#### Network structure

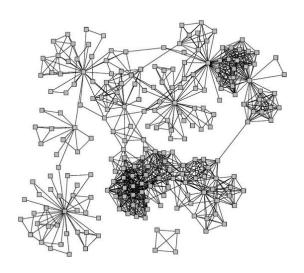
I. Makarov & L.E. Zhukov

### 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

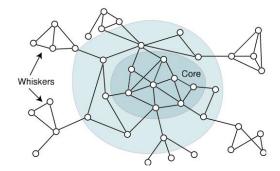
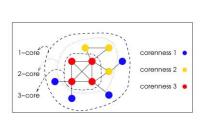


image from J. Leskovec, K. Lang, 2010

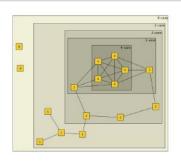
### Graph cores

#### **Definition**

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



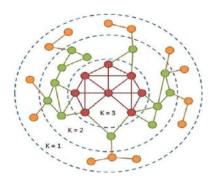
Every vertex in k-core has a degree  $k_i > k$ 



(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

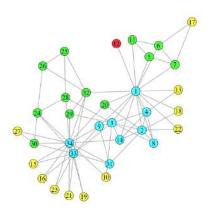
### k-core decomposition

- 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.

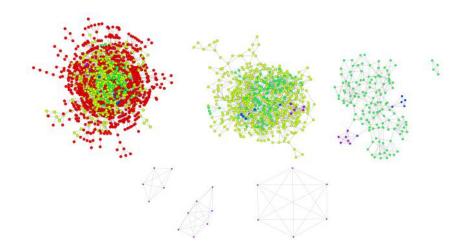


### K-cores

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



#### k-cores

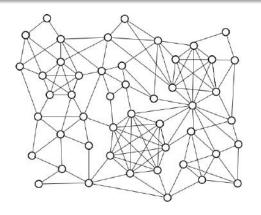


k-cores: 1:1458, 2:594, 3:142, 4:12, 5:6

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

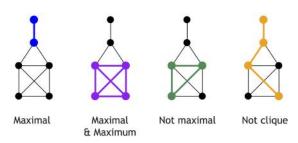
#### **Definition**

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



#### Cliques can overlap

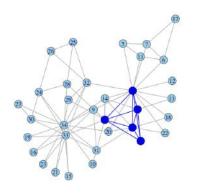
- A maximal clique is a clique that cannot be extended by including one more adjacent vertex (not included in larger one)
- A maximum clique is a clique of the largest possible size in a given graph

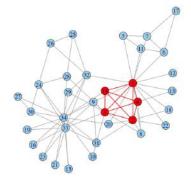


• Graph clique number is the size of the maximum clique

image from D. Eppstein

#### Maximum cliques





Maximal cliques:

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

Zachary, 1977

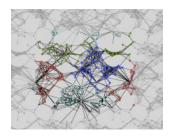
#### Computational issues:

- 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

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

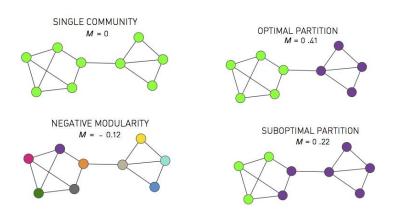
Modularity score

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

 $m_u$  - 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

#### Newman-Girvan, 2004

**Algorithm:** Edge Betweenness

Input: graph G(V,E)

Output: Dendrogram

repeat

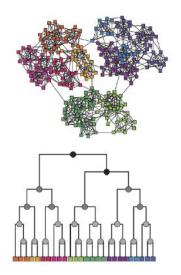
For all  $e \in E$  compute edge betweenness  $C_B(e)$ ;

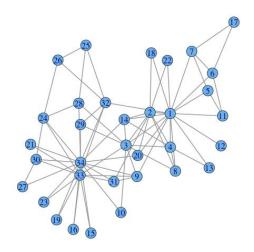
remove edge  $e_i$  with largest  $C_B(e_i)$ ;

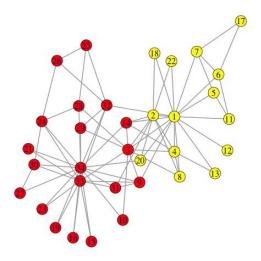
until edges left;

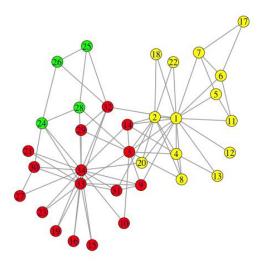
If bi-partition, then stop when graph splits in two components (check for connectedness)

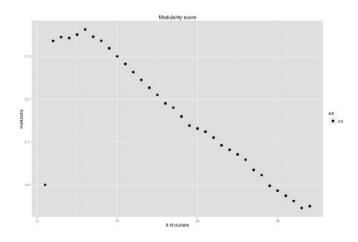
Hierarchical algorithm, dendrogram



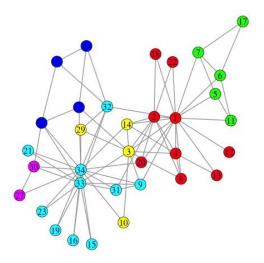


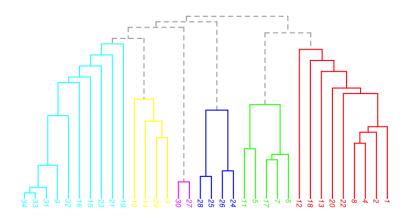






best: clusters = 6, modularity = 0.345





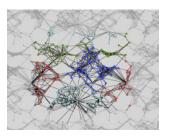
### Lecture outline

- Network cores
- 2 Cliques
- Network communities
- Graph paritioning
- Spectral optimization
  - Min cut
  - Normalized cut
  - Modularity maximization
- Multilevel spectral
- Overlapping communities
- Multi-level optimization
- Random walk methods

#### 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):

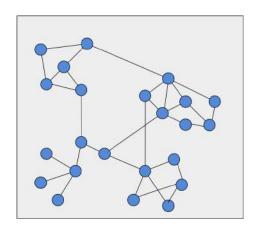
$$B_n = \sum_{k=1}^n S(n,k)$$

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

# 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):

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

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  $\mathbf{s} = \{+1, -1, +1, \dots -1, +1\}^T$  indicator vector

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

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

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

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

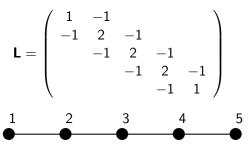
$$cut(V^{+}, V^{-}) = \frac{1}{4} \sum_{i,j} (D_{ij} - A_{ij}) s(i) s(j)$$

### Graph cuts

• Graph Laplacian:  $\mathbf{L}_{ij} = \mathbf{D}_{ij} - \mathbf{A}_{ij}$ , where  $\mathbf{D}_{ii} = diag(k_i)$ 

$$\mathbf{L}_{ij} = \begin{cases} k(i), & \text{if } i = j \\ -1, & \text{if } \exists \ e(i,j) \\ 0, & \text{otherwise} \end{cases}$$

• Laplacian matrix 5x5:



## Graph cuts

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

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

• Minimal cut:

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

Balanced cut constraint:

$$\sum_{i} s(i) = 0$$

Integer minimization problem, exact solution is NP-hard!

# Spectral method - relaxation

- ullet Discrete problem o continuous problem
- Discrete problem: find

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

under constraints:  $s(i) = \pm 1$ ,  $\sum_{i} s(i) = 0$ ;

• Relaxation - continuous problem: find

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

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):

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

• Eigenvalue problem:

$$\mathbf{L}\mathbf{x} = \lambda \mathbf{x}, \ \mathbf{x} \perp \mathbf{e}$$

Solution:

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

• First (smallest) eigenvector:

**Le** = 0, 
$$\lambda$$
 = 0,  $x_1$  = **e**

- Looking for the second smallest eigenvalue/eigenvector  $\lambda_2$  and  $\mathbf{x}_2$
- Minimization of Rayleigh-Ritz quotient:

$$\min_{\mathbf{x} \perp \mathbf{x}_1} (\frac{\mathbf{x}^T \mathbf{L} \mathbf{x}}{\mathbf{x}^T \mathbf{x}})$$

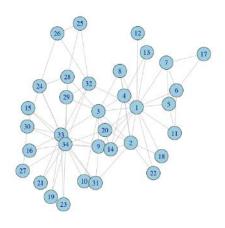
## Spectral graph theory

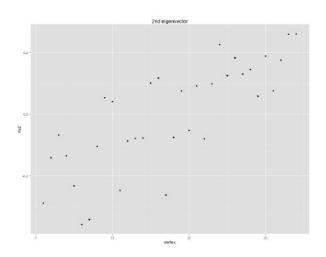
- $\lambda_1 = 0$
- Number of  $\lambda_i = 0$  equal to the number of connected components
- $0 \le \lambda_2 \le 2$   $\lambda_2 = 0$ , disconnected graph  $\lambda_2 = 1$ , totally connected
- Graph diameter (longest shortest path)

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

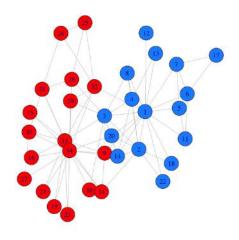
#### Spectral graph partitioning algorithm

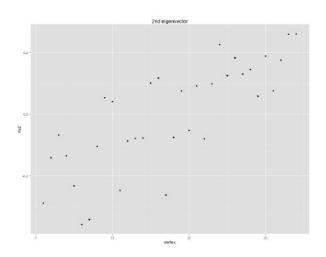
```
Algorithm: Spectral graph partitioning - normalized cuts
Input: adjacency matrix A
Output: class indicator vector s
compute \mathbf{D} = diag(deg(\mathbf{A}));
compute \mathbf{L} = \mathbf{D} - \mathbf{A}:
solve for second smallest eigenvector:
min cut: \mathbf{L}\mathbf{x} = \lambda \mathbf{x}:
normalized cut : Lx = \lambda Dx;
set \mathbf{s} = sign(\mathbf{x}_2)
```



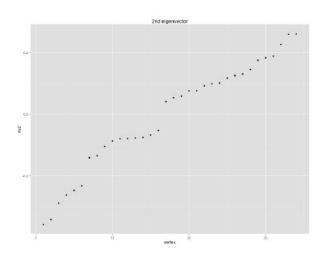


Eigenvalues:  $\lambda_1=$  0,  $\lambda_2=$  0.2,  $\lambda_3=$  0.25 ...

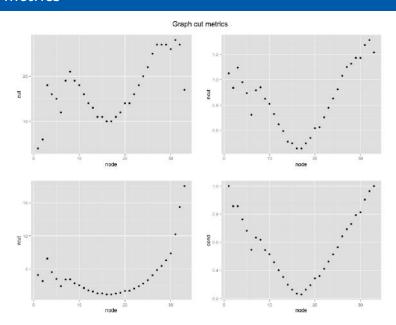




## Spectral ordering



#### Cut metrics



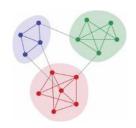
#### Optimization criterion: modularity

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

$$\delta(c_i,c_j) = \left\{ egin{array}{ll} 1: & ext{if} & c_i = c_j \\ 0: & ext{if} & c_i 
eq c_j \end{array} 
ight. ext{- kronecker delta}$$



[Maximization!]

### Spectral modularity maximization

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

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

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:

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

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

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

Eigenvector problem

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

Approximate modularity

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

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

#### Modularity maximization

Algorithm: Spectral modularity maximization: two-way partition

Input: adjacency matrix A

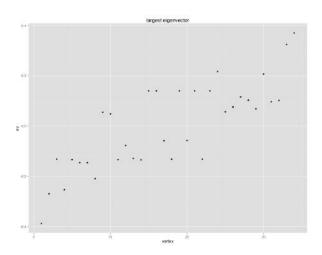
Output: class indicator vector s

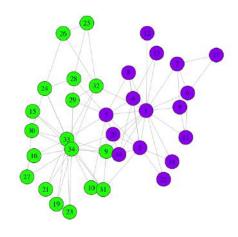
compute  $\mathbf{k} = deg(\mathbf{A})$ ;

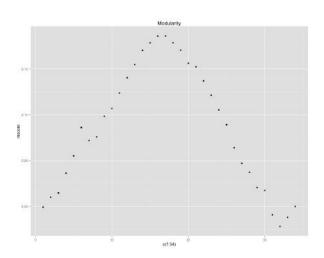
compute  $\mathbf{B} = \mathbf{A} - \frac{1}{2m} \mathbf{k} \mathbf{k}^T$ ;

solve for maximal eigenvector  $\mathbf{B}\mathbf{x} = \lambda \mathbf{x}$ ;

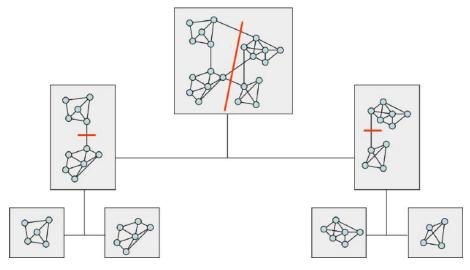
 $\mathsf{set}\ \mathbf{s} = \mathit{sign}(\mathbf{x}_{\mathit{max}})$ 





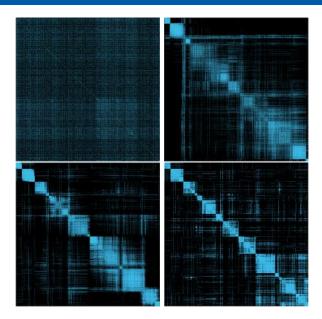


## Multilevel spectral



recursive partitioning

# Multilevel spectral



#### Lecture outline

- Network cores
- 2 Cliques
- Network communities
- Graph paritioning
- Spectral optimization
  - Min cut
  - Normalized cut
  - Modularity maximization
- Multilevel spectral
- Overlapping communities
- Multi-level optimization
- Random walk methods

### Community detection

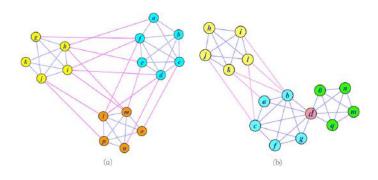
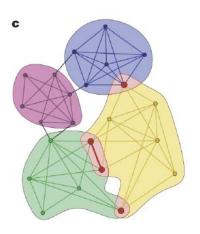


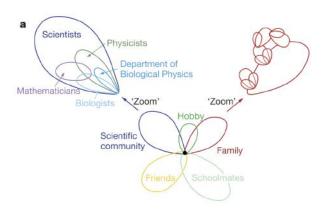
image from W. Liu, 2014

# Overlapping communities



Palla, 2005

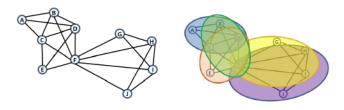
#### Overlapping communities



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.



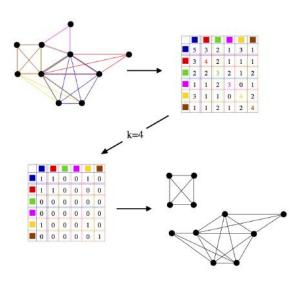
Adjacent 4-cliques

#### k-clique percolation

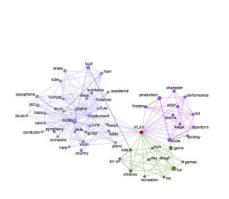
- Find all maximal cliques
- Create clique overlap matrix
- Threshold matrix at value k-1
- Communities = connected components

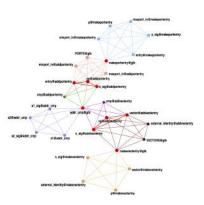
Palla, 2005

### k-clique percolation



#### *k*-clique percolation



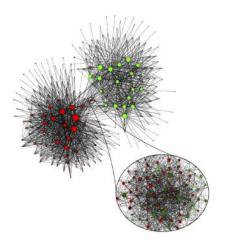


$$k = 4$$

$$k = 5$$

Palla, 2005

#### Multi-resolution scalable method



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

"The Louvain method"

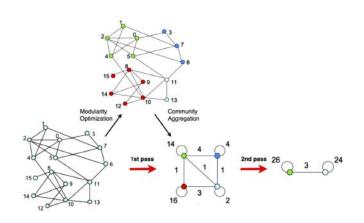
- Heuristic method for greedy modularity optimization
- Find partitions with high modularity
- Multi-level (multi-resolution) hierarchical scheme
- Scalable

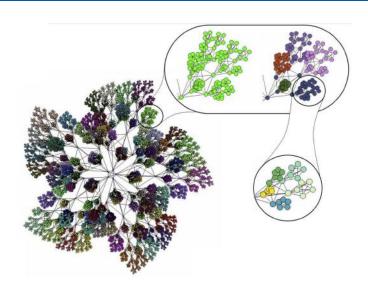
#### Modularity:

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

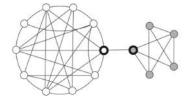
#### Algorithm

- 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)





#### 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  $P_{ij} = \frac{A_{ij}}{d(i)}$ ,  $P = D^{-1}A$ ,  $D_{ii} = diag(d(i))$
- ullet  $P_{ij}^t$  probability to get from i to j in t steps,  $t \ll t_{ extit{mixing}}$
- ullet Assumptions: for two i and j in the same community  $P_{ij}^t$  is high
- if i and j are in the same community, then  $\forall k$ ,  $P_{ik}^t \approx P_{jk}^t$
- Distance between nodes:

$$r_{ij}(t) = \sqrt{\sum_{k=1}^{n} \frac{(P_{ik}^{t} - P_{jk}^{t})^{2}}{d(k)}} = ||D^{-1/2}P_{i}^{t} - D^{-1/2}P_{j}^{t}||$$

#### Walktrap

Computing node distance  $r_{ij}$ 

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

Distance between communities:

$$P_{Cj}^t = \frac{1}{|C|} \sum_{i \in C} P_{ij}^t$$

$$r_{C_1C_2}(t) = \sqrt{\sum_{k=1}^n \frac{(P_{C_1k}^t - P_{C_2k}^t)^2}{d(k)}} = ||D^{-1/2}P_{C_1}^t - D^{-1/2}P_{C_2}^t||$$

#### Walktrap

Algorithm (hierarchical clustering)

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

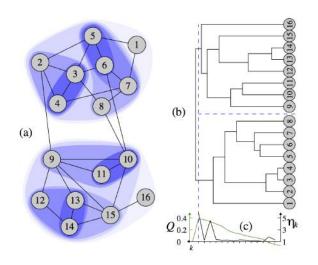
$$\Delta\sigma(C_1, C_2) = \frac{1}{n} \left( \sum_{i \in C_3} r_{iC_3}^2 - \sum_{i \in C_1} r_{iC_1}^2 - \sum_{i \in C_2} r_{iC_2}^2 \right)$$

and merge them  $S_{k+1} = (S_k \setminus \{C_1, C_2\}) \cup C_3$ ,  $C_3 = C_1 \cup C_2$ 

update distance between communities

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

### Walktrap



#### Community detection algorithms

Author	Ref.	Label	Order
Eckmann & Moses	(Eckmann and Moses, 2002)	EM	$O(m(k^2))$
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.	(Radiochi 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.	$O(n \log^3 n)$
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	$O(nk^3)$ , $k < n$ 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	$O(m^{\beta} \log n), \beta \sim 1.3$

#### 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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