


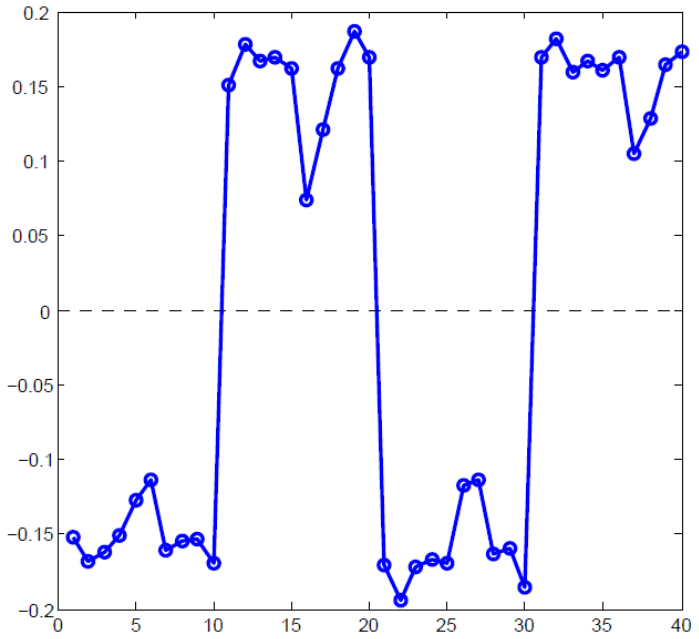
Components of x_2



Example: Spectral partitioning







Components of x_3

Example using R

Example #1


```
ComputeDegreeMatrix <- function(v) {
    n <- max(dim(v))
    m <- diag(n)
    d = v %*% rep(1,n)
    for(i in 1:n ) {
       m[i,i] = d[i,1]
    }
    return(m)
}

ComputeLaplacianMatrix <- function(v) {
  D = ComputeDegreeMatrix(v)
  L = D-v
  return(L)
}
```

Example #1


```
####    2 ----6
####  /   \    |
#### 1     4   |
####  \   /  \ |
####   3       5
```

```
G = rbind(
  c(0, 1, 1, 0, 0, 0),
  c(1, 0, 0, 1, 0, 1),
  c(1, 0, 0, 1, 0, 0),
  c(0, 1, 1, 0, 1, 0),
  c(0, 0, 0, 1, 0, 1),
  c(0, 1, 0, 0, 1, 0)
)
L = ComputeLaplacianMatrix(G)
E = eigen(L)
second_eigen_value = (E$value)[max(dim(L))-1]
second_eigen_vector = (E$vectors)[,max(dim(L))-1]
```

```
5.000000e-01  1.165734e-15  5.000000e-01  4.718448e-16 -5.000000e-01 -
5.000000e-01
```

Example #2


```
G = rbind(
  c(0, 0, 1, 0, 0, 1, 0, 0),
  c(0, 0, 0, 0, 1, 0, 0, 1),
  c(1, 0, 0, 1, 0, 1, 0, 0),
  c(0, 0, 1, 0, 1, 0, 1, 0),
  c(0, 1, 0, 1, 0, 0, 0, 1),
  c(1, 0, 1, 0, 0, 0, 1, 0),
  c(0, 0, 0, 1, 0, 1, 0, 1),
  c(0, 1, 0, 0, 1, 0, 1, 0)
)

L = ComputeLaplacianMatrix(G)

E = eigen(L)

second_eigen_value = (E$value)[max(dim(L))-1]
second_eigen_vector = (E$vectors)[,max(dim(L))-1]
```

```
5.000000e-01 -5.000000e-01  3.535534e-01 -3.885781e-16 -3.535534e-01
3.535534e-01 -4.996004e-16  -3.535534e-01
```

How Do We Partition a Graph into k Clusters?

- Two basic approaches:
- Recursive bi-partitioning [Hagen et al., '92]
  - Recursively apply bi-partitioning algorithm in a hierarchical divisive manner
  - Disadvantages: inefficient, unstable
- Cluster multiple eigenvectors [Shi-Malik, '00]
  - Build a reduced space from multiple eigenvectors
  - Commonly used in recent papers
  - A preferable approach…

Why Use Multiple Eigenvectors?

- Approximates the optimal cut [Shi-Malik, '00]
  - Can be used to approximate optimal k-way normalized cut
- Emphasizes cohesive clusters
  - Increases the unevenness in the distribution of the data
  - Associations between similar points are amplified, associations between dissimilar points are attenuated
  - The data begins to "approximate a clustering"
- Well-separated space
  - Transforms data to a new "embedded space", consisting of k orthogonal basis vectors
- Multiple eigenvectors prevent instability due to information loss

Run the Python notebooks
for this lecture