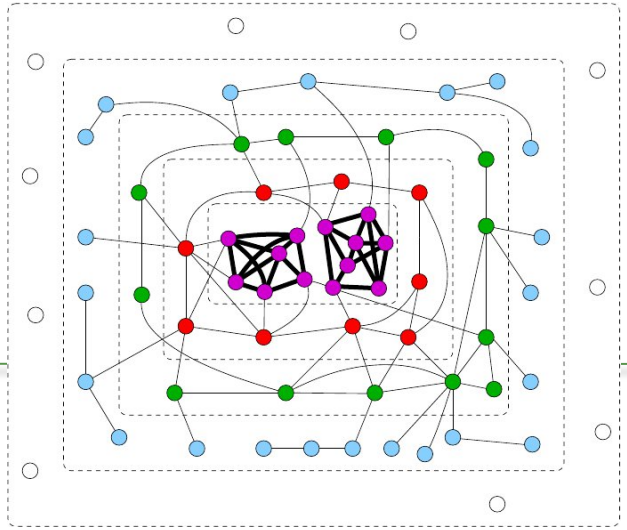
Graph Mining



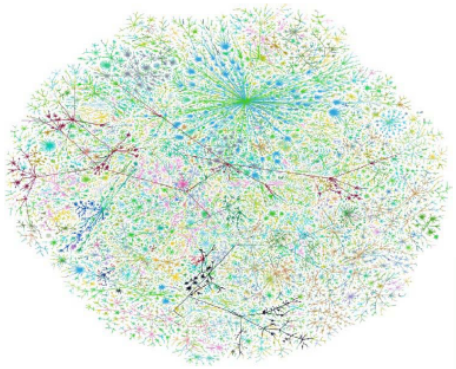
Michalis Vazirgiannis

LIX @ Ecole Polytechnique

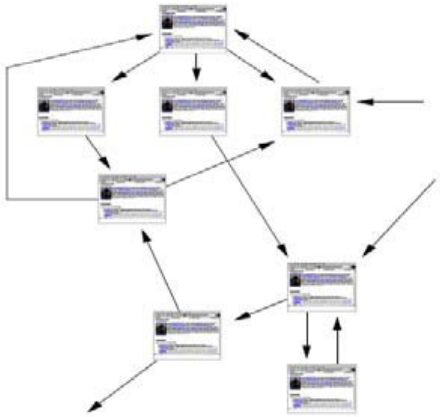
Outline

1. **Introduction & Motivation**
2. Community evaluation measures
3. Graph clustering
4. Graph classification

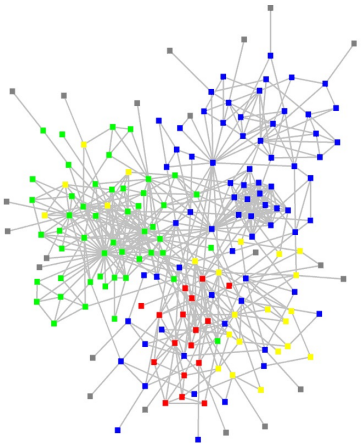
Networks are Everywhere



(a) Internet

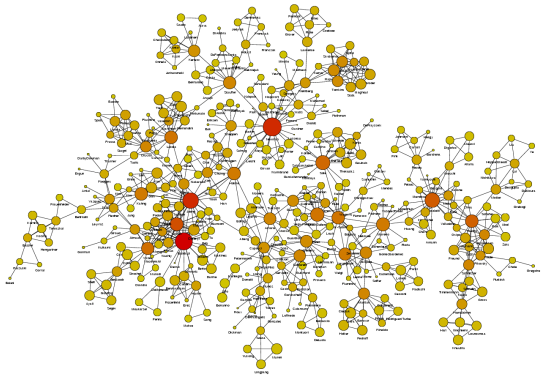


(b) World Wide Web

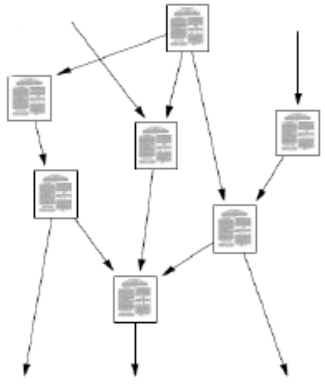


(c) Email network

(d) Social network



(e) Collaboration network



(f) Citation network

Social Networks Growth

- Social networking accounts for 1 of every 6 minutes spent online [http://blog.comscore.com/]
- One out of seven people on Earth is on Facebook
- People on Facebook install 20 million “Apps” every day
- YouTube has more than on billion unique users who visit every month (Oct. 2014)
- Users on YouTube spend a total of 6 billion hours per month (almost an hour for every person on Earth!
- Wikipedia hosts ~34 million articles and has over 91,000 contributors
- 500 million average Tweets per day occur on Twitter (Oct. 2014)

[http://www.jeffbullas.com/2011/09/02/20-stunning-social-media-tatistics/#q3eTJhr64rtD0tLF.99]

Graphs are ubiquitous!

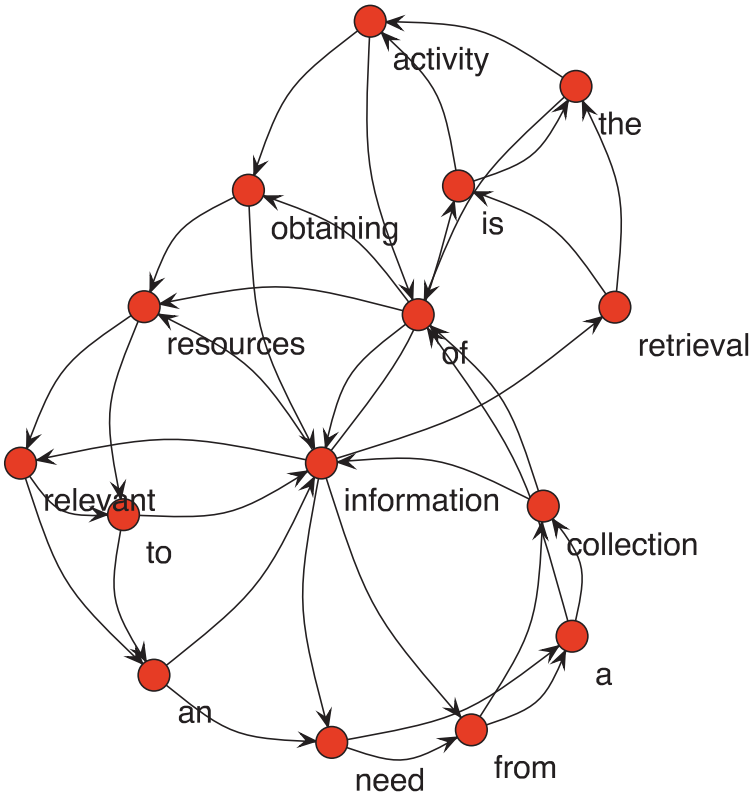
- **Technological networks:**
  - Internet
  - Telephone networks
  - Power grid
  - Road, airline and rail networks
- **Information networks:**
  - World Wide Web
  - Blog networks
  - Citation networks
- **Social networks:**
  - Collaboration networks
  - Organizational networks
  - Communication networks
- **Biological networks:**
  - Networks from Neuroscience
  - Protein-protein interaction networks
  - Gene regulatory networks
  - Food webs
- **Software networks:**
  - Call graphs
  - Software module/component interaction networks

Even representing text - Graph-of-word

information retrieval is the activity of obtaining

information resources relevant to an information need

from a collection of information resources



"Graph of word approach for ad-hoc information retrieval", F. Rousseau, M. Vazirgiannis, Best paper mention award ACM CIKM 2013

How Big are the graphs?

- AS by Skitter (AS-Skitter) - internet topology in 2005 (n = router, m = traceroute)
- LiveJournal (LJ) - social network (n = members, m = friendship)
- U.S. Road Network (USRD) - road network (n = intersections, m = roads)
- Billion Triple Challenge (BTC) - RDF dataset 2009 (n = object, m = relationship)
- WWW of UK (WebUK) - Yahoo Web spam dataset (n = pages, m = hyperlinks)
- Twitter graph (Twitter) - Twitter network (n = users, m = tweets)
- Yahoo! Web Graph (YahooWeb) - WWW pages in 2002 (n = pages, m = hyperlinks

AS-Skitter	**1.7**	**11**	**142 MB**
LJ	**4.8**	**69**	**337.2 MB**
USRD	**24**	**58**	**586.7 MB**
BTC	**165**	**773**	**5.3 GB**
WebUK	**106**	**1877**	**8.6 GB**
Twitter	**42**	**1470**	**24 GB**
YahooWeb	**1413**	**6636**	**120 GB**

Space/Time Complexity

Undirected graph space complexity

Adjaceny matrix: $\Theta(n^2)$

Adjacency list: $\Theta(n+4m)$

Edge List: $O(4m)$

Social scale...
1 billion vertices, 100 billion edges
111 PB adjacency matrix
2.92 TB adjacency list
2.92 TB edge list

Time complexity

Pagerank: $O(n^2)$

all shortest path (Floyd–Warshall algorithm): $O(n^3)$

...

Why Graph Mining

Understand the structure and dynamics of complex interaction systems

- Rich data (in terms of semantics)
- Large scale (big) data

Several application domains

- Community detection
- Web search
- Recommender systems
- Anomaly detection
- Prediction
- ...

Elements og Learning from Graph data

- **Graph models/ graph generators** graph generators (erdos reyni, preferential attachment, kronecker graphs)
- **Node base metrics**: - Ranking algorithms (Pagerank), Ranking evaluation measures (Kendal Tau, NDCG),
- **Graph exploration/preprocessing**: degree distributions, visualization
- **Supervised learning for graphs**: link prediction, graph kernels, graph classification
- **Unsupervised learning:** clustering, community mining, degeneracy.
- **Learning theory in graphs:** model ensembling/selection…

Communities in Real Networks

- Real networks are not **random graphs** (e.g., the Erdos-Renyi random graph model)
- Present fascinating patterns and properties:
  - The **degree distribution** is skewed, following a power-law
  - The **average distance** between the nodes of the network is short (the small-world phenomenon)
  - The edges between the nodes may not represent reciprocal relations, forming **directed networks with non-symmetric links**
  - **Edge density** is inhomogeneous (groups of nodes with high concentration of edges within them and low concentration between different groups

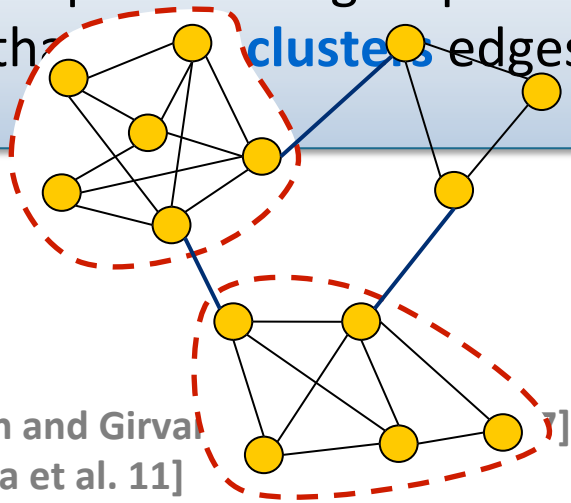
Outline

1. Introduction & Motivation
2. **Community evaluation measures**
3. Graph clustering
4. Graph classification

Basics

- The notion of **community structure** captures the tendency of nodes to be organized into modules (communities, clusters, groups)
  - Members within a community are **more similar** among each other
- Typically, the communities in graphs (networks) correspond to **densely connected** entities (nodes)

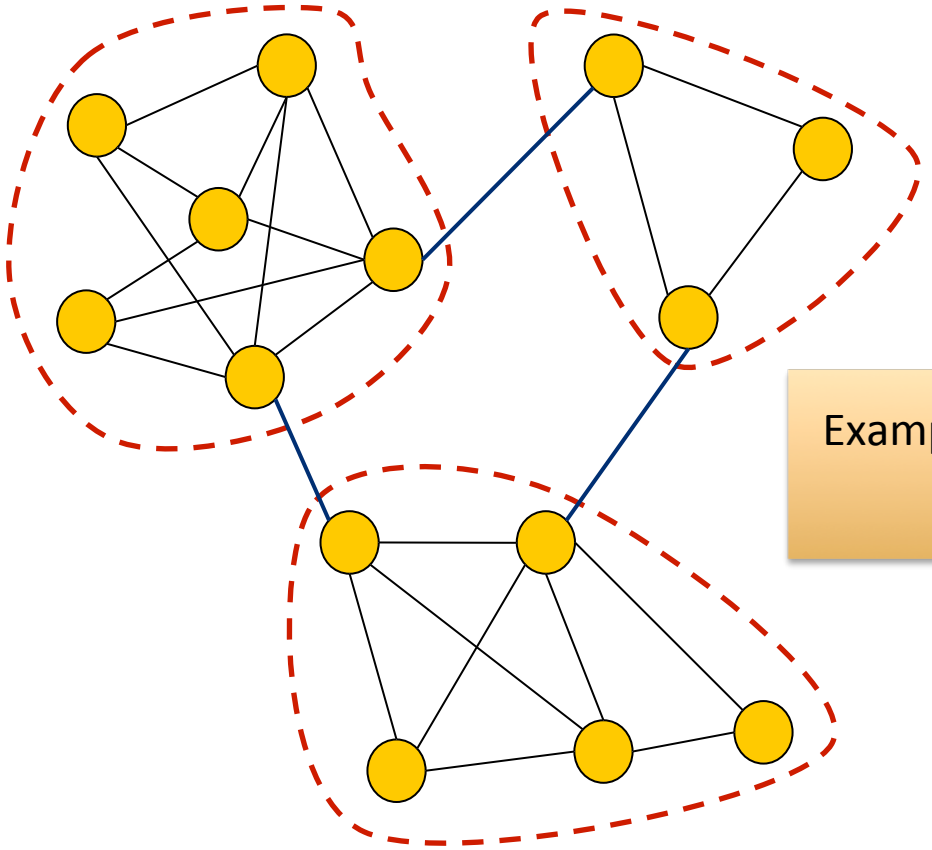
A community corresponds to a group of nodes with more **intra-cluster** edges than **inter-cluster** edges



Example graph with three communities

[Newman '03], [Newman and Girvan], [Fortunato '10], [Danon et al. '05], [Coscia et al. 11]

Schematic representation of communities



Example graph with three communities

Community detection in graphs

- How can we extract the inherent communities of graphs?
- Typically, a two-step approach
  1. Specify a **quality measure** (evaluation measure, objective function) that quantifies the desired properties of communities
  2. Apply **algorithmic techniques** to assign the nodes of graph into communities, optimizing the objective function
- Several measures for quantifying the quality of communities have been proposed
- They mostly consider that communities are set of nodes with many edges between them and few connections with nodes of different communities
  - Many possible ways to formalize it

Community evaluation measures

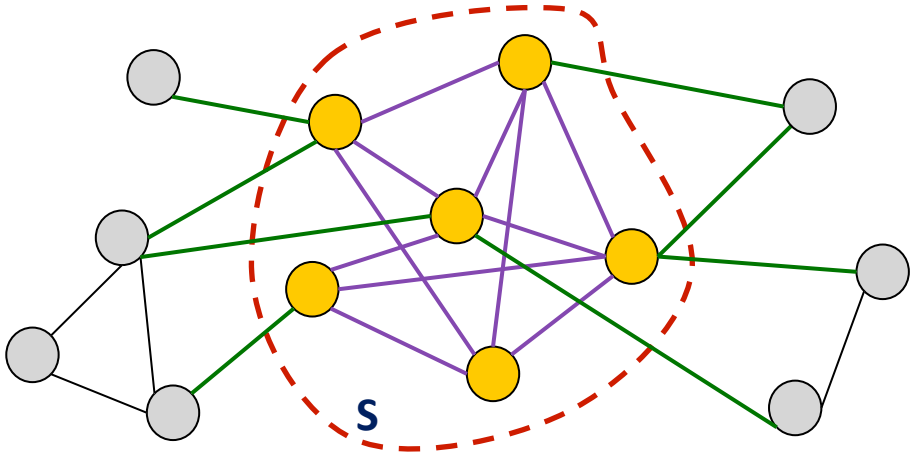
- Focus on
  - Intra-cluster edge density (# of edges within community),
  - Inter-cluster edge density (# of edges across communities)
  - Both two criteria

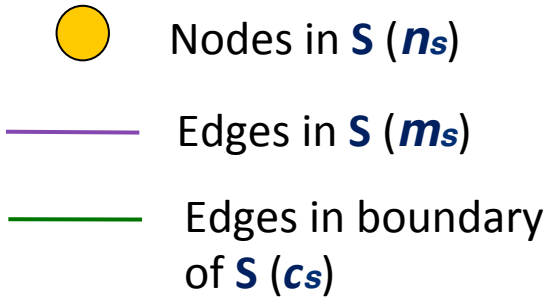
- We group the community evaluation measures according to
  - Evaluation based on **internal** connectivity
  - Evaluation based on **external** connectivity
  - Evaluation based on **internal and external** connectivity
  - Evaluation based on **network model**

[Leskovec et al. '10], [Yang and Leskovec '12], [Fortunato '10]

Notation

- **G = (V, E)** is an undirected graph, **|V| = n**, **|E| = m**
- **S** is the set of nodes in the cluster
- $n_S = |S|$ is the number of nodes in **S**
- m_S is the number of edges in **S**, $m_s = \left|\{(u,v): u \in S, v \in S\}\right|$
- c_S is the number of edges on the boundary of **S**, $c_s = \left|\{(u,v): u \in S, v \notin S\}\right|$
- d_u is the degree of node u
- $f(S)$ represent the clustering quality of set S



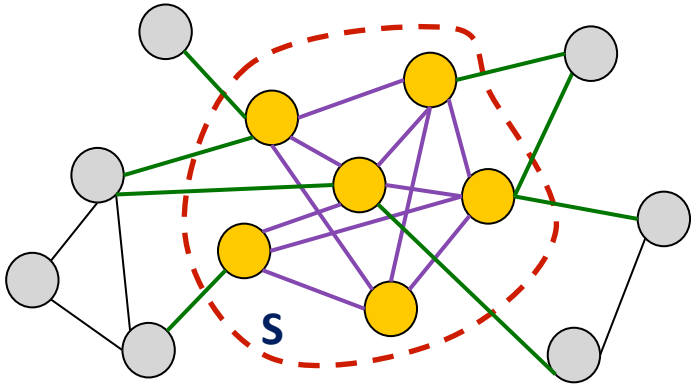


Evaluation based on internal connectivity (1)

- **Internal density** [Radicchi et al. '04]

$$f(S) = \frac{m_s}{n_s(n_s - 1)/2}$$

Captures the internal edge density of community **S**



- **Edges inside** [Radicchi et al. '04]

$$f(S) = m_s$$

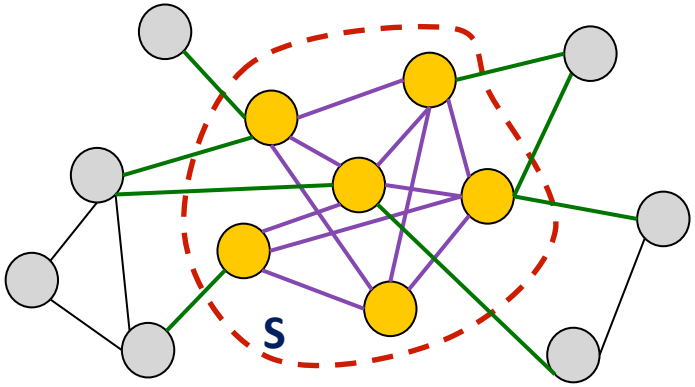
Number of edges between the nodes of **S**

Evaluation based on external connectivity

- **Expansion** [Radicchi et al. '04]

$$f(S) = \frac{c_s}{n_s}$$

Measures the number of edges per node that point outside **S**



- **Cut ratio** [Fortunato '10]

$$f(S) = \frac{c_s}{n_s(n - n_s)}$$

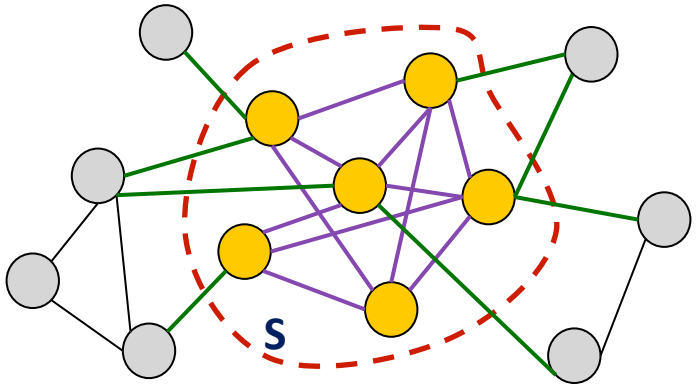
Fraction of existing edges – out of all possible edges – that leaving **S**

Evaluation based on internal and external connectivity (1)

Conductance [Chung '97]

$$f(S) = \frac{c_s}{2m_s + c_s}$$

Measures the fraction of total edge volume that points outside **S**



Normalized cut [Shi and Malic '00]

$$f(S) = \frac{c_s}{2m_s + c_s} + \frac{c_s}{2(m - m_s) + c_s}$$

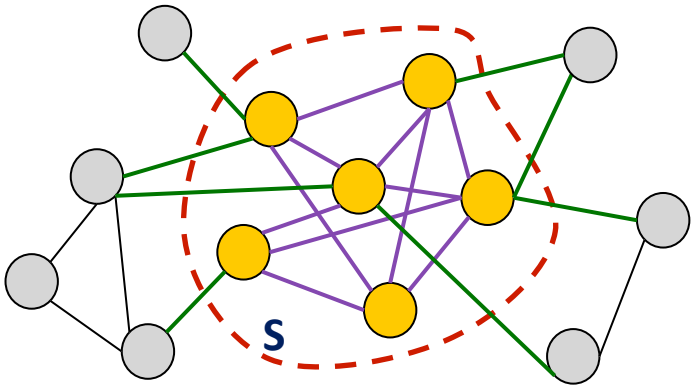
Measures the fraction of total edge volume that points outside **S** normalized by the size of **S**

Evaluation based on internal connectivity (3)

- **Triangle participation ratio (TPR)** [Yang and Leskovec '12]

$$f(S) = \frac{\left|\left\{u : u \in S, \left\{(v,w) : v,w \in S, (u,v) \in E, (u,w) \in E, (v,w) \in E\right\} \neq \varnothing\right\}\right|}{n_s}$$

Fraction of nodes in **S** that belong to a triangle



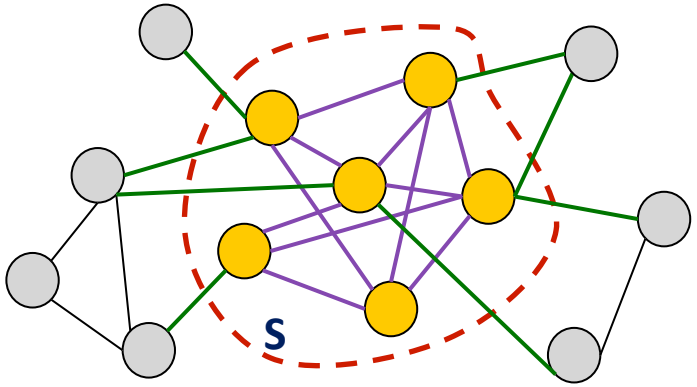
Evaluation based on network model

Modularity [Newman and Girvan '04], [Newman '06]

$$f(S) = \frac{1}{4}\left(m_s - E\left(m_s\right)\right)$$

Measures the difference between the number of edges in **S** and the expected number of edges **E(m_s)** in case of a configuration model

- Typically, a random graph model with the same degree sequence



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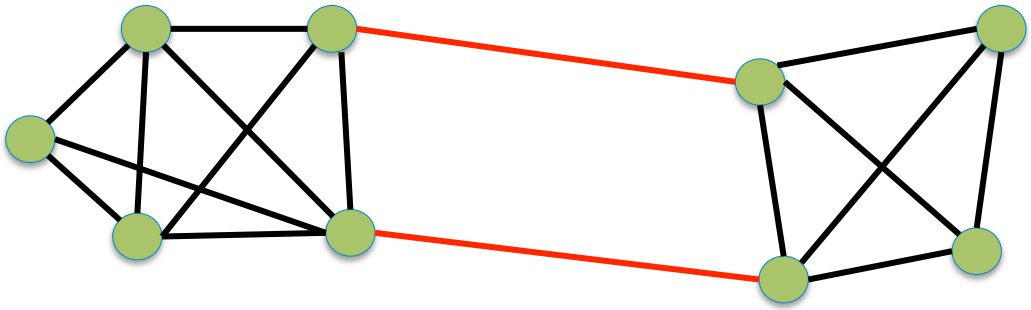
Notations

- Given Graph G=(V,E) undirected:
  - Vertex Set V={v_1,…..v_n}, Edge e_{ij} between v_i and v_j
    - we assume weight $w_{ij}>0$ for e_{ij}
  - |V| : number of vertices
  - d_i degree of v_i : $d_i = \sum_{v_j \in V} w_{ij}$
  - $v(V) = \sum_{v_i \in V} d_i$
  - for $A \subset V$ $\bar{A} = V - A$
  - Given $A, B \subset V$ & $A \cap B = \emptyset, w(A,B) = \sum_{v_i \in A, vj \in B} w_{ij}$
  - D : Diagonal matrix where $D(i,i) = d_i$
  - W : Adjacency matrix $W(i,j) = w_{ij}$

Graph-Cut

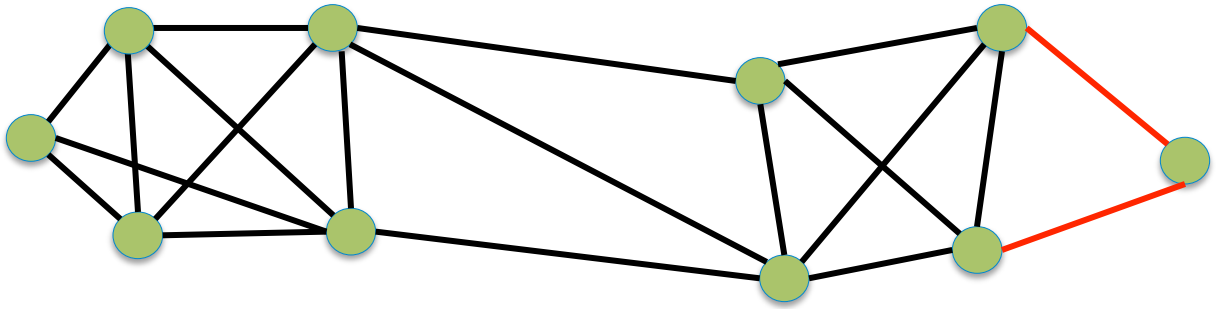
- For k clusters:
  - $cut(A_1, .., Ak) = 1/2 \sum_{i=1}^{k} w(Ai, \overline{A_i})$
    - undirected graph:1/2 we count twice each edge



- Min-cut:Minimize the edges' weight a cluster shares with the rest of the graph

Min-Cut

- Easy for k=2 : Mincut(A_1,A_2)
  - Stoer and Wagner: "A Simple Min-Cut Algorithm"
- In practice one vertex is separated from the rest
  - The algorithm is drawn to outliers



Normalized Graph Cuts

- We can normalize by the size of the cluster (size of sub-graph) :
  - number of Vertices (Hagen and Kahng, 1992):

    $$Ratiocut(A_1, \dots Ak) = \sum_{i=1}^{k} \frac{cut(Ai, \overline{A_i})}{|Ai|}$$

  - sum of weights (Shi and Malik, 2000) :

    $$Ncut(A_1, \dots Ak) = \sum_{i=1}^{k} \frac{cut(Ai, \overline{A_i})}{v(A_i)}$$

- Optimizing these functions is NP-hard
- Spectral Clustering provides solution to a relaxed version of the above

From Graph Cuts to Spectral Clustering

- For simplicity assume k=2:
  - Define $f: V \to \mathbb{R}$ for Graph G :

$$f_i = \begin{cases} 1 & v_i \in A \\ -1 & v_i \in \overline{A} \end{cases}$$

- Optimizing the original cut is equivalent to an optimization of:

$$\sum_{i,j=1}^{n} w_{ij}\left(f_i - f_j\right)^2$$

$$= \sum_{v_i \in A, vj \in \overline{A}} w_{ij}(1+1)^2 + \sum_{v_i \in \overline{A}, vj \in A} w_{ij}(-1-1)^2$$

$$= \mathbf{8} * \boldsymbol{cut}\left(\boldsymbol{A}, \overline{\boldsymbol{A}}\right)$$

Graph Laplacian

- How is the previous useful in Spectral clustering?

$$\sum_{i,j=1}^{n} w_{ij}(f_i - fj)^2$$

$$= \sum_{i,j=1}^{n} w_{ij} {f_i}^2 - 2\sum_{i,j=1}^{n} w_{ij} f_i f_j + \sum_{i,j=1}^{n} w_{ij} {f_j}^2$$

$$= \sum_{i,j=1}^{n} d_i {f_i}^2 - 2\sum_{i,j=1}^{n} w_{ij} f_i f_j + \sum_{i,j=1}^{n} d_j {f_j}^2$$

$$= 2\left(\sum_{i,j=1}^{n} d_{ii} {f_i}^2 - \sum_{i,j=1}^{n} w_{ij} f_i f_j\right)$$

$$= 2\left(\boldsymbol{f^T D f} - \boldsymbol{f^T W f}\right) = 2\boldsymbol{f^T}(\boldsymbol{D} - \boldsymbol{W})\boldsymbol{f} = 2\boldsymbol{f^T L f}$$

- **f:**a single vector with the cluster assignments of the vertices
- **L=D-W :** the Laplacian of a graph

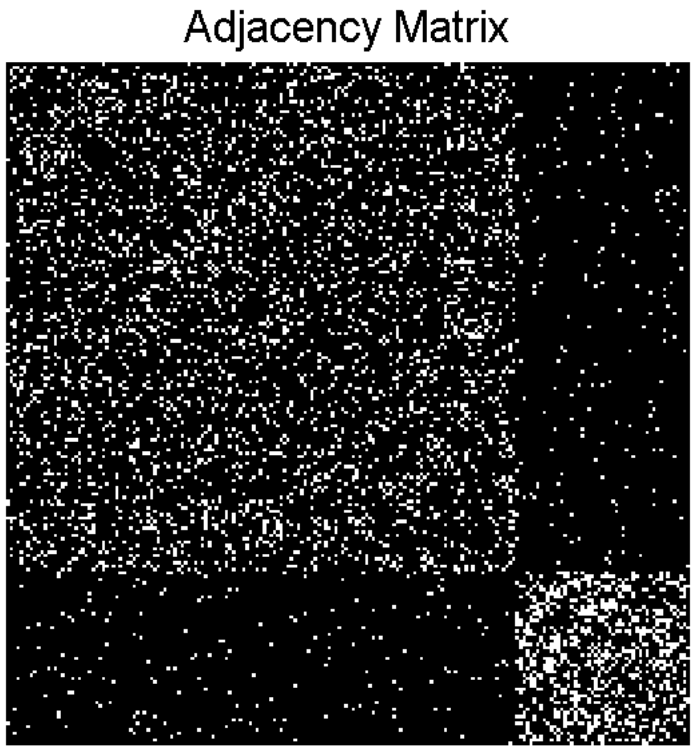
Properties of L

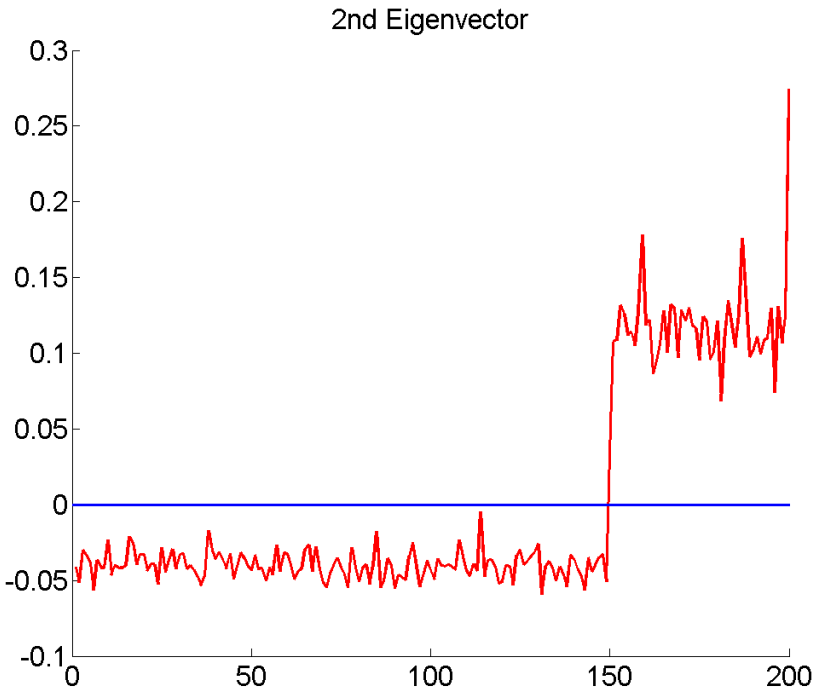
- L is
  - Symmetric
  - Positive
  - Semi-definite
- The smallest eigenvalue of L is 0
  - The corresponding eigenvector is $\mathbb{1}$
- L has n non-negative, real valued eigenvalues
  - $0 = \lambda 1 \leq \lambda 2 \leq \ldots \leq \lambda n$

Two Way Cut from the Laplacian

- We could solve $min_f f^T L f$ where $f \in \{-1,1\}^n$
- NP-Hard for discrete cluster assignments
  - Relax the constraint $to\ f \in R^n$:
    $min_f f^T L f$ subject to $f^T f = n$
- The solution to this problem is given by:
  - (**Rayleigh-Ritz Theorem**) the eigenvector corresponding to smallest eigenvalue: 0 and the corresponding eigenvector (full of 1s) offers no information
- We use the second eigenvector as an approximation
  - $f_i > 0$ the vertex belongs to one cluster , $f_i < 0$ to the other

Example


Adjacency Matrix


2nd Eigenvector
0.3
0.25
0.2
0.15
0.1
0.05
0
-0.05
-0.1
0
50
100
150
200

Ratio Cut

- $Ratiocut(A_1, \dots Ak) = \sum_{i=1}^{k} \frac{cut(Ai, \overline{A_i})}{|Ai|}$
  - Define $f: V \to \mathbb{R}$ for Graph G :

$$f_i = \begin{cases} \sqrt{\frac{|\overline{A}|}{|A|}} & vi \in A \\ -\sqrt{\frac{|A|}{|\overline{A}|}} & v_i \in \overline{A} \end{cases}$$

  - $\sum_{i,j=1}^{n} w_{ij}(f_i - fj)^2 = 2cut(\mathrm{A}, \overline{A}) \left(\sqrt{\frac{|\overline{A}|}{|A|}} + \sqrt{\frac{|A|}{|\overline{A}|}} + 2 \right)$

    $= 2|V|Ratiocut(A, \overline{A})$

Ratio Cut

- We have $min_f f^T L f$ subject to

$$f^T 1 = 0, \; fTf = n$$

$$f^T 1 = \sum_i^n f_i = \sum_{v_i \in A} \sqrt{\frac{|\bar{A}|}{|A|}} + \sum_{v_i \in \bar{A}} - \sqrt{\frac{|A|}{|\bar{A}|}} = |A| \sqrt{\frac{|\bar{A}|}{|A|}} - |\bar{A}| \sqrt{\frac{|A|}{|\bar{A}|}} = 0$$

$$f^T f = \sum_i^n f_i^2 = |\bar{A}| + |A| = n$$

- The second smallest eigenvalue of $Lf = \lambda f$ approximates the solution

Normalized Cut

- $Ncut(A_1, \dots Ak) = \sum_{i=1}^{k} \frac{cut(Ai, \overline{A_i})}{v(A_i)}$
- Define $f: V \rightarrow \mathbb{R}$ for Graph G :

$$f_i = \begin{cases} \sqrt{\frac{v(\overline{A})}{v(A)}} & vi \in A \\ -\sqrt{\frac{v(A)}{v(\overline{A})}} & vi \in \overline{A} \end{cases}$$

- $\sum_{i,j=1}^{n} w_{ij}(f_i - fj)^2 = 2cut(\mathrm{A}, \overline{A}) \left(\sqrt{\frac{v(\overline{A})}{v(A)}} + \sqrt{\frac{v(A)}{v(\overline{A})}} + 2 \right)$

$$= 2v(\mathrm{V})\mathrm{Ncut}(\mathrm{A}, \overline{A})$$

Normalized Cut

- Similarly: $\min_f f^T L f$ subject to

$$f^T D 1 = 0, f^T D f = v(V)$$

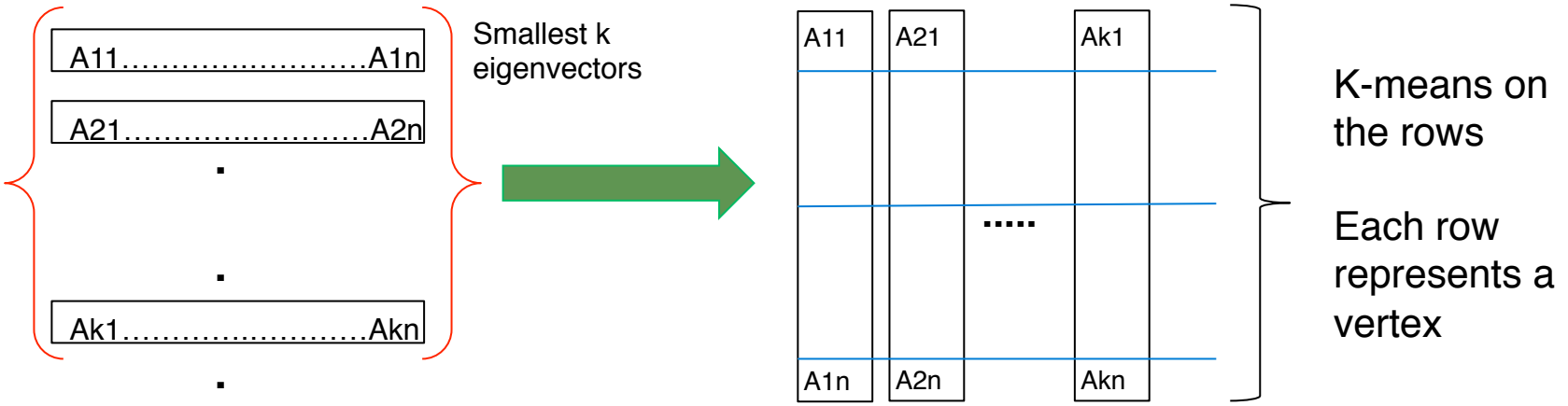
- Assume $h = D^{1/2} f$
  - $min_h h^T D^{-1/2} L D^{-1/2} h$ subject to

$$h^T D^{1/2} 1 = 0, \qquad h^T h = v(V)$$

  - The answer is in the eigenvector of the second smallest eigenvalue of $L_{sym} = D^{-1/2} L D^{-1/2}$
    Shi and Malik (2000)
- L_{sym} is the normalized Laplacian
  - has n non-negative, real valued eigenvalues
  - $0 = \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$

Multi-Way Graph Partition

- The cluster assignment is given by the smallest k eigenvectors of L
- The real values need to be converted to cluster assignments
  - We use k-means to cluster the rows
  - We can substitute *L* with L_{sym}



References – Graph clustering

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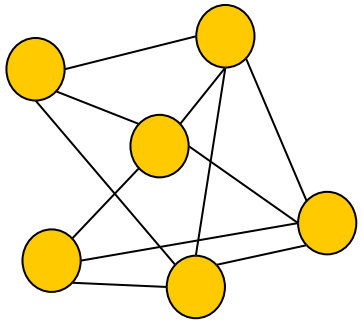
Graph Clustering Algorithms

- Spectral Clustering
- **Modularity Based Methods**

Main idea

- **Modularity** function [Newman and Girvan '04], [Newman '06]
- Initially introduced as a measure for assessing the strength of communities
  - **Q = (fraction of edges within communities) –**

    (expected number of edges within communities)
- What is the **expected** number of edges?
- Consider a configuration model
  - **Random graph** model with the same degree distribution
  - Let P_{ij} = probability of an edge between nodes **i** and **j** with degrees k_i and k_j respectively
  - Then $P_{ij} = k_i k_j / 2m$, where $m = |E| = \frac{1}{2} \sum_i k_i$



Formal definition of modularity

Modularity Q

$$Q = \frac{1}{2m} \sum_{ij} \left(A_{ij} - \frac{k_i k_j}{2m} \right) \delta(C_i, C_j)$$

where

- **A** is the adjacency matrix
- k_i, k_j the degrees of nodes **i** and **j** respectively
- **m** is the number of edges
- C_i is the community of node **i**
- **δ(.)** is the Kronecker function: 1 if both nodes **i** and **j** belong on the same community ($C_i = C_j$), 0 otherwise

[Newman and Girvan '04], [Newman '06]

Properties of modularity

$$Q = \frac{1}{2m}\sum_{ij}\left(A_{ij} - \frac{k_i k_j}{2m}\right)\delta(c_i, c_j)$$

- **Larger** modularity **Q** indicates **better** communities (more than random intra-cluster density)
  - The community structure would be better if the number of internal edges exceed the expected number
- Modularity value is always **smaller than 1**
- It can also take **negative values**
  - E.g., if each node is a community itself
  - No partitions with positive modularity → No community structure
  - Partitions with large negative modularity → Existence of subgraphs with small internal number of edges and large number of inter-community edges

[Newman and Girvan '04], [Newman '06], [Fortunato '10]

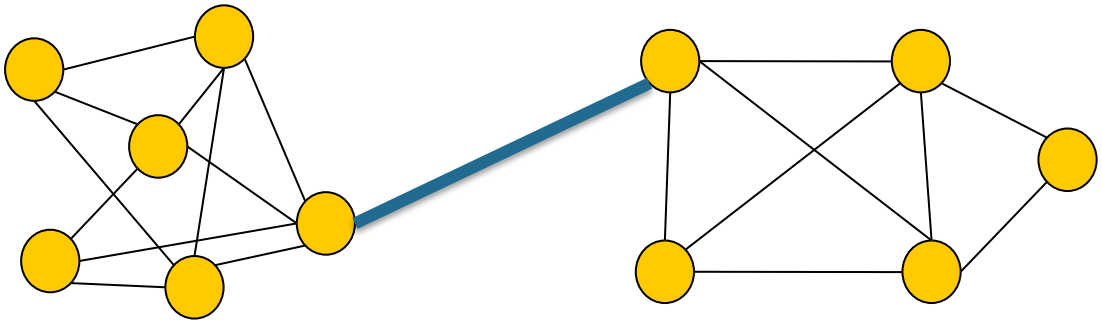
Applications of modularity

- Modularity can be applied:
  - As **quality function** in clustering algorithms
  - As **evaluation measure** for comparison of different partitions or algorithms
  - As a community detection tool itself
    - **Modularity optimization**
  - As criterion for reducing the size of a graph
    - Size reduction preserving modularity [Arenas et al. '07]

[Newman and Girvan '04], [Newman '06], [Fortunato '10]

Modularity-based community detection

- Modularity was first applied as a **stopping criterion** in the Newman-Girvan algorithm
- Newman-Girvan algorithm [Newman and Girvan '04]
  - A **divisive** algorithm (detect and remove edges that connect vertices of different communities)
  - **Idea:** try to identify the edges of the graph that are most between other vertices → responsible for connecting many node pairs
  - Select and remove edges based to the value of **betweenness centrality**
  - **Betweenness centrality:** number of **shortest paths** between every pair of nodes, that pass through an edge



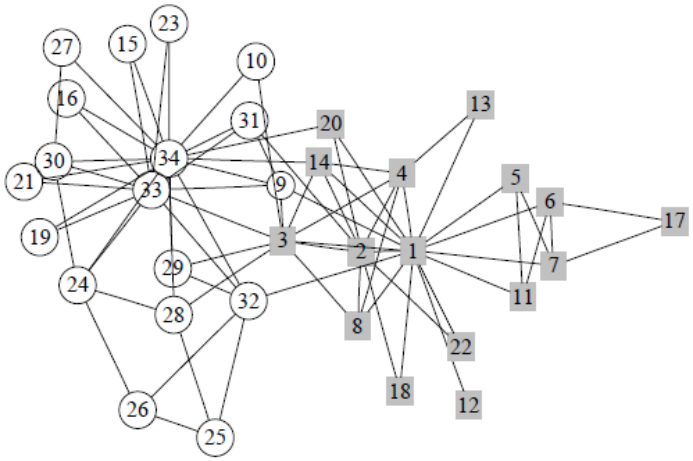
Edge betweenness is higher for edges that connect different communities

Newman-Girvan algorithm (1)

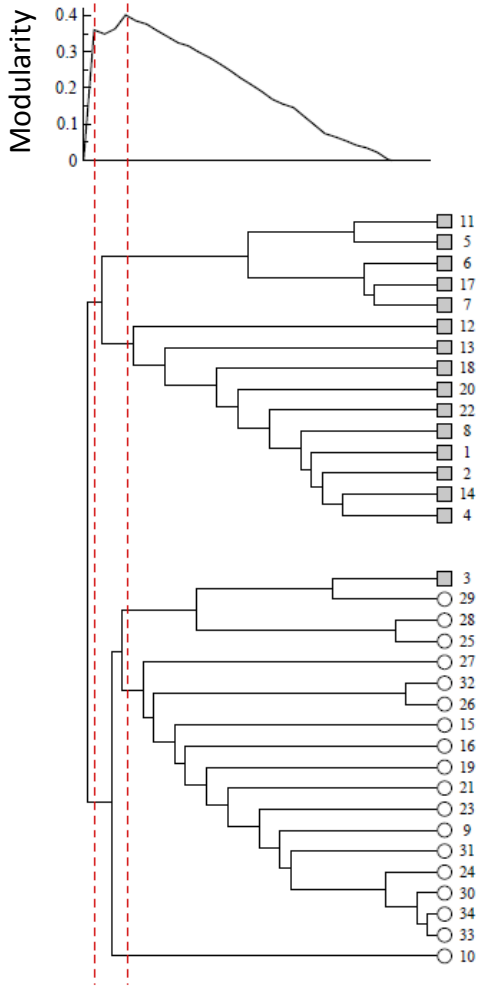
- **Basic steps:**
  1. Compute betweenness centrality for all edges in the graph
  2. Find and remove the edge with the highest score
  3. Recalculate betweenness centrality score for the remaining edges
  4. Go to step 2
- How do we know if the produced communities are **good ones** and stop the algorithm?
  - The output of the algorithm is in the form of a **dendrogram**
  - Use **modularity** as a criterion to cut the dendrogram and terminate the algorithm (Q ~= 0.3-0.7 indicates good partitions)
- Complexity: **$O(m^2n)$** (or **$O(n^3)$** on a sparse graph)

[Newman and Girvan '04], [Girvan and Newman '02]

Newman-Girvan algorithm (2)



Zachary's karate club



Community structure

[Newman and Girvan '04]

Modularity optimization

- High values of modularity indicate good quality of partitions
- **Goal:** find the partition that corresponds to the maximum value of modularity
- **Modularity maximization** problem
  - Computational difficult problem **[Brandes et al. '06]**
  - Appoximation techniques and heuristics
- Four main categories of techniques
  1. Greedy techniques
  2. **Spectral optimization**
  3. Simulated annealing
  4. Extremal optimization

[Fortunato '10]

Spectral optimization (1)

- **Idea:** Spectral techniques for modularity optimization
- **Goal:** Assign the nodes into two communities, **X** and **Y**
- Let $s_i, \forall i \in V$ be an indicator variable where **s_i = +1** if **i** is assigned to **X** and **s_i = -1** if **i** is assigned to **Y**

$$Q = \frac{1}{2m}\sum_{ij}\left(A_{ij} - \frac{k_i k_j}{2m}\right)\delta(C_i, C_j)$$

$$= \frac{1}{4m}\sum_{ij}\left(A_{ij} - \frac{k_i k_j}{2m}\right)(s_i s_j + 1)$$

$$= \frac{1}{4m}\sum_{ij} B_{ij} s_i s_j = \frac{1}{4m} s^T \mathrm{B} s$$

- **B** is the **modularity matrix**

$$B_{ij} = A_{ij} - \frac{k_i k_j}{2m}$$

[Newman '06], [Newman '06b]

Spectral optimization (2)

- Modularity matrix **B**

$$B_{ij} = A_{ij} - \frac{k_i k_j}{2m}$$

- Vector **s** can be written as a linear combination of the eigenvectors u_i of the modularity matrix **B**

$$s = \sum_i a_i u_i \quad \text{where} \quad a_i = u_i^T s$$

- Modularity can now expressed as

$$Q = \frac{1}{4m} \sum_i a_i u_i^T B \sum_j a_j u_j^T = \frac{1}{4m} \sum_{i=1}^{n} \left(u_i^T s \right)^2 \beta_i$$

Where β_i is the eigenvalue of **B** corresponding to eigenvector u_i

[Newman '06], [Newman '06b]

Spectral optimization (3)

- Spectral modularity optimization algorithm
  1. Consider the eigenvector $\mathbf{u_1}$ of **B** corresponding to the largest eigenvalue
  2. Assign the nodes of the graph in one of the two communities **X** ($\mathbf{s_i = +1}$) and **Y** ($\mathbf{s_i = -1}$) based on the **signs** of the corresponding components of the eigenvector

$$s_i = \begin{cases} 1 & if\ u_1(i) \geq 0 \\ -1 & if\ u_1(i) < 0 \end{cases}$$

  - More than two partitions?
  1. **Iteratively**, divide the produced partitions into two parts
  2. If at any step the split does not contribute to the modularity, leave the corresponding subgraph as is
  3. End when the entire graph has been splinted into no further divisible subgraphs
  - Complexity: **$O(n^2 \log n)$** for sparse graphs

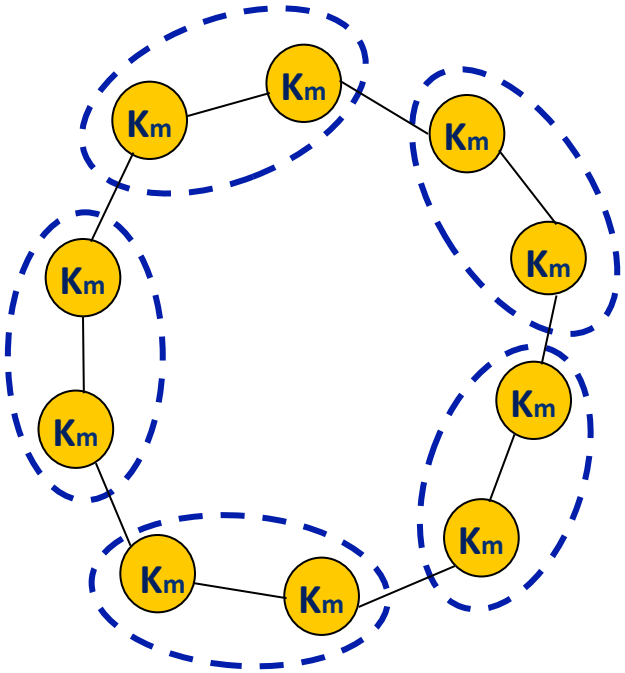
[Newman '06], [Newman '06b]

Extensions of modularity

- Modularity has been extended in several directions
  - Weighted graphs **[Newman '04]**
  - Bipartite graphs **[Guimera et al '07]**
  - Directed graphs (next in this tutorial) **[Arenas et al. '07], [Leicht and Newman '08]**
  - Overlapping community detection (next in this tutorial) **[Nicosia et al. '09]**
  - Modifications in the configuration model – local definition of modularity **[Muff et al. '05]**

Resolution limit of modularity

- **Resolution Limit** of modularity **[Fortunato and Barthelemy '07]**
- The method of modularity optimization may not detect communities with relatively small size, which depends on the total number of edges in the graph



- K_m are cliques with **m** edges (**$m \leq \sqrt{|E|}$**)
- K_m represent well-defined clusters
- However, the maximum modularity corresponds to clusters formed by two or more cliques
- It is difficult to know if the community returned by modularity optimization corresponds to a **single community** or a **union of smaller communities**

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Outline

- Modularity Based Methods
- **Louvain algorithm**
- Graph kernels - classification

Louvain algorithm

- method to extract the community structure of networks
- heuristic method based on modularity optimization.
- Relatively low cost in terms of computation time.
- quality of the communities good, as measured by modularity.

The algorithm

- Assume a weighted undirected graph $G(E,V)$ and a splitting G in $\{Ci\}$ communities. Then the modularity of the community splitting is:

$$Q = \frac{1}{2m}\sum_{ij}\left(A_{ij} - \frac{k_i k_j}{2m}\right)\delta\left(C_i, C_j\right)$$

- A_{ij} is the weight among nodes i and j, k_i is the sum of weight of the edges attached to vertex i, c_i the community to which i belongs and the δ function $\delta(u,v)$ is 1 if u-v and 0 otherwise. Finally $m = \frac{1}{2}\sum_{ij} A_{ij}$
- **Phase 1:**
- weighted graph. Create for each node i a community .
- For each node i consider all its neighbors j. For each of them evaluate the gain in modularity if we place i in the community of j.
- The node i is placed in the community that maximizes the gain
- The process is repeated until there is no further gain for any reassignment.

$$\Delta Q = \left[\frac{\sum_{in} + k_{i,in}}{2m} - \left(\frac{\sum_{tot} + k_i}{2m}\right)^2\right] - \left[\frac{\sum_{in}}{2m} - \left(\frac{\sum_{tot}}{2m}\right)^2 - \left(\frac{k_i}{2m}\right)^2\right]$$

Phase1: re-assignment of nodes – modularity gain

- Reassigning a node i to a cluster C incurs a gain in modularity:

$$\Delta Q = \left[\frac{\sum_{in} + k_{i,in}}{2m} - \left(\frac{\sum_{tot} + k_i}{2m} \right)^2 \right] - \left[\frac{\sum_{in}}{2m} - \left(\frac{\sum_{tot}}{2m} \right)^2 - \left(\frac{k_i}{2m} \right)^2 \right]$$

$\sum_{in}$ sum of the weights of links in cluster C,

$\sum_{tot}$ sum of weights of the links incident to nodes in C ,

κ_i sum weights of links incident node i,

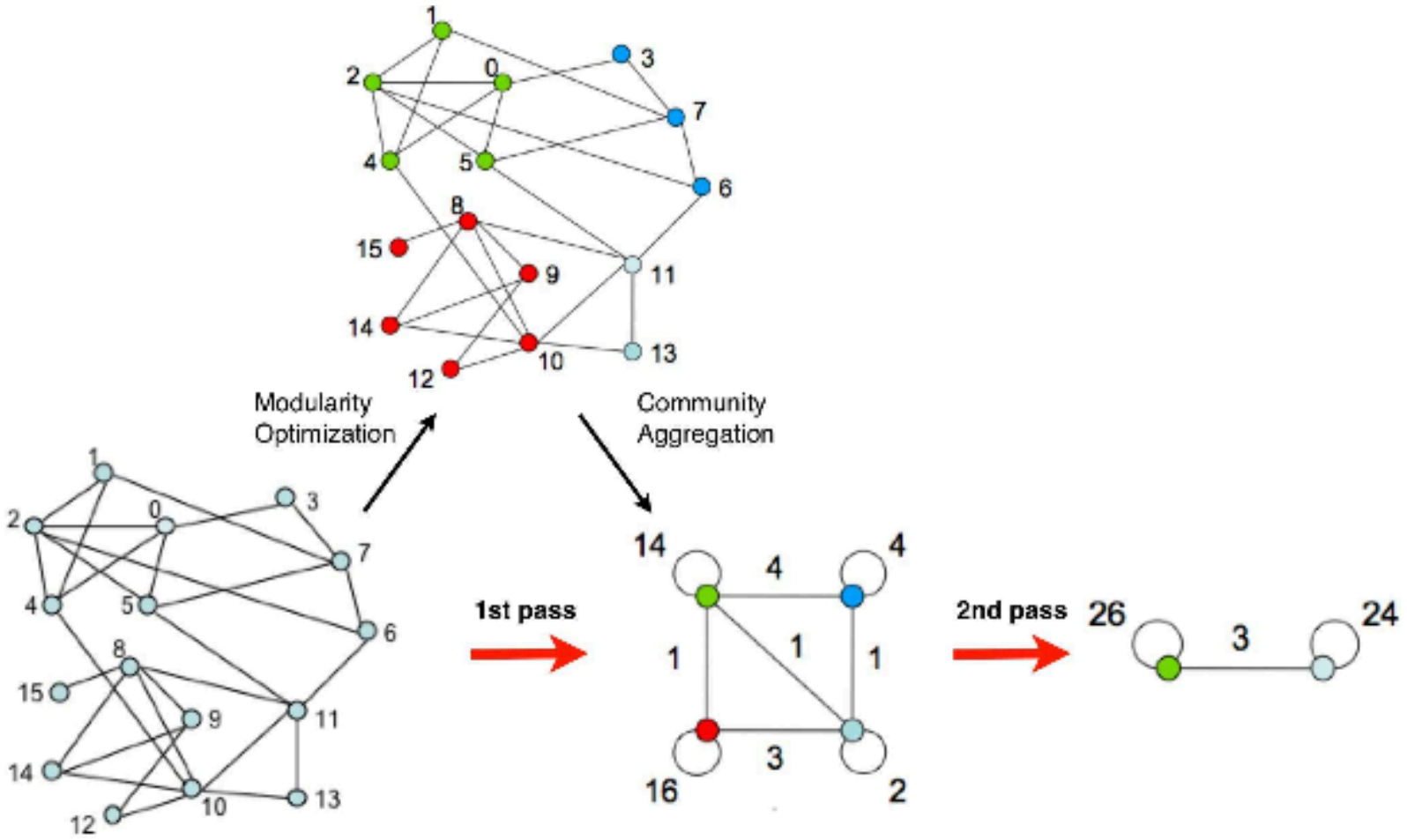
$\kappa_{i,in}$ sum weights of links from i to nodes in C

m sum of the weights of all the links in the network.

Phase 2: collapsing communities

- For each community c_i all nodes i in collapse in to one super-node c_i
- Inter community links weight: sum of the weights of the links among the communities nodes.
- Within community links collapse to a self link
- Go to phase 1

Iterative passes



Example

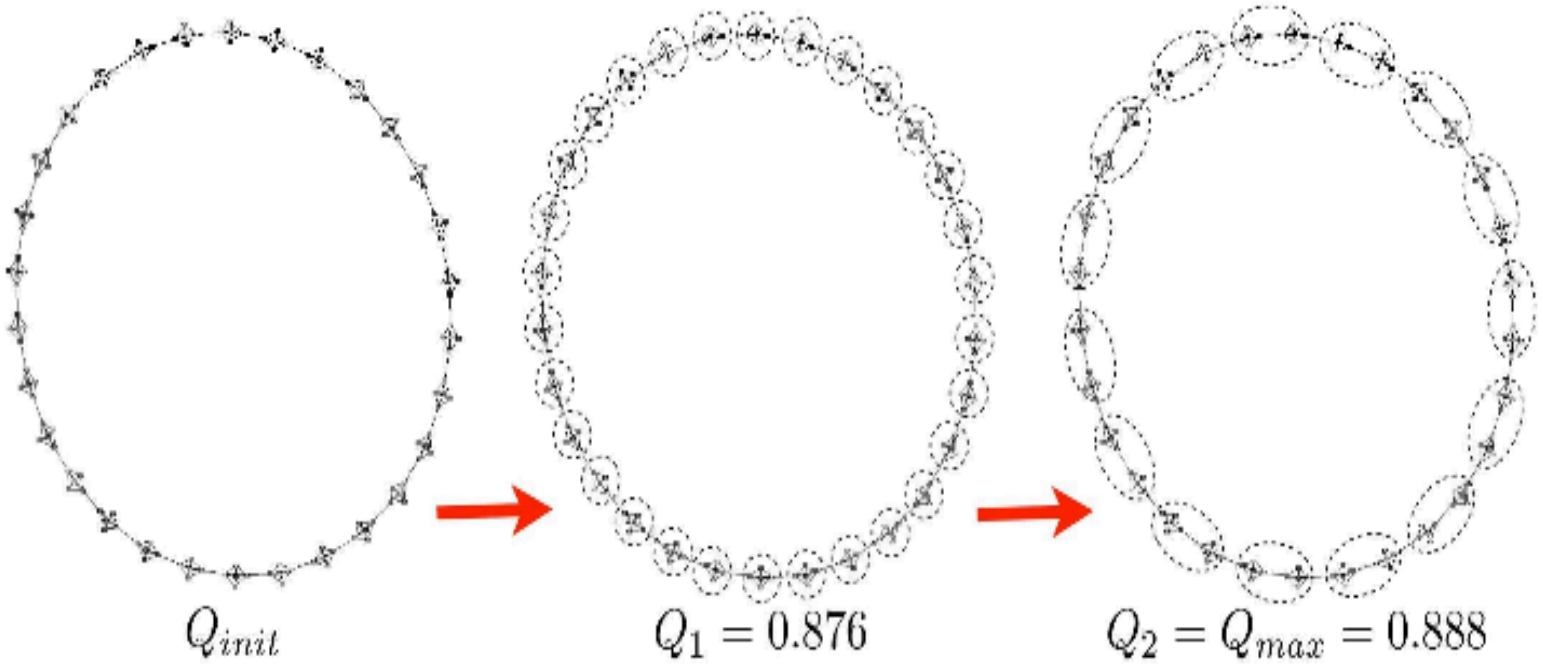


Figure 2. We have applied our method to the ring of 30 cliques discussed in [23]. The cliques are composed of 5 nodes and are inter-connected through single links. The first pass of the algorithm finds the natural partition of the network. The second pass finds the global maximum of modularity where cliques are combined into groups of two.

Performance considerations

Performance on large scale graphs (2008)

- sub-network of the .uk domain (39 M nodes, 783 M links
- Stanford WebBase crawler (118 million nodes and 1Bn links.
- Time: 12 minutes and 152 minutes respectively

Almost linear complexity for sparse data

- Number of communities decreases drastically after just a few passes
- Running time is concentrated on the first iterations.

Resolution limit problem modularity circumvented

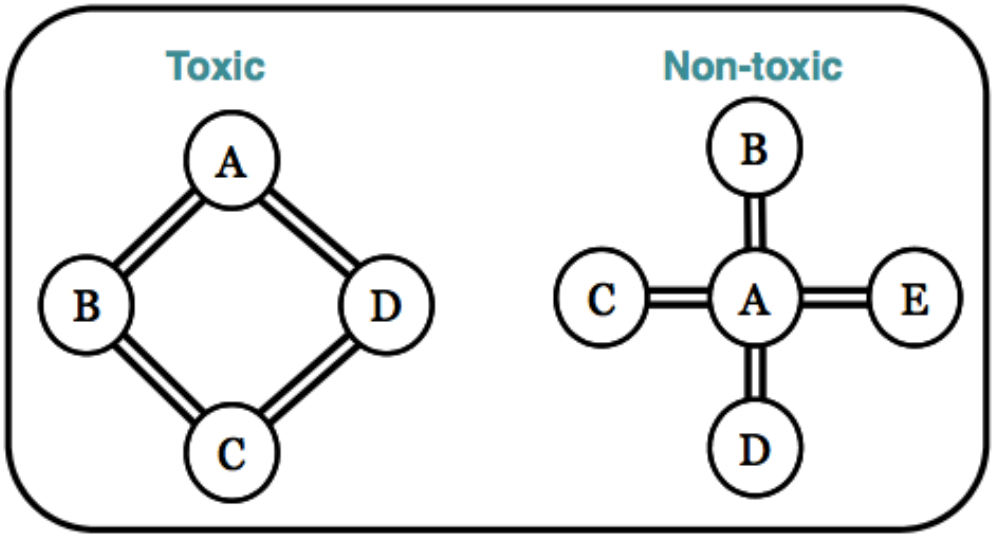
- intrinsic multi-level nature

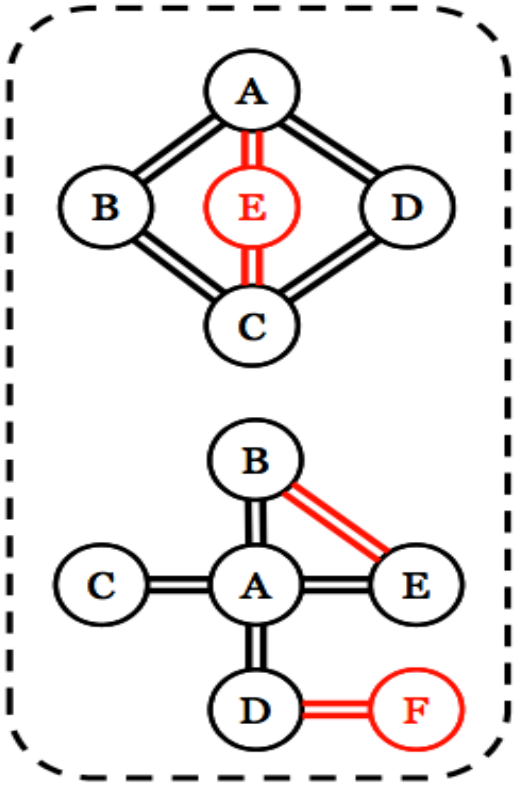
Outline

- Modularity Based Methods
- Louvain algorithm
- **Graph kernels - classification**

Graph classification

Chemical compounds





known

Predict toxic molecules assuming the known toxic ones

http://www.csc.ncsu.edu/faculty/samatova/practical-graph-mining-with-R/slides/pdf/Classification.pdf

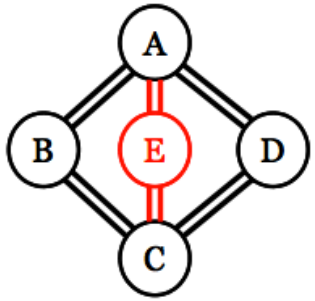
Graph classification

Graphs classification applications

- Chemical compounds
- Molecular structures
- Textual data – text categorization, opinion mining, sentiment analysis, metaphor detection …
- Social networks – community similarity

Classification based on graph structures

- Graph classification – i.e. recognize graph topologies
  - i.e. molecular graphs:



Toxic

- Vertex classification – label prediction
  - i.e. predict in a social graph is the node is male/ female.

Graph Isomorphism

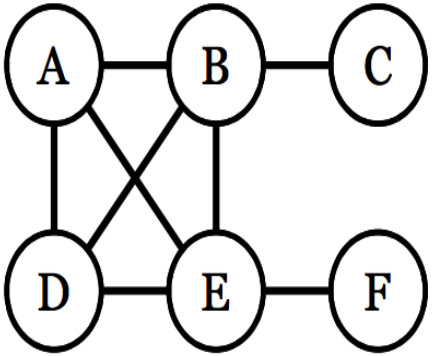
- $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ are isomorphic if
  - there exists a bijection(isomorphism) $f : V_1 \rightarrow V_2$ such that $(v_i , v_j) \in E_1$ if and only if $(f (v_i), f (v_j)) \in E_2$
- *Subgraph isomorphism:*
- try sub-graph isomorphism between two graphs
- could be a potential solution to graph similarity
- the problem is NP-complete
- finding the largest isomorphic subgraphs is NP-hard

Graph kernels

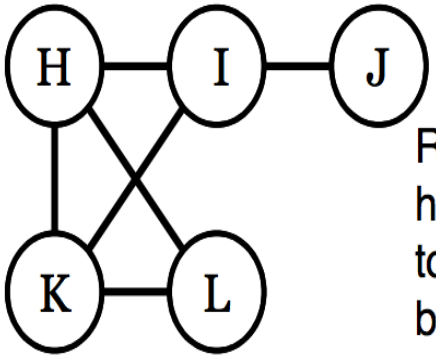
- Define a similarity measure between graphs computable in polynomial time
- Desired Properties of Graph Kernels
  - Symmetric, Semi-positive definite
  - Fast to compute
  - Expressive (captures topological similarity between graphs)
- Categories of Graph Kernels – based on:
  - walks and paths
  - limited-sized subgraphs
  - Sub tree patterns
  - others (based on graph edit distance etc.)

Random walk Graph kernels

Random walk vertices heavily distributed towards A,B,D,E

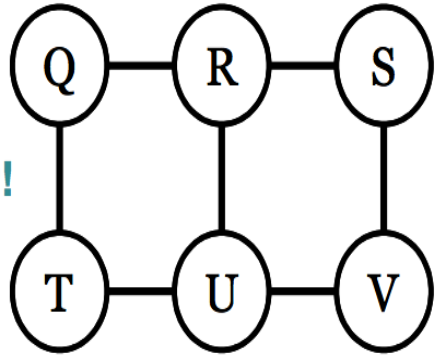


Similar!



Random walk vertices heavily distributed towards H,I,K with slight bias towards L

Not Similar!



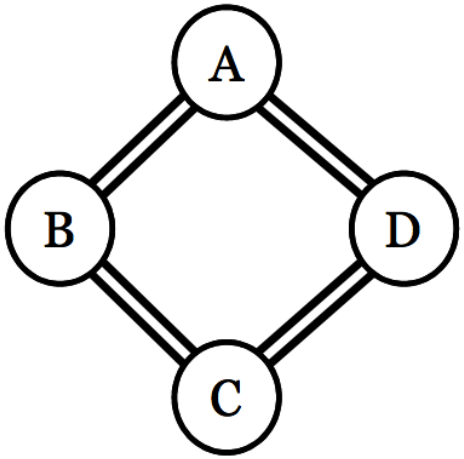
Random walk vertices evenly distributed

http://www.csc.ncsu.edu/faculty/samatova/practical-graph-mining-with-R/slides/pdf/Classification.pdf

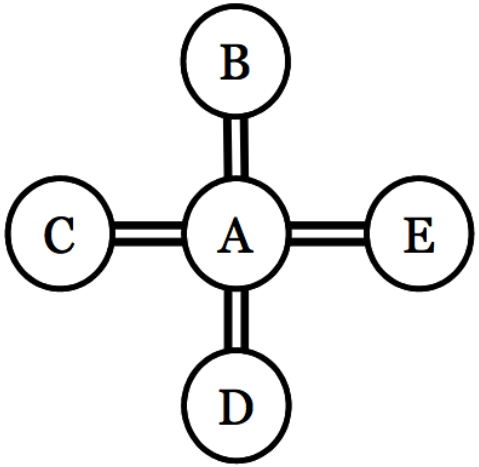
Product graph

- Assume two graphs $G_1(V_1, E_1)$, $G_2(V_2, E_2)$
- Direct Product notation: $G_x = G_1 x\ G_2$
- Direct product vertices: $V(G_x) = \{(a,b) \in (V_1 x V_2)\}$
- Direct product edges: $E(G_x) = \{(a,b),(c,d) |$ $(a,c) \in E_1$ & $(b,d) \in E_2\}$

Graph Product - example



Type-A



Type-B

Type-A	A	B	C	D
A	0	1	1	0
B	1	0	0	1
C	1	0	0	1
D	0	1	1	0

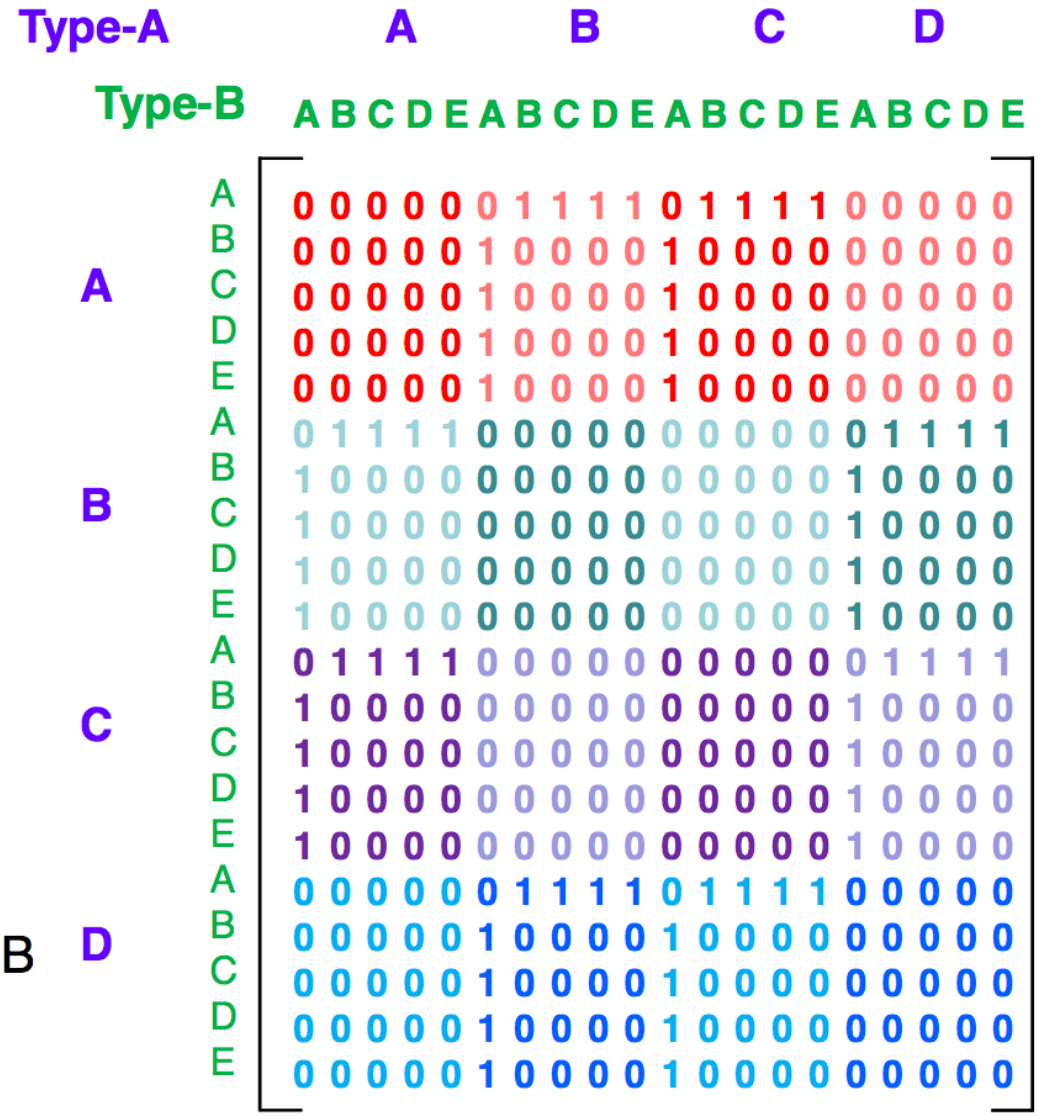
Type-B	A	B	C	D	E
A	0	1	1	1	1
B	1	0	0	0	0
C	1	0	0	0	0
D	1	0	0	0	0
E	1	0	0	0	0

Graph Product - example

Type-A	A	B	C	D
A	0	1	1	0
B	1	0	0	1
C	1	0	0	1
D	0	1	1	0

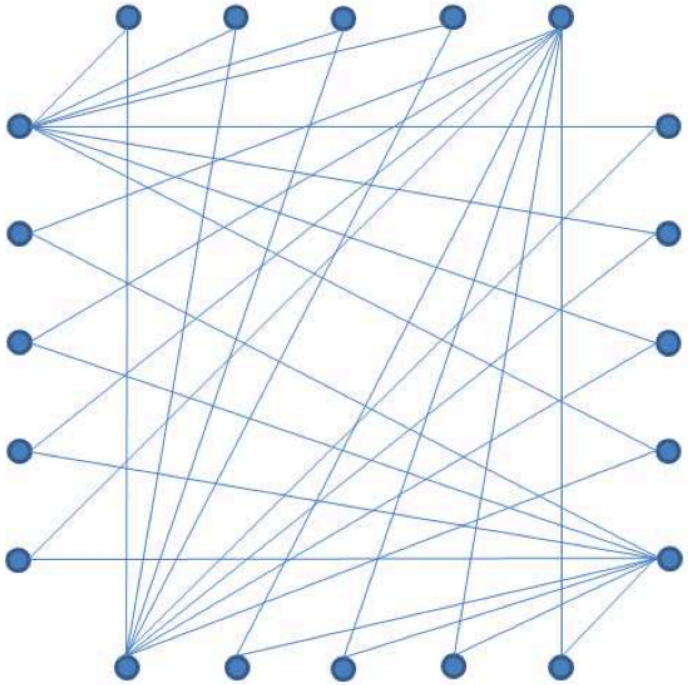
Type-B	A	B	C	D	E
A	0	1	1	1	1
B	1	0	0	0	0
C	1	0	0	0	0
D	1	0	0	0	0
E	1	0	0	0	0

Intuition: multiply each entry of Type-A by ***entire matrix*** of Type-B



Direct Product Kernel

- Compute direct product graph
- Decay constant $\gamma < 1/\min(d_i, d_o)$
  - d_i/d_o: max in/out degree in G_x
- Compute the weighted geometric series of walks (array A).
- Sum over all vertex pairs.



$$k(G_1, G_2) = \sum_{ij} \left(I - \frac{A_{ij}}{\gamma} \right)^{-1}$$

Random Walk Kernels - Preliminaries

- graph $G = (V,E)$, $V = \{v_1, v_2, \cdots, v_n\}$ ordered set of n vertices, $E \subset V \times V$ set of edges
- The adjacency matrix A of G is defined as $[A_{ij}] = \{1 \text{ if } (v_i, v_j) \in E, 0 \text{ otherwise}\}$
- A walk w on the graph is a sequence of nodes $w = (v_1, v_2, \cdots, v_n)$, $(v_i, v_{i+1},) \in E$

Random Walk Kernel

- Graphs with matching walks are similar
- Performing a random walk on the direct product graph G_x is equivalent to simultaneous random walk on the graphs G_1 and G_2

  - The A^k_X entry represents the probability of simultaneous length-k random walks on G and G'.

- Number of walks of length *k* from v_i to v_j can be computed by A^k_{ij}
- Discount longer walks by the factor of λ

How to compute common walks between two graphs?

- The product graph $G\times = (V_\times, E_\times)$ of G1 and G2:

$$V_\times = \{(v,w) \in V_1 \times V_2 : l(v)=l(w)\},\ l(v)\text{: label of vertex } v$$

$$E_\times = \{((v_1,w_1),(v_2,w_2)) \in V_\times^2 : (v1,v2) \in E1$$

$$\text{and } (w_1,w_2) \in E_2 \text{ and } l(v_1,w_1) = l(v_2,w_2)\}$$

- Common walks can be thought of as walks within the product graph

Random Walk Kernel

- Random walk kernel between two graphs G1 and G2 is defined as

$$k_x\left(G_1, G_2\right) = \sum_{i,j=1}^{|V_x|} [\sum_{n=0}^{\infty} \lambda^n A_X^n]_{ij} = e^T (I - \lambda \mathrm{A}_x)^{-1} e$$

- where $e = (1,1,\cdots,1)^T$ start/termination prob distribution
- A_x, un-normalized adjacency matrix of the direct product graph.
- A_X^n represents similarity between simultaneous length *n* walks on G and G', measured via the kernel function κ

- Requires matrix inversion of $n^2 \times n^2$ matrix
- Time complexity $O(n^6)$
- Can be improved to $O(n^3)$ (Vishwanathan et al., 2010)
  - Employ Sylvester equation $M = SMT + M_0$ where $S,T,M_0 \in Rn \times n$ are given and we need to solve for $M \in Rn \times n$

Random walk kernels alternatives

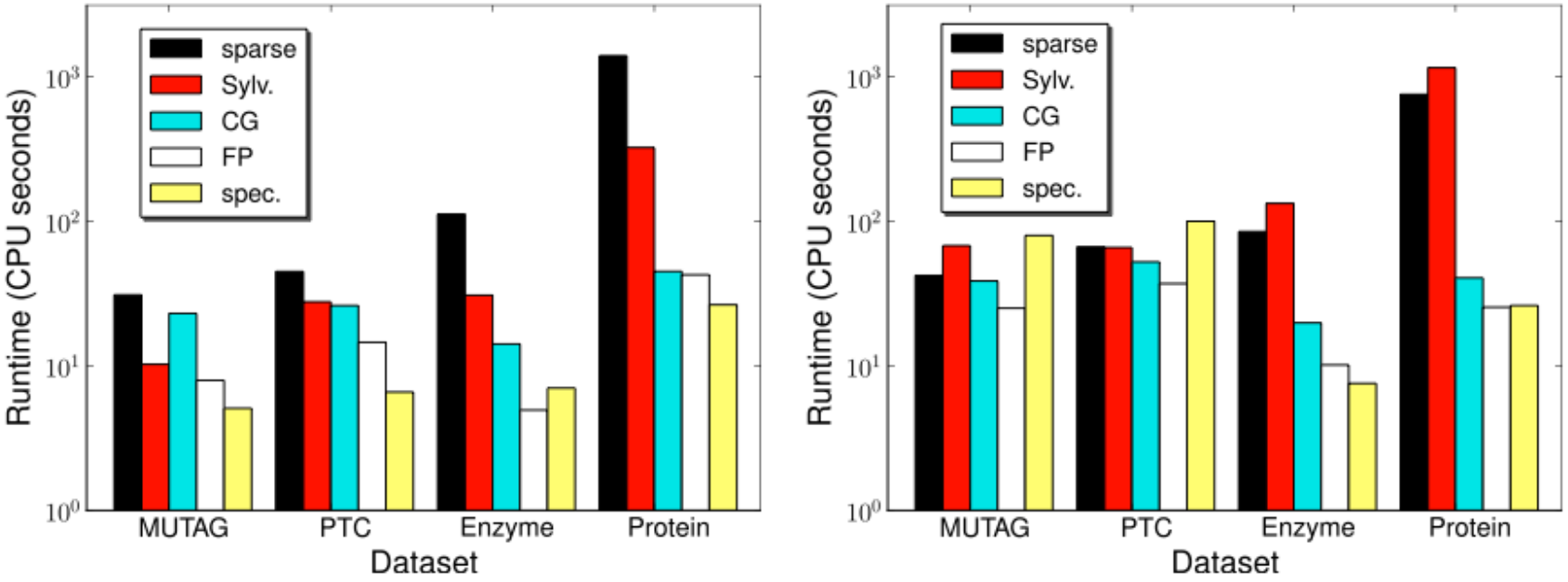


Figure 5: Time (in seconds on a log-scale) to compute 100×100 kernel matrix for unlabeled (left) *resp*. labeled (right) graphs from several data sets, comparing the conventional sparse method to our fast Sylvester equation, conjugate gradient (CG), fixed-point iteration (FP), and spectral approaches.

Kernel Matrix

- Assuming a set {G1, …Gn} graphs

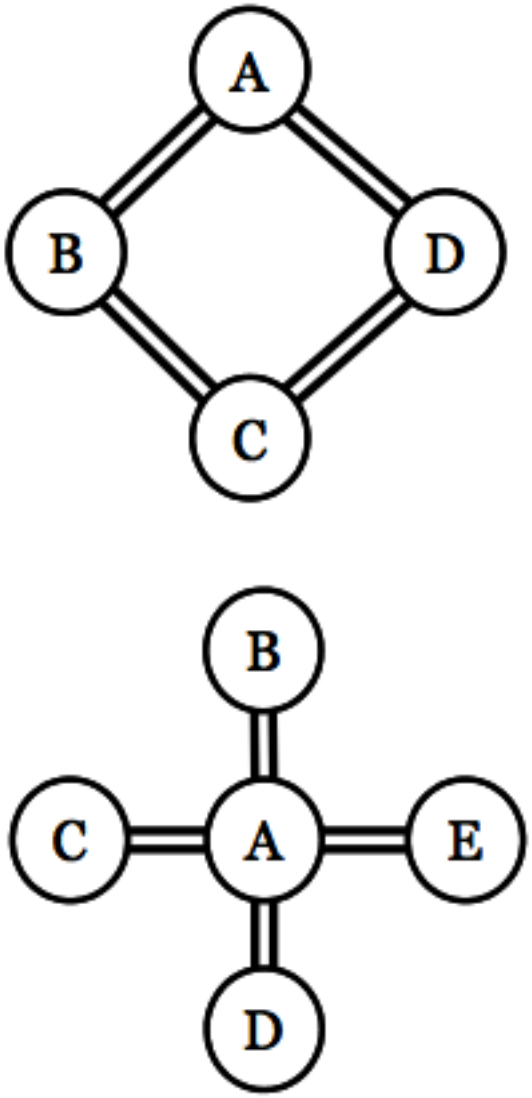
$$\begin{bmatrix} K(G_1,G_1), K(G_1,G_2), \dots, K(G_1,G_n) \\ K(G_2,G_1), K(G_2,G_2), \dots, K(G_2,G_n) \\ \dots \\ K(G_n,G_1), K(G_n,G_2), \dots, K(G_n,G_n) \end{bmatrix}$$

- This matrix is used as input to the classification learning method (i.e. SVM) function to learn the model.

Predicting toxic compounds

Assume the PTC dataset of molecules tested for positive or negative toxicity

```
# Learning pipeline (SVM ) in R
data("PTCData") # graph data
data("PTCLabels") # toxicity information
# select 5 molecules to build model on
sTrain= sample(1:length(PTCData),5)
PTCDataSmall<-PTCData[sTrain]
PTCLabelsSmall<-PTCLabels[sTrain]
# generate kernel matrix
K = generateKernelMatrix(PTCDataSmall,
PTCDataSmall)
# create SVM model
model =ksvm(K, PTCLabelsSmall,
kernel='matrix')
```



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