Network structure

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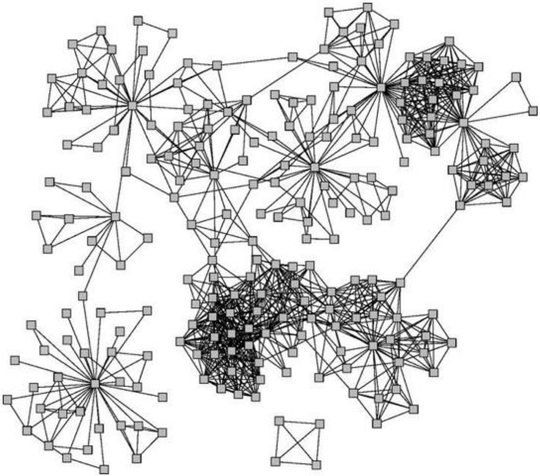
BigData Academy MADE from Mail.ru Group

Social Network Analysis and Machine Learning on Graphs

Network structure



Typical network structure

Core-periphery structure of a network

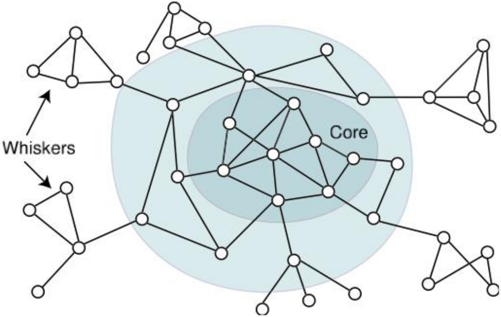
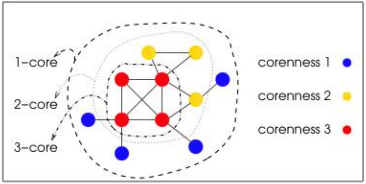


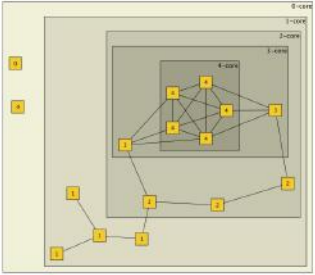
image from J. Leskovec, K. Lang, 2010

Graph cores

Definition

A *k-core* is the largest subgraph such that each vertex is connected to at least k others in subset





Every vertex in k-core has a degree $k_i \geq k$

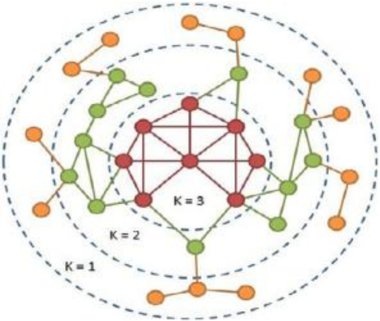
$(k+1)$-core is always subgraph of k-core

The core number of a vertex is the highest order of a core that contains this vertex

k-core decomposition

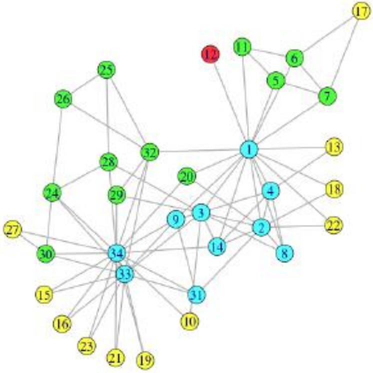
V. Batageli, M. Zaversnik, 2002

- If from a given graph G = (V, E) recursively delete all vertices, and lines incident with them, of degree less than k, the remaining graph is the k-core.

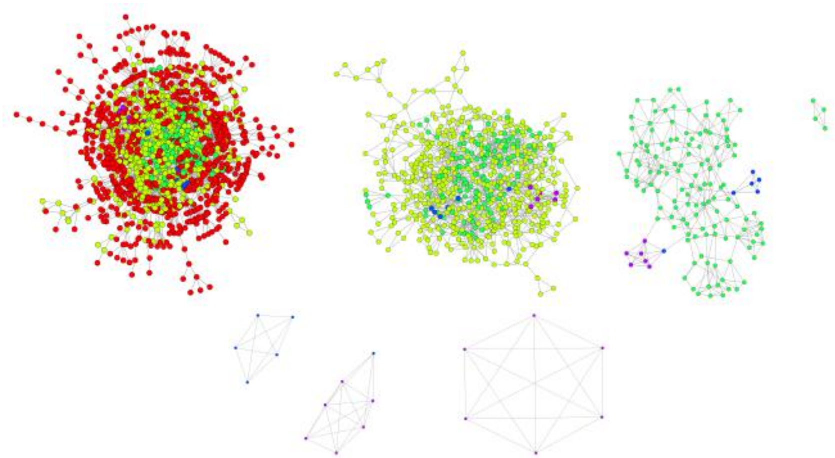


K-cores

Zachary karate club: 1,2,3,4 - cores



k-cores



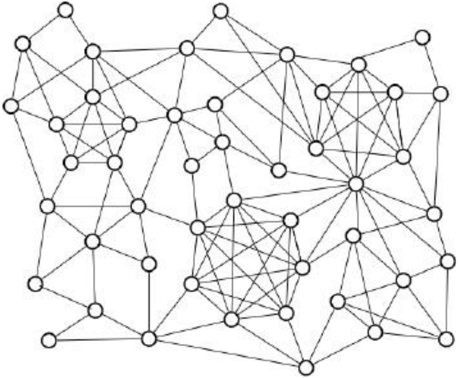
k-cores: 1:1458, 2:594, 3:142, 4:12, 5:6

k-shells: 1:864-red, 2:452-pale green, 3:130-green, 5:6-blue, 6:6-purple

Graph cliques

Definition

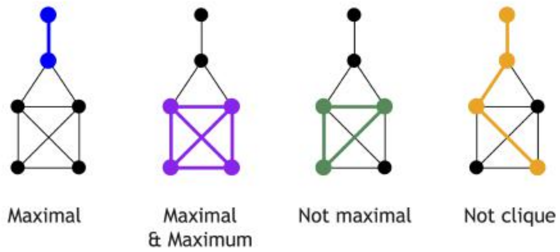
A *clique* is a complete (fully connected) subgraph, i.e. a set of vertices where each pair of vertices is connected.



Cliques can overlap

Graph cliques

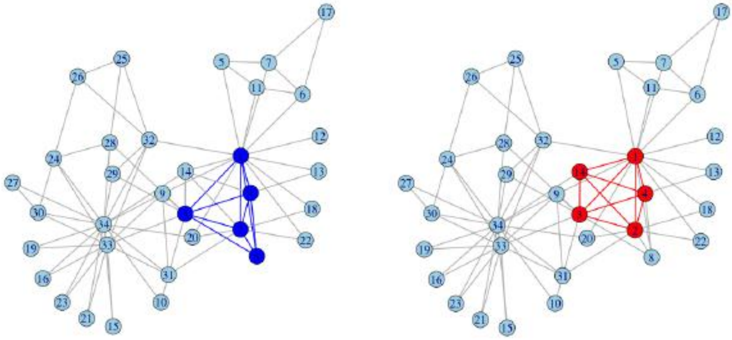
- A **maximal clique** is a clique that cannot be extended by including one more adjacent vertex (not included in larger one)
- A **maximum clique** is a clique of the largest possible size in a given graph



- Graph clique number is the size of the maximum clique

image from D. Eppstein

Maximum cliques



Maximal cliques:

Clique size:	2	3	4	5
Number of cliques:	11	21	2	2

Zachary, 1977

Graph cliques

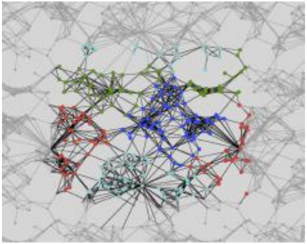
Computational issues:

- Finding click of fixed given size k - $O(n^k k^2)$
- Finding maximum clique $O(3^{n/3})$
- But in sparse graphs...

Network communities

Definition

Network communities are groups of vertices such that vertices inside the group connected with many more edges than between groups.



- Community detection is an assignment of vertices to communities.
- Will consider non-overlapping communities
- Graph partitioning problem

Network communities

What makes a community (cohesive subgroup):

- Mutuality of ties. Almost everyone in the group has ties (edges) to one another
- Compactness. Closeness or reachability of group members in small number of steps, not necessarily adjacency
- Density of edges. High frequency of ties within the group
- Separation. Higher frequency of ties among group members compared to non-members

Wasserman and Faust

Community density

- Graph $G(V, E)$, $n = |V|$, $m = |E|$
- Community - set of nodes S
  n_s-number of nodes in S, m_s - number of edges in S
- Graph density
$$\rho = \frac{m}{n(n-1)/2}$$
- community internal density
$$\delta_{int} = \frac{m_s}{n_s(n_s-1)/2}$$
- external edges density
$$\delta_{ext} = \frac{m_{ext}}{n_s(n-n_s)}$$
- community (cluster): $\delta_{int} > \rho$, $\delta_{ext} < \rho$

Modularity

- Compare fraction of edges within the cluster to expected fraction in random graph with identical degree sequence

$$Q = \frac{1}{4}(m_s - E(m_s))$$

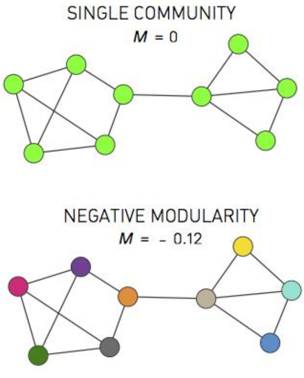
- Modularity score

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

m_u - number of internal edges in a community u,
k_u - sum of node degrees within a community

- Modularity score range $Q \in [-1/2, 1)$, single community $Q = 0$

Modularity



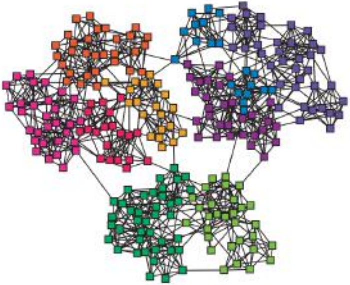
- The higher the modularity score - the better are communities

from A.L. Barabasi 2016

Heuristic approach

Focus on edges that connect communities.
Edge betweenness -number of shortest paths $\sigma_{st}(e)$ going through edge e

$$C_B(e) = \sum_{s \neq t} \frac{\sigma_{st}(e)}{\sigma_{st}}$$



Construct communities by progressively removing edges

Edge betweenness

Newman-Girvan, 2004

Algorithm: Edge Betweenness

Input: graph G(V,E)

Output: Dendrogram

repeat

  For all $e \in E$ compute edge betweenness $C_B(e)$;

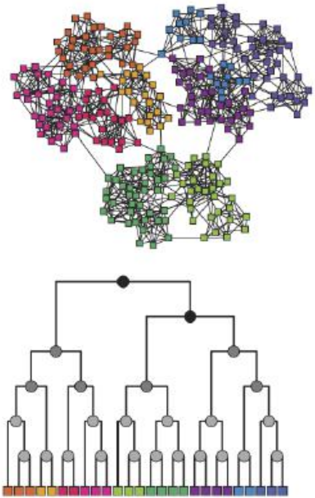
  remove edge e_i with largest $C_B(e_i)$;

until *edges left*;

If bi-partition, then stop when graph splits in two components (check for connectedness)

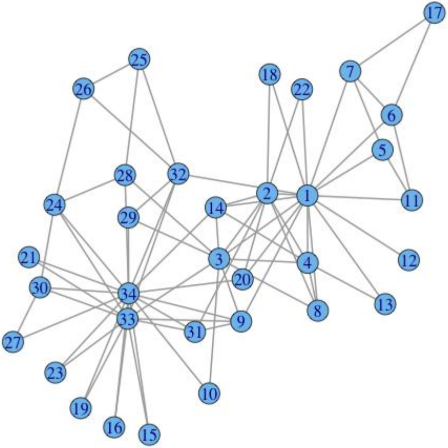
Edge betweenness

Hierarchical algorithm, dendrogram



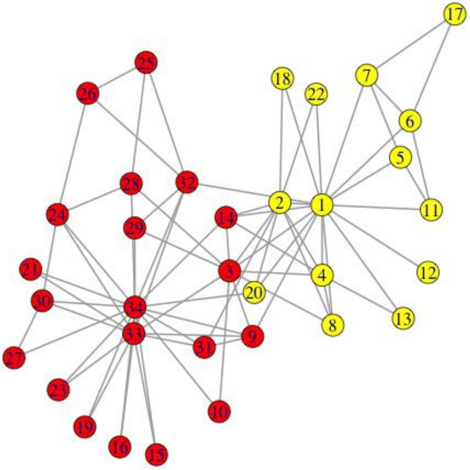
Edge betweenness

Zachary karate club



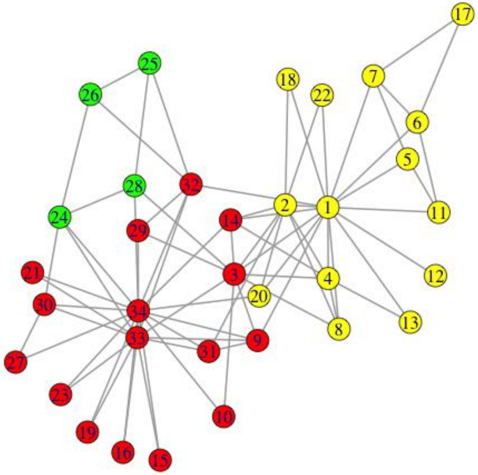
Edge betweenness

Zachary karate club

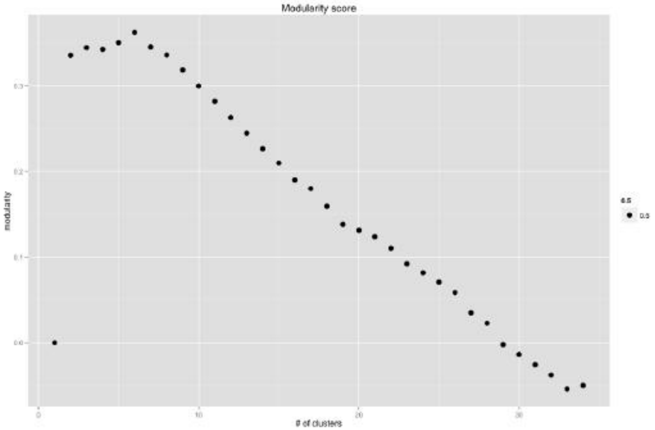


Edge betweenness

Zachary karate club

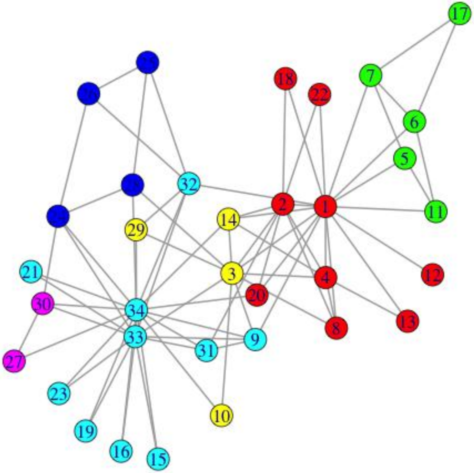


Edge betweenness



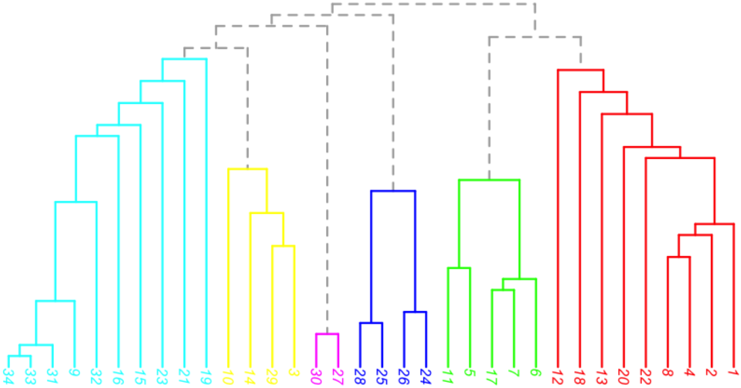
Edge betweenness

best: clusters = 6, modularity = 0.345



Edge betweenness

Zachary karate club

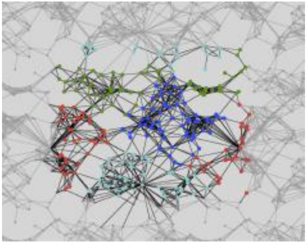


Lecture outline

Network communities

Definition

Network communities are groups of vertices such that vertices inside the group connected with many more edges than between groups.



- Graph partitioning problem

Graph partitioning

Combinatorial problem:

- Number of ways to divide network of n nodes in 2 groups (bi-partition):

$$\frac{n!}{n_1!n_2!}, \quad n = n_1 + n_2$$

- Dividing into k non-empty groups (Stirling numbers of the second kind)

$$S(n,k) = \frac{1}{k!}\sum_{j=0}^{n}(-1)^j C_k^j (k-j)^n$$

- Number of all possible partitions (n-th Bell number):

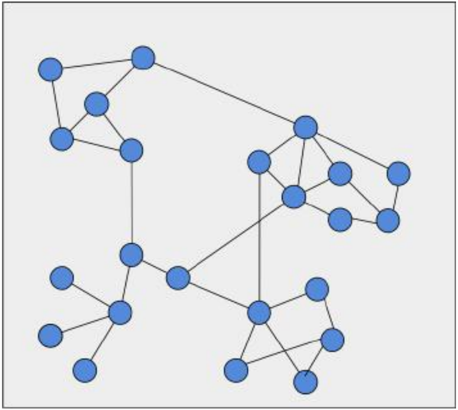
$$B_n = \sum_{k=1}^{n} S(n,k)$$

$B_{20} = 5,832,742,205,057$

Community detection

- Consider only sparse graphs $m \ll n^2$
- Each community should be connected
- Combinatorial optimization problem:
  - optimization criterion
  - optimization method
- Exact solution NP-hard
  (bi-partition: $n = n_1 + n_2$, $n!/(n_1!n_2!)$ combinations)
- Solved by greedy, approximate algorithms or heuristics
- Recursive top-down 2-way partition, multiway partiton
- Balanced class partition vs communities

Graph cut



Optimization criterion: graph cut

Graph $G(E, V)$ partition: $V = V_1 + V_2$

- Graph cut

$$Q = cut(V_1, V_2) = \sum_{i \in V_1, j \in V_2} e_{ij}$$

- Ratio cut:

$$Q = \frac{cut(V_1, V_2)}{||V_1||} + \frac{cut(V_1, V_2)}{||V_2||}$$

- Normalized cut:

$$Q = \frac{cut(V_1, V_2)}{Vol(V_1)} + \frac{cut(V_1, V_2)}{Vol(V_2)}$$

- Quotient cut (conductance):

$$Q = \frac{cut(V_1, V_2)}{\min\left(Vol(V_1), Vol(V_2)\right)}$$

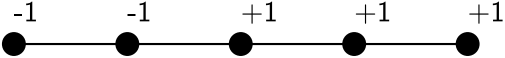
where: $Vol(V_1) = \sum_{i \in V_1, j \in V} e_{ij} = \sum_{i \in V_1} k_i$

Optimization methods

- Greedy optimization:
  – Local search [Kernighan and Lin, 1970], [Fidducia and Mettheyses, 1982]
- Approximate optimization:
  – Spectral graph partitioning [M. Fiedler, 1972], [Pothen et al 1990], [Shi and Malik, 2000]
  – Multicommodity flow [Leighton and Rao, 1988]
- Heuristics algorithms:
  – Multilevel graph partitioning (METIS) [G. Karypis, Kumar 1998]
- Randomized algorithms:
  –Randomized min cut [D. Karger, 1993]

Graph cuts

- Let $V = V^+ + V^-$ be partitioning of the nodes
- Let $s = \{+1, -1, +1, ... -1, +1\}^T$ - indicator vector



$$s(i) = \begin{cases} +1: & \text{if} \quad v(i) \in V^+ \\ -1: & \text{if} \quad v(i) \in V^- \end{cases}$$

- Number of edges, connecting V^+ and V^-

$$cut(V^+, V^-) = \frac{1}{4} \sum_{e(i,j)} (s(i) - s(j))^2 = \frac{1}{8} \sum_{i,j} A_{ij} (s(i) - s(j))^2 =$$

$$= \frac{1}{4} \sum_{i,j} (k_i \delta_{ij} s(i)^2 - A_{ij} s(i) s(j)) = \frac{1}{4} \sum_{i,j} (k_i \delta_{ij} - A_{ij}) s(i) s(j)$$

$$cut(V^+, V^-) = \frac{1}{4} \sum_{i,j} (D_{ij} - A_{ij}) s(i) s(j)$$

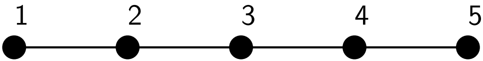
Graph cuts

- Graph Laplacian: $L_{ij} = D_{ij} - A_{ij}$, where $D_{ii} = diag(k_i)$

$$L_{ij} = \begin{cases} k(i)\,, & if \;\; i = j \\ -1\,, & if \; \exists \; e(i,j) \\ 0\,, & otherwise \end{cases}$$

- Laplacian matrix 5x5:

$$L = \begin{pmatrix} 1 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & -1 & 2 & -1 \\ & & & -1 & 1 \end{pmatrix}$$



Graph cuts

- Graph Laplacian: $\mathrm{L} = \mathrm{D} - \mathrm{A}$
- Graph cut:

$$Q(\mathrm{s}) = cut(V^+, V^-) = \frac{1}{4}\sum_{i,j} L_{ij} s(i) s(j) = \frac{\mathrm{s}^T \mathrm{L} \mathrm{s}}{4}$$

- Minimal cut:

$$\min_{\mathrm{s}} Q(\mathrm{s})$$

- Balanced cut constraint:

$$\sum_i s(i) = 0$$

- Integer minimization problem, exact solution is NP-hard!

Spectral method - relaxation

- Discrete problem $\to$ continuous problem
- Discrete problem: find

$$\min_{s}(\frac{1}{4}s^T Ls)$$

  under constraints: $s(i) = \pm 1$, $\sum_i s(i) = 0$;
- Relaxation - continuous problem: find

$$\min_{x}(\frac{1}{4}x^T Lx)$$

  under constraints: $\sum_i x(i)^2 = n$, $\sum_i x(i) = 0$
- Given $x(i)$, round them up by $s(i) = sign(x(i))$
- Exact constraint satisfies relaxed equation, but not other way around!

Spectral method - computations

- Constraint optimization problem (Lagrange multipliers):

$$Q(\mathrm{x}) = \frac{1}{4}\mathrm{x}^T \mathrm{L}\mathrm{x} - \lambda(\mathrm{x}^T\mathrm{x} - n), \quad \mathrm{x}^T\mathrm{e} = 0$$

- Eigenvalue problem:

$$\mathrm{L}\mathrm{x} = \lambda\mathrm{x}, \quad \mathrm{x} \perp \mathrm{e}$$

- Solution:

$$Q(\mathrm{x_i}) = \frac{n}{4}\lambda_i$$

- First (smallest) eigenvector:

$$\mathrm{L}\mathrm{e} = 0, \quad \lambda = 0, \quad \mathrm{x}_1 = \mathrm{e}$$

- Looking for the second smallest eigenvalue/eigenvector λ_2 and x_2
- Minimization of Rayleigh-Ritz quotient:

$$\min_{\mathrm{x} \perp \mathrm{x}_1}\left(\frac{\mathrm{x}^T\mathrm{L}\mathrm{x}}{\mathrm{x}^T\mathrm{x}}\right)$$

Spectral graph theory

- $\lambda_1 = 0$
- Number of $\lambda_i = 0$ equal to the number of connected components

- $0 \leq \lambda_2 \leq 2$
  $\lambda_2 = 0$, disconnected graph
  $\lambda_2 = 1$, totally connected

- Graph diameter (longest shortest path)

$$D(G) >= \frac{4}{n\lambda_2}$$

Spectral graph partitioning algorithm

Algorithm: Spectral graph partitioning - normalized cuts

Input: adjacency matrix A

Output: class indicator vector s

compute $D = diag(deg(A))$;

compute $L = D - A$;

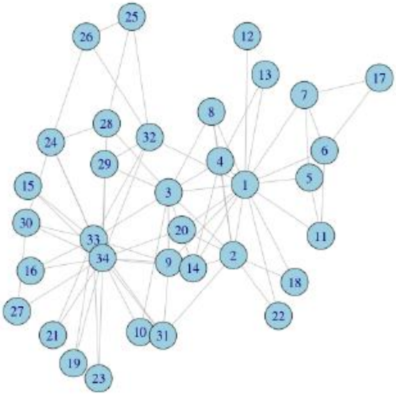
solve for second smallest eigenvector:

min cut: $Lx = \lambda x$;

normalized cut : $Lx = \lambda Dx$;

set $s = sign(x_2)$

Example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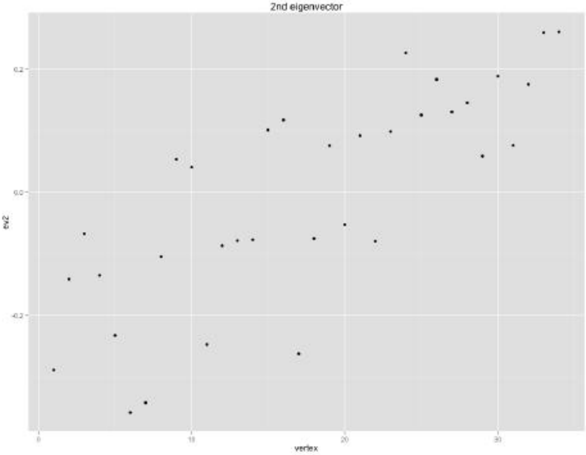
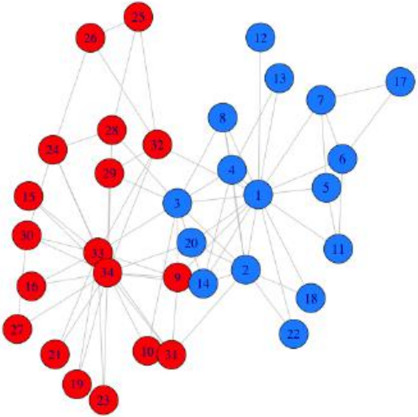
Example



Eigenvalues: $\lambda_1 = 0,\ \lambda_2 = 0.2,\ \lambda_3 = 0.25\ ...$

Example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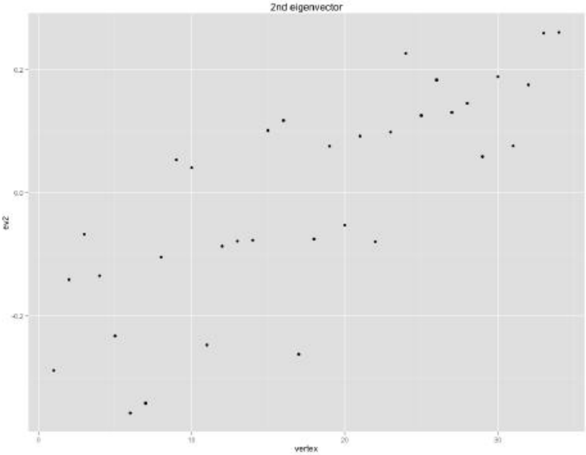
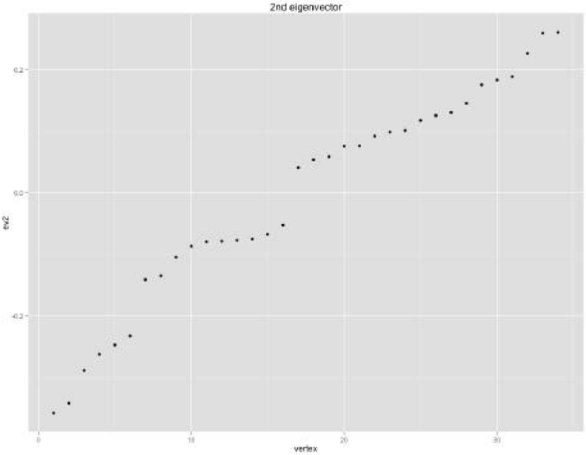
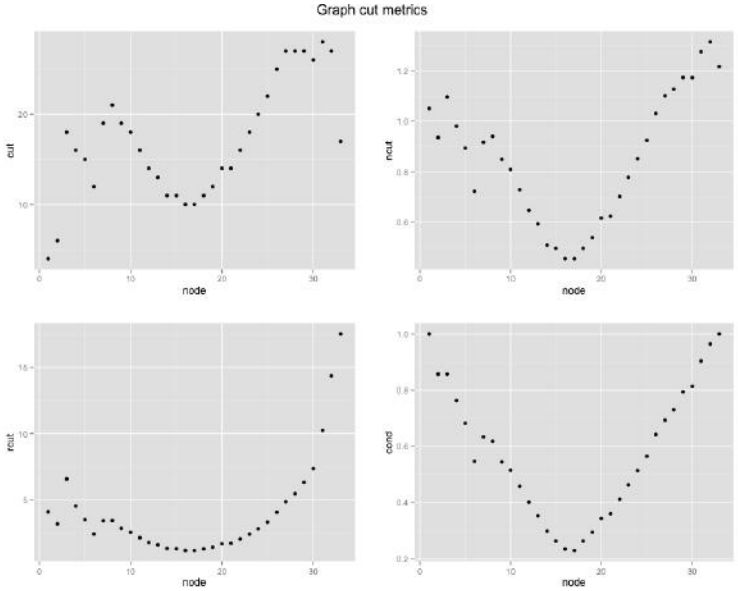
Example



Spectral ordering



Cut metrics



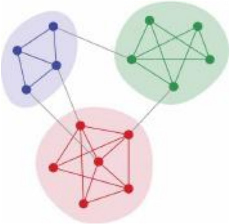
Optimization criterion: modularity

- Modularity:

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

where n_c - number of classes and

$$\delta(c_i, c_j) = \begin{cases} 1: & \text{if} \quad c_i = c_j \\ 0: & \text{if} \quad c_i \neq c_j \end{cases}$$ - kronecker delta



[Maximization!]

Spectral modularity maximization

- Direct modularity maximization for bi-partitioning, [Newman, 2006]
- Let two classes $c_1 = V^+$, $c_2 = V^-$, indicator variable $s = \pm 1$

$$\delta(c_i, c_j) = \frac{1}{2}(s_i s_j + 1)$$

- Modularity

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

where

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

M. Newman, 2006

Spectral modularity maximization

- Qudratic form:

$$Q(\mathrm{s}) = \frac{1}{4m}\mathrm{s}^T \mathrm{B}\mathrm{s}$$

- Integer optimization - NP, relaxation $s \to x$, $x \in R$
- Keep norm $||x||^2 = \sum_i x_i^2 = \mathrm{x}^T\mathrm{x} = n$
- Quadratic optimization

$$Q(\mathrm{x}) = \frac{1}{4m}\mathrm{x}^T \mathrm{B}\mathrm{x} - \lambda(\mathrm{x}^T\mathrm{x} - n)$$

- Eigenvector problem

$$\mathrm{B}\mathrm{x}_i = \lambda_i \mathrm{x}_i$$

- Approximate modularity

$$Q(\mathrm{x_i}) = \frac{n}{4m}\lambda_i$$

- Modularity maximization - largest $\lambda = \lambda_{max}$

Modularity maximization

Algorithm: Spectral modularity maximization: two-way partition

Input: adjacency matrix A

Output: class indicator vector s

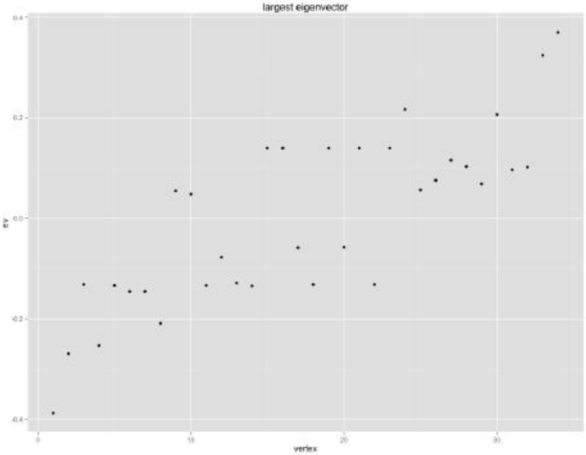
compute $\mathrm{k} = deg(\mathrm{A})$;

compute $\mathrm{B} = \mathrm{A} - \frac{1}{2m}\mathrm{k}\mathrm{k}^T$;

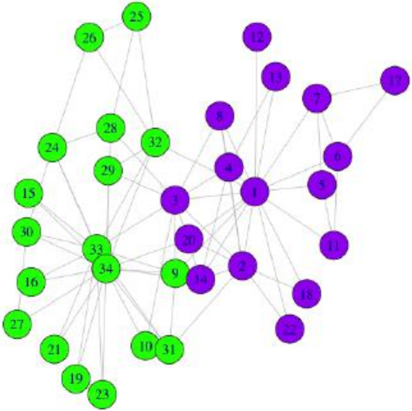
solve for maximal eigenvector $\mathrm{Bx} = \lambda \mathrm{x}$;

set $\mathrm{s} = sign(\mathrm{x}_{max})$

Example



Example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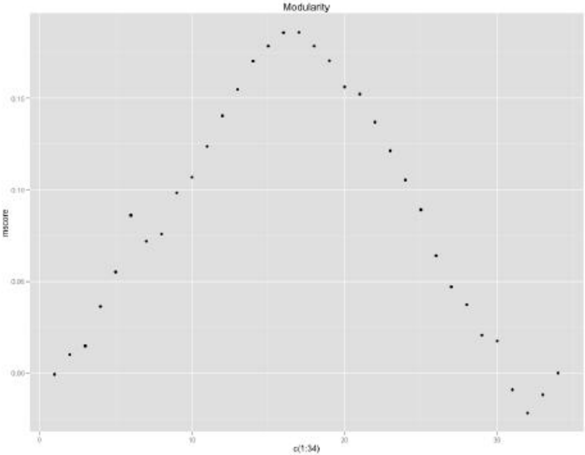
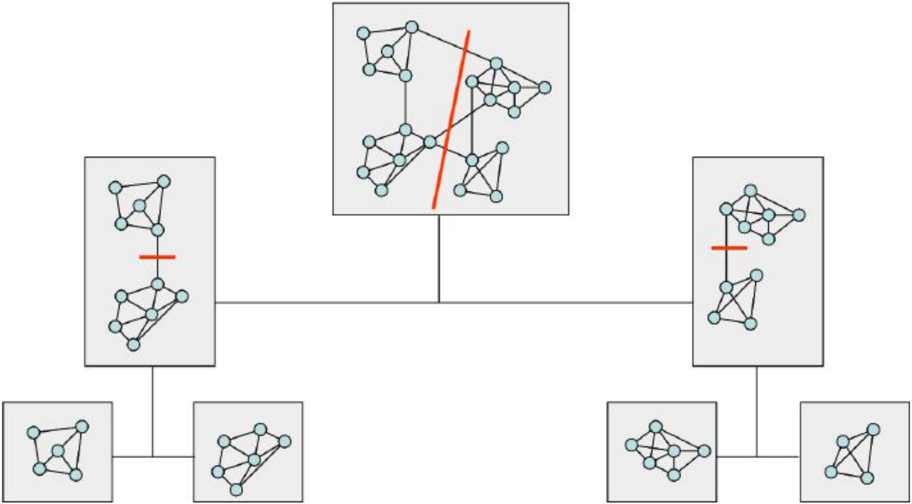
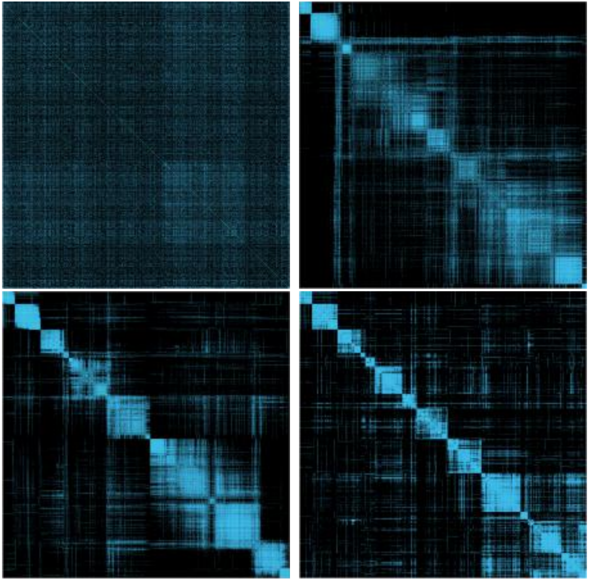


Multilevel spectral



recursive partitioning

Multilevel spectral



Lecture outline

1. Network cores
2. Cliques
3. Network communities
4. Graph paritioning
5. Spectral optimization
   - Min cut
   - Normalized cut
   - Modularity maximization
6. Multilevel spectral
7. Overlapping commmunities
8. Multi-level optimization
9. Random walk methods

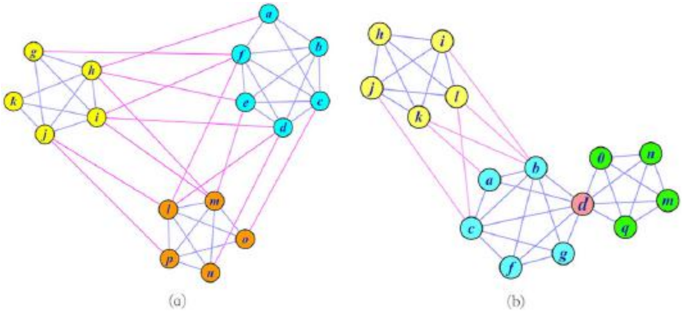
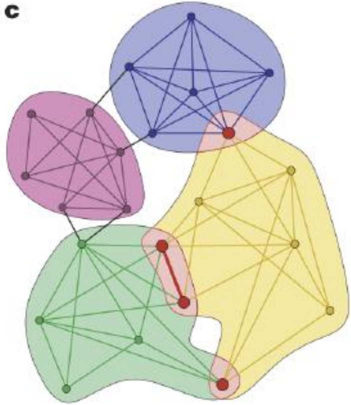


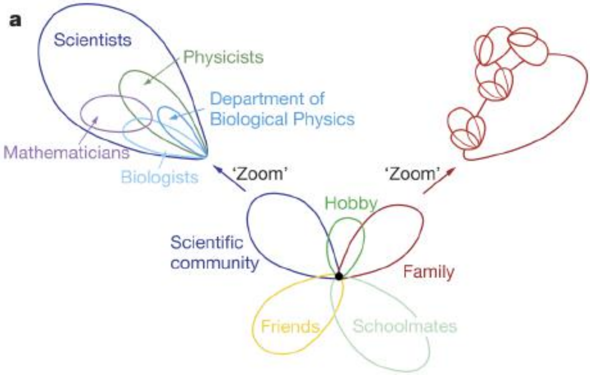
image from W. Liu , 2014

Overlapping communities



Palla, 2005

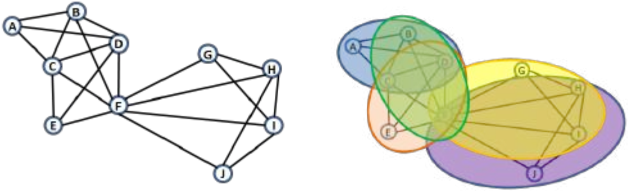
Overlapping communities



Palla, 2005

k-clique community

- k-clique is a clique (complete subgraph) with k nodes
- k-clique community a union of all k-cliques that can be reached from each other through a series of adjacent k-cliques
- two k-cliques are said to be adjacent if they share $k-1$ nodes.



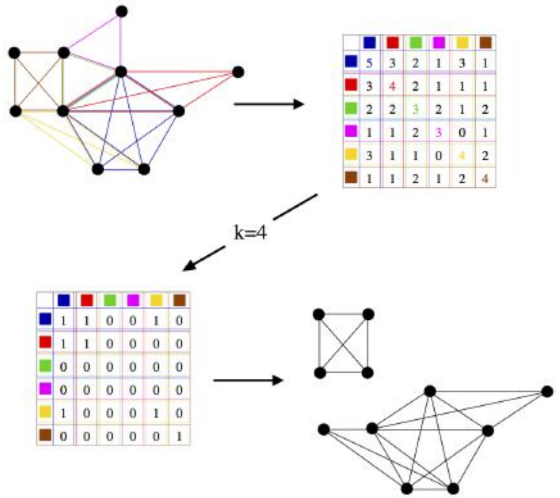
Adjacent 4-cliques

k-clique percolation

- Find all maximal cliques
- Create clique overlap matrix
- Threshold matrix at value $k-1$
- Communities = connected components

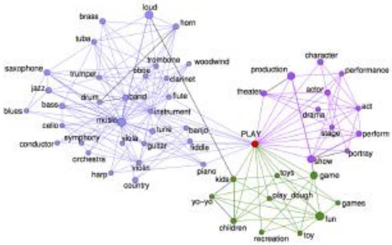
Palla, 2005

k-clique percolation

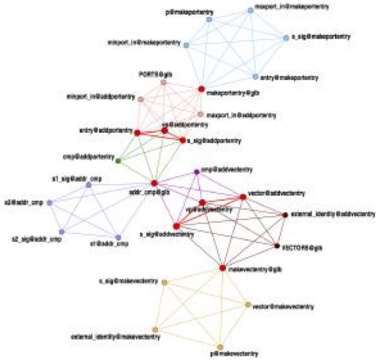


Palla, 2005

k-clique percolation



$k = 4$

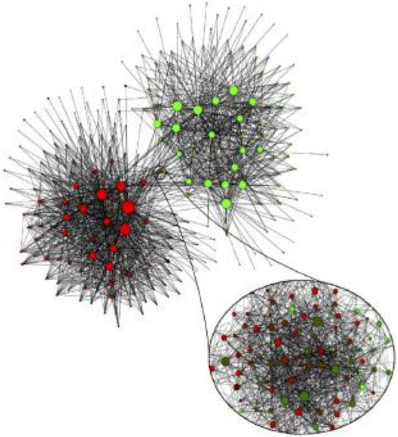


$k = 5$

Palla, 2005

Fast community unfolding

Multi-resolution scalable method



2 mln mobile phone network
V. Blondel et.al., 2008

Fast community unfolding

"The Louvain method"

- Heuristic method for greedy modularity optimization
- Find partitions with high modularity
- Multi-level (multi-resolution) hierarchical scheme
- Scalable

Modularity:

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

V. Blondel et.al., 2008

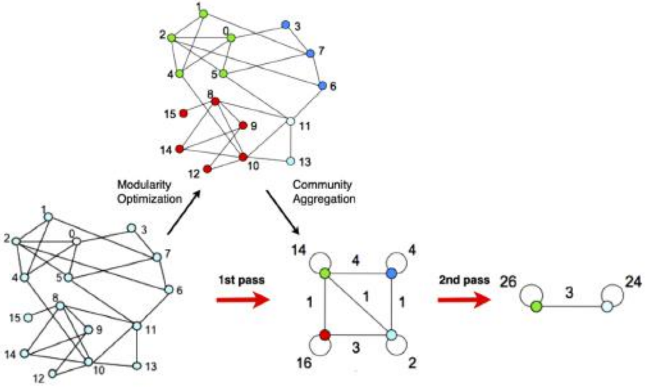
Fast community unfolding

Algorithm

- Assign every node to its own community
- Phase I
  - For every node evaluate modularity gain from removing node from its community and placing it in the community of its neighbor
  - Place node in the community maximizing modularity gain
  - repeat until no more improvement (local max of modularity)
- Phase II
  - Nodes from communities merged into "super nodes"
  - Weight on the links added up
- Repeat until no more changes (max modularity)

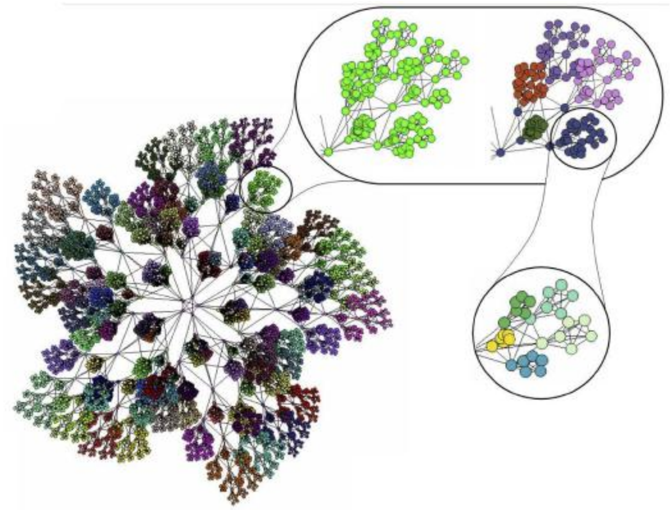
V. Blondel et.al., 2008

Fast community unfolding



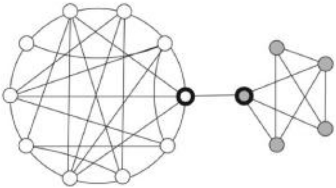
V. Blondel et.al., 2008

Fast community unfolding



V. Blondel et.al., 2008

Communities and random walks



- Random walks on a graph tend to get trapped into densely connected parts corresponding to communities.

Walktrap community

Walktrap

- Consider random walk on graph
- At each time step walk moves to NN uniformly at random $P_{ij} = \frac{A_{ij}}{d(i)}$, $P = D^{-1}A$, $D_{ii} = diag(d(i))$
- P^t_{ij} - probability to get from i to j in t steps, $t \ll t_{mixing}$
- Assumptions: for two i and j in the same community P^t_{ij} is high
- if i and j are in the same community, then $\forall k$, $P^t_{ik} \approx P^t_{jk}$
- Distance between nodes:

$$r_{ij}(t) = \sqrt{\sum_{k=1}^{n} \frac{(P^t_{ik} - P^t_{jk})^2}{d(k)}} = ||D^{-1/2}P^t_i - D^{-1/2}P^t_j||$$

P. Pons and M. Latapy, 2006

Walktrap

Computing node distance r_{ij}

- Direct (exact) computation: $P^t_{ij} = (P^t)_{ij}$ or $P^t_i = P^t p^0_i$, $p^0_i(k) = \delta_{ik}$
- Approximate computation (simulation):
  - Compute K random walks of length t starting form node i
  - Approximate $P^t_{ik} \approx \frac{N_{ik}}{K}$, number of walks end up on k

Distance between communities:

$$P^t_{Cj} = \frac{1}{|C|} \sum_{i \in C} P^t_{ij}$$

$$r_{C_1 C_2}(t) = \sqrt{\sum_{k=1}^{n} \frac{(P^t_{C_1 k} - P^t_{C_2 k})^2}{d(k)}} = ||D^{-1/2} P^t_{C_1} - D^{-1/2} P^t_{C_2}||$$

P. Pons and M. Latapy, 2006

Walktrap

Algorithm (hierarchical clustering)

- Assign each vertex to its own community $S_1 = \{\{v\}, v \in V\}$
- Compute distance between all adjacent communities $r_{C_i C_j}$
- Choose two "closest" communities that minimizes (Ward's methods):

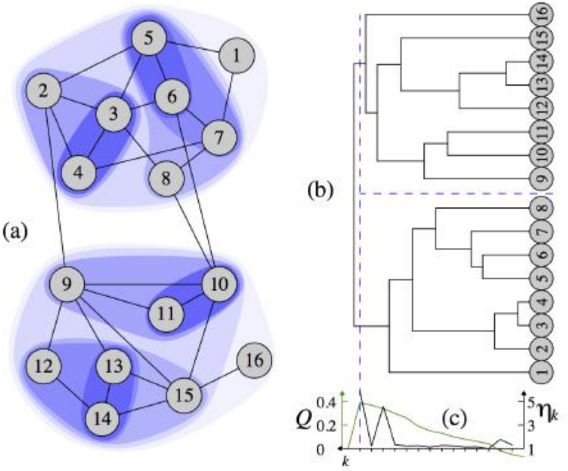
$$\Delta\sigma(C_1, C_2) = \frac{1}{n}\left(\sum_{i \in C_3} r^2_{iC_3} - \sum_{i \in C_1} r^2_{iC_1} - \sum_{i \in C_2} r^2_{iC_2}\right)$$

  and merge them $S_{k+1} = (S_k \backslash \{C_1, C_2\}) \cup C_3,\ C_3 = C_1 \cup C_2$
- update distance between communities

After $n-1$ steps finish with one community $S_n = \{V\}$

P. Pons and M. Latapy, 2006

Walktrap



P. Pons and M. Latapy, 2006

Community detection algorithms

Author	Ref.	Label	Order
Eckmann & Moses	(Eckmann and Moses, 2002)	EM	$O(m\langle k^2\rangle)$
Zhou & Lipowsky	(Zhou and Lipowsky, 2004)	ZL	$O(n^3)$
Latapy & Pons	(Latapy and Pons, 2005)	LP	$O(n^3)$
Clauset et al.	(Clauset *et al.*, 2004)	NF	$O(n\log^2 n)$
Newman & Girvan	(Newman and Girvan, 2004)	NG	$O(nm^2)$
Girvan & Newman	(Girvan and Newman, 2002)	GN	$O(n^2m)$
Guimerà et al.	(Guimerà and Amaral, 2005; Guimerà *et al.*, 2004)	SA	parameter dependent
Duch & Arenas	(Duch and Arenas, 2005)	DA	$O(n^2\log n)$
Fortunato et al.	(Fortunato *et al.*, 2004)	FLM	$O(m^3n)$
Radicchi et al.	(Radicchi *et al.*, 2004)	RCCLP	$O(m^4/n^2)$
Donetti & Muñoz	(Donetti and Muñoz, 2004, 2005)	DM/DMN	$O(n^3)$
Bagrow & Bollt	(Bagrow and Bollt, 2005)	BB	$O(n^3)$
Capocci et al.	(Capocci *et al.*, 2005)	CSCC	$O(n^2)$
Wu & Huberman	(Wu and Huberman, 2004)	WH	$O(n+m)$
Palla et al.	(Palla *et al.*, 2005)	PK	$O(\exp(n))$
Reichardt & Bornholdt	(Reichardt and Bornholdt, 2004)	RB	parameter dependent

Author	Ref.	Label	Order
Girvan & Newman	(Girvan and Newman, 2002; Newman and Girvan, 2004)	GN	$O(nm^2)$
Clauset et al.	(Clauset *et al.*, 2004)	Clauset et al.	$O(n\log^2 n)$
Blondel et al.	(Blondel *et al.*, 2008)	Blondel et al.	$O(m)$
Guimerà et al.	(Guimerà and Amaral, 2005; Guimerà *et al.*, 2004)	Sim. Ann.	parameter dependent
Radicchi et al.	(Radicchi *et al.*, 2004)	Radicchi et al.	$O(m^4/n^2)$
Palla et al.	(Palla *et al.*, 2005)	Cfinder	$O(\exp(n))$
Van Dongen	(Dongen, 2000a)	MCL	$O(nk^2)$, $k<n$ parameter
Rosvall & Bergstrom	(Rosvall and Bergstrom, 2007)	Infomod	parameter dependent
Rosvall & Bergstrom	(Rosvall and Bergstrom, 2008)	Infomap	$O(m)$
Donetti & Muñoz	(Donetti and Muñoz, 2004, 2005)	DM	$O(n^3)$
Newman & Leicht	(Newman and Leicht, 2007)	EM	parameter dependent
Ronhovde & Nussinov	(Ronhovde and Nussinov, 2009)	RN	$O(m^\beta\log n)$, $\beta\sim 1.3$

Fortunato, 2010

Summary

Lectures 1-5 Descriptive Network Analysis

- Network characteristics:
  – Power law node degree distribution
  – Small diameter
  – High clustering coefficient (transitivity)
- Network models:
  – Random graphs
  – Preferential attachment
  – Small world
- Centrality measures:
  – Degree centrality
  – Closeness centrality
  – Betweenness centrality
- Link analysis:
  – Page rank
  – HITS

Summary

Lectures 1-5 Descriptive Network Analysis

- Structural equivalence
  – Vertex equivalence
  – Vertex similarity
- Assortative mixing
  – Assortative and disassortative networks
  – Mixing by node degree
  – Modularity
- Network structures:
  – Cliques
  – k-cores
- Network communities:
  – Graph partitioning
  – Overlapping communities
  – Heuristic methods
  – Random walk based methods

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