### Quality Functions in Graph Clustering

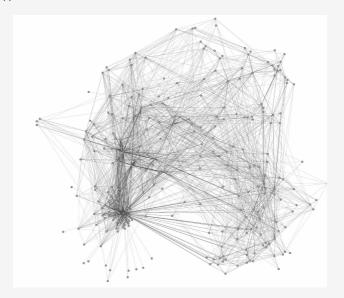
#### Leonidas Pitsoulis

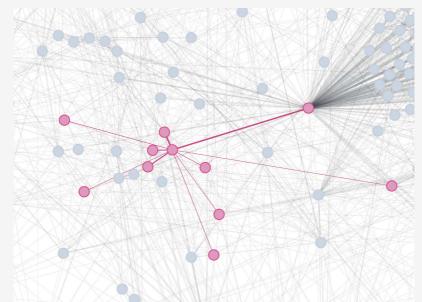
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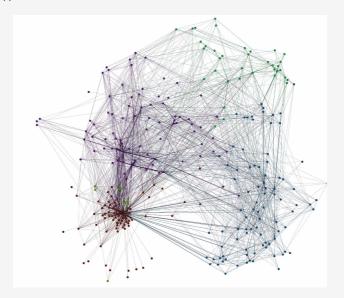
Workshop on clustering and search techniques in large scale networks
Nizhny Novgorod, Russia
3-8 November 2014

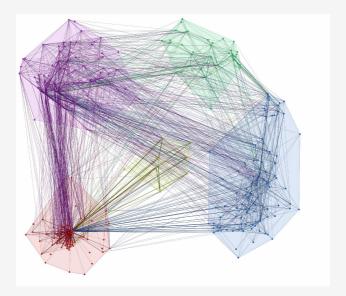
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- 1 Preliminaries
- 2 Axioms for distance based clustering
- 3 Axioms for graph clustering
- 4 Graph clustering quality functions
- 5 Modularity negative results
- 6 Computational experiments
- 7 Clustering criteria





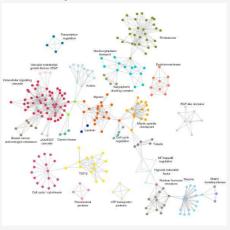




## Community Detection

### Community detection appears as a problem in many real-life networks

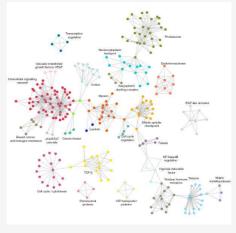
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- metabolic networks
- social networks
- WWW (search engines)
- scientific collaboration networks
- mobile phone networks



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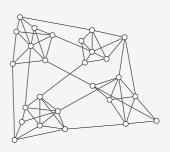


In all cases we are interested in mesoscopic system behavior, derived from the known microscopic dynamics.

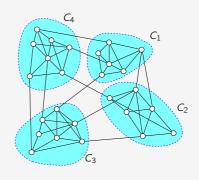
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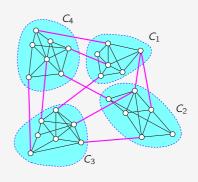
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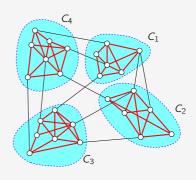
- Graph G = (V, E) and let |V(G)| = n while |E(G)| = m
- A clustering  $C = \{C_1, C_2, ..., C_k\}$  is a partition of V(G)
- The  $C_i \in \mathcal{C}$  are the **clusters**



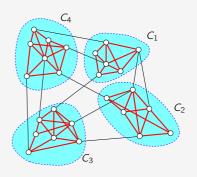
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A network exhibits community structure, if there is a partition of the vertices into groups where the **density** of edges joining the vertices within the groups is higher than the density of edges joining the groups themselves

# Comparing clusterings

### Definition (Jaccard similarity coefficient)

Given G(V, E) and two clusterings  $C_1, C_2$  let

 $a_{1,1}$  = number of vertex pairs which belong to same cluster in both  $C_1$  and  $C_2$ 

 $a_{1,0}$  = number of vertex pairs which belong to same cluster in  $C_1$  only

 $a_{0,1}$  = number of vertex pairs which belong to same cluster in  $C_2$  only

The Jaccard similarity coefficient is defined as

$$J(\mathcal{C}_1, \mathcal{C}_2) = \frac{a_{1,1}}{a_{1,0} + a_{0,1} + a_{1,1}}$$

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- $J(C_1, C_2) \in [0, 1]$  with higher values directly proportional to similarity
- more *exact* algebraic metric for clusterings in Pitsoulis Nanscimento (COR 2013) but requires  $\mathcal{O}(n^3)$  time.

## Distance between clusterings

### Definition

A matrix  $S = (s_{ii}) \in \{0, 1\}^{k \times n}$  is called a basic clustering matrix if

- i) it has no zero rows
- ii)  $\sum_{i=1}^{k} s_{ij} = 1$  for all j = 1, ..., n
- iii) if  $s_{ij}$  is the first nonzero element of row i then  $s_{lt}=0$  for  $l=i+1,\ldots,n$  and  $t=1,\ldots,j$ .

If only conditions i) and ii) are satisfied then the matrix is called clustering matrix.

 $\Rightarrow$  there is a one-to-one correspondence between the set of clusterings of size k and the  $\{0,1\}^{k\times n}$  basic clustering matrices

Given any two clustering matrices  $S \in \{0,1\}^{k_1 \times n}$  and  $T \in \{0,1\}^{k_2 \times n}$  we define their difference set as the set

$$\Delta(S,T) := \{j : S_{ij} \neq T_{ij}, i = 1, \dots, \min\{k_1, k_2\}, j = 1, \dots, n\},\$$

which is the set of columns that these matrices differ.

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## Distance beween clusterings

The distance between any two basic clustering matrices  $S^1 \in \{0, 1\}^{k_1 \times n}$  and  $S^2 \in \{0, 1\}^{k_2 \times n}$  is thus defined as

$$d(S^1, S^2) := \min\{|\Delta(S, T)| : S \in \mathcal{M}(S^1), T \in \mathcal{M}(S^2)\}.$$

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 $\Rightarrow$   $d(S^1, S^2)$  is the minimum number of *moves* of elements between the clusters in the clusterings associated with the basic clustering matrices  $S^1$  and  $S^2$ , needed to transform one clustering to another

#### Lemma

For some graph G(V, E) and any three clusterings  $C_1$ ,  $C_2$  and  $C_3$  the following statements are true:

- i)  $d(S_{C_1}, S_{C_2}) \ge 0$  with equality iff  $S_{C_1} = S_{C_2}$
- ii)  $d(S_{\mathcal{C}_1}, S_{\mathcal{C}_2}) = d(S_{\mathcal{C}_2}, S_{\mathcal{C}_1})$
- iii)  $d(S_{\mathcal{C}_1}, S_{\mathcal{C}_2}) + d(S_{\mathcal{C}_2}, S_{\mathcal{C}_3}) \geq d(S_{\mathcal{C}_1}, S_{\mathcal{C}_3})$

### Clusterings - Distance

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### Proof.

Given the two basic clustering matrices  $S^1=(s^1_{ij})$  and  $S^2=(s^2_{ij})$ , construct a  $k\times k$  cost matrix  $C=(c_{ij})$ 

$$c_{ij} := \sum_{l=1}^{n} |s_{il}^{1} - s_{jl}^{2}|,$$

for i, j = 1, ..., k. Then optimum solution to related LAP gives the distance.

### Example

Say we have n = 10 vertices and two clusterings

$$\mathcal{C}_1 = \{\{1,4,5\},\{2\},\{3,8\},\{6,7\},\{9,10\}\},$$

$$C_2 = \{\{1, 2, 9\}, \{3, 8\}, \{4, 5, 10\}, \{6, 7\}\}$$

Then the basic clustering matrices

For the distance computation

$$C = \begin{bmatrix} 4 & 2 & 5 & 5 \\ 5 & 3 & 0 & 4 \\ 2 & 4 & 4 & 5 \\ 5 & 3 & 4 & 0 \end{bmatrix},$$

### Example

So the optimum permutation is p = (3, 1, 2, 4) and

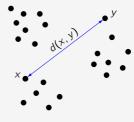
So we have  $\Delta^*(S_{\mathcal{C}_1}, S_{\mathcal{C}_2}) = \Delta(S_{\mathcal{C}_1}, S) = \{1, 9, 10\}$ , which implies that  $d(S_{\mathcal{C}_1}, S_{\mathcal{C}_2}) = 3$ .

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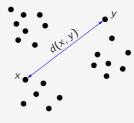
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- lacktriangle A **clustering**  $\mathcal{C}$  is a partition of X







# Clustering functions

### Definition

■ A **clustering function** is a function F which given a data set X and a distance function d it returns a partition C of X.

$$F:(X,d)\to \mathcal{C}$$

■ A **clustering quality function** is any function Q which given a data set X, a partioning C of X and a distance function d it returns a real number.

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Given Q we can define F as the extrema

$$F(X, d) = \arg\max_{\mathcal{C}} Q(X, d, \mathcal{C})$$

⇒ any property of *clustering functions* can stated for *clustering quality functions* 

### Kleinberg's Impossibility Theorem

### Kleinberg's axioms for clustering functions F(X, d)

- i. Scale Invariance: *F* produces the same clustering if distances between points are scaled uniformly.
- ii. Richness: if any clustering of the points can be produced by modifying the distances between the points.
- iii. Consistency: for any clustering that F produces, decreasing inner cluster distances or increasing outer cluster distances gives a set of points that F produces the same clustering.

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### Theorem (Kleinberg (NIPS 2002))

There is no clustering function that satisfies scale invariance, richness and consistency at the same time.

## Consistency through quality functions

Ackerman and Ben-David (NIPS 2009) properties for quality functions.

i. Scale Invariance: Q is **scale invariant** if for every clustering  $\mathcal{C}$  of (X,d) and every positive  $\lambda$ 

$$Q(X, d, \mathcal{C}) = Q(X, \lambda d, \mathcal{C})$$

ii. Richness: Q is **rich** if for any  $C^*$  of X there exists some d over X such that

$$C^* = \underset{C}{\operatorname{arg max}} Q(X, d, C)$$

iii. Consistency: Q is **consistent** if for any C of X, if  $d_C$  corresponds to d where intra (extra) cluster distances are decreased (increased) then

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- presented a number of quality functions which constitute the above set of axioms consistent
- propose a set of axioms which include relaxations of the above plus isomorphism invariance
- the above results can be extended to graph clustering quality functions

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# Properties of graph clustering quality functions

#### We have identified the following properties

- i. Isomorphism invariance
- ii. Scale invariance
- iii. Richness
- iv. Monotonicity
- v. Perfectness
- vi. Connectivity
- vii. Convexity
- viii. Complementarity
- ix. Resolution limit free

#### Isomorphism

#### Property (Isomorphism invariance)

A quality function Q is **isomorphism invariant** if for any pair of isomorphic graphs  $G_1 \cong G_2$  with isomorphism  $\phi$ , we have

$$Q(G_1, \mathcal{C}) = Q(G_2, \phi(\mathcal{C})), \quad \text{for all } \mathcal{C} \in 2^{|\mathcal{V}|}$$
 (1)

where  $\phi(C)$  = {{ $\phi(v)$  :  $v \in C$ } :  $C \in C$ }.

quality function values of two isomorphic graphs should be equal for clusterings under the same isomorphism

# Scaling

#### Property (Scale invariance)

A quality function Q is **scale invariant** if for a graph G with weight function  $w : E(G) \to \mathbb{R}$  and a constant  $\alpha > 0$ , we have

$$Q(G, \mathcal{C}) = Q(\alpha G, \mathcal{C}), \quad \text{for all } \mathcal{C} \in 2^{|V|},$$
 (2)

where the weighted graph  $\alpha G$  is defined as  $E(\alpha G) = E(G)$ ,  $V(\alpha G) = V(G)$  with weight function  $z(e) = \alpha w(e)$ ,  $e \in E(\alpha G)$ .

quality function should be invariant under a uniform scaling of the edge weights in a graph

#### **Richness**

#### Property (Richness)

A quality function Q is **rich** if for any finite set of vertices V and a partition  $C^* \in 2^{|V|}$  there exists a set of edges E such that for G = (V, E)

$$C^* = \arg\max\{Q(G, C) : C \in 2^{|V|}\}.$$
(3)

for any partition of a finite set V we can find a graph with V as its vertex set such that the partition will be the maximum value of the clustering quality function

# Monotonicity

#### Property (Monotonicity)

A quality function is **monotone** if for any graph G, clustering C of V(G), and any graph G' satisfying:

(i) 
$$V(G') = V(G)$$
,

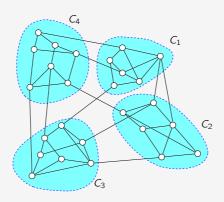
(ii) 
$$E^+(G, \mathcal{C}) \subseteq E^+(G', \mathcal{C})$$
 and  $E^-(G', \mathcal{C}) \subseteq E^-(G, \mathcal{C})$ ,

we have

$$Q(G,\mathcal{C}) \le Q(G',\mathcal{C}). \tag{4}$$

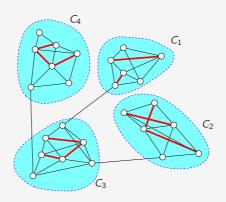
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#### Perfectness

#### Property (Perfectness)

A quality function is **perfect** if for any graph G(V, E), the following are true

(i) if  $C^*$  is a clustering on V(G) such that we cannot add an intra-cluster edge nor remove an extra-cluster edge, then

$$Q(G, \mathcal{C}^*) = \max\{Q(G', \mathcal{C}) : \text{all } G' \text{ such that } V(G') = V, \mathcal{C} \in 2^{|V|}\}.$$

(ii) if  $C^*$  is a clustering on V(G) such that we cannot add an extra-cluster edge nor remove an intra-cluster edge, then

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quality function should provide the maximum value among all possible graphs and clusterings on this vertex set

# Connectivity

#### Property (Connectivity)

Let a graph G, a clustering C that contains a dissconnected cluster C with a partition  $\{C_1, C_2, \ldots, C_k\}$  such that  $G[C_1], \ldots, G[C_k]$  are the connected components of G[C], and a clustering D obtained from C by replacing C with  $\{C_1, C_2, \ldots, C_k\}$ . A quality function Q is called **connected** if for any such triple G, C, D we have

$$Q(G, C) \leq Q(G, D)$$

minimum requirement for a cluster to be be classified as a community is that the associated induced subgraph should be connected

### Convexity

#### Definition

Given a graph G(V, E) some set of vertices  $X \subseteq V(G)$  is called **convex** in G if for any pair of vertices  $v, w \in X$  the shortest v - w path contains vertices only from X.

#### Property (Convexity)

Let a graph G, a clustering C that contains a nonconvex cluster C with a partition  $\{C_1, C_2, \ldots, C_k\}$  such that  $C_1, \ldots, C_k$  are convex, and a clustering D obtained from C by replacing C with  $\{C_1, C_2, \ldots, C_k\}$ . A quality function Q is called **convex** if for any such triple G, C, D we have

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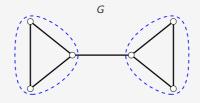
# Complentarity

#### Property (Complementarity)

A quality function Q is **complementary** if for any graph G, its complement  $\overline{G}$ , and any clustering C of V(G),

$$Q'(G,\mathcal{C})=1-Q'(\bar{G},\mathcal{C})$$

where Q' the function which results as a uniform scaling on the range of Q in the interval [0,1].



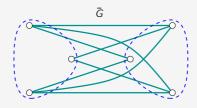
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#### Resolution-limit-free

Introduced by Traag, van Dooren, and Nesterov (2011)

#### Property (**Resolution-limit-freedom**)

Let  $C = \{C_1, C_2, ..., C_k\}$  be a Q-optimal clustering of a graph G, for some quality function Q. Then, Q is called **resolution-limit-free** if for each subgraph of G induced by  $\mathcal{D} \subset C$ , the partition  $\mathcal{D}$  is also Q-optimal.

attempt to rigorously define the resolution limit of some quality functions

### Axiomatic system

Consider that we have an axiomatic system say AQF. Then it should be:

- **consistent**: there exists at least one quality function which satisfies all axioms
- independent: there does not exist a set of axioms  $\mathcal{A}$  of AQF and an axiom A of AQF such that  $\mathcal{A} \not\Rightarrow A$ .

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Consider that we have an axiomatic system say AQF. Then it should be:

- **consistent**: there exists at least one quality function which satisfies all axioms
- independent: there does not exist a set of axioms  $\mathcal{A}$  of AQF and an axiom A of AQF such that  $\mathcal{A} \not\Rightarrow A$ .

But we would like to have results of the form

#### Theorem

Let  $Q_1$  and  $Q_2$  be two graph clustering quality functions which satisfy AQF and G a graph. Then

$$\arg\max\{Q_1(G,\mathcal{C}):\mathcal{C}\in 2^{|V(G)|}\}=\arg\max\{Q_2(G,\mathcal{C}):\mathcal{C}\in 2^{|V(G)|}\}.$$

#### Outline of the talk

- 1 Preliminaries
- 2 Axioms for distance based clustering
- 3 Axioms for graph clustering
- 4 Graph clustering quality functions
- 5 Modularity negative results
- 6 Computational experiments
- 7 Clustering criteria

### Graph clustering quality functions

We have examined the following types of graph clustering quality functions

- i. modularity
- ii. density
- iii. distance
- iv. node membership
- v. connectivity

### Graph clustering quality functions

We have examined the following types of graph clustering quality functions

- i. modularity
- ii. density
- iii. distance
- iv. node membership
- v. connectivity
- all functions other than the modularity are new
- in each type of function we can formulated it based on a random model

# Modularity

Modularity is a quality function introduced by Newman and Girvan that quantifies the community structure by providing a value for every clustering of a given graph.

■ Newman MJ, Girvan M. Finding and evaluating community structure in networks, Physical Review E 2004, 69(026113).

### Modularity - Main Idea

Employ a random graph on the same vertex set that does not have any community structure and compare the edge densities of the clusters in the original graph and the random graph.

The modularity of a clustering  ${\cal C}$  for some graph  $\,{\cal G}_{\cdot}$  is defined by the following normalized sum of differences

$$Q_m(\mathcal{C},G) := \frac{1}{2m} \sum_{C \in \mathcal{C}} \sum_{i,j \in C} (a_{ij} - p_{ij})$$

- $a_{ii} =$  number of edges between vertices i and j in G
- $p_{ij} = is$  the expected number of edges between vertices i and j in the random graph

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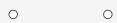
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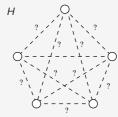
$$Q_m(\mathcal{C},G) := \frac{1}{2m} \sum_{C \in \mathcal{C}} \sum_{i,j \in C} (a_{ij} - p_{ij})$$

- $a_{ij} = \text{number of edges between vertices } i \text{ and } j \text{ in } G$
- $\mathbf{p}_{ij} =$ is the expected number of edges between vertices i and j in the random graph

# Modularity - Main Idea

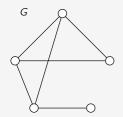
Question: How do we define the random graph (equivalently the  $p_{ij}$ )?

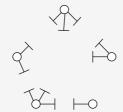


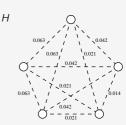


# Modularity - the Random Graph

Random Graph Property: Keep the same degree distribution as in the original graph

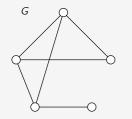




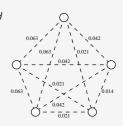


# Modularity - the Random Graph

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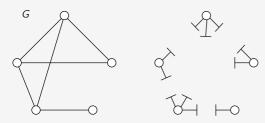


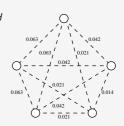
Random graph H will have V(H) = V(G) and E(G) defined by

$$Pr[(i,j) \in E(H)] = \frac{d_G(i)}{2m} \cdot \frac{d_G(j)}{2m}.$$

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 $\Rightarrow$  expected number of edges between i and j then is

$$p_{ij} = 2m \times Pr[(i,j) \in E(H)] = \frac{d_G(i)d_G(j)}{2m}$$

# Modularity - unweighted graphs

we thus have

$$Q_m(G,C) = \frac{1}{2m} \sum_{C \in C} \sum_{i,j \in C} \left( a_{ij} - \frac{d_G(i)d_G(j)}{2m} \right)$$

where  $a_{ij}$  is the number of edges between vertices i and j in G. Its is *straighforward* to show that

$$Q_m(G,C) = \sum_{C \in C} \left[ \frac{m_C}{m} - \left( \frac{d_G(C)}{2m} \right)^2 \right]$$
 (5)

where m = |E(G)| and  $m_C = |E(G[C])|$ , and the terms

 $\frac{m_C}{m}$  : fraction of edges within cluster C

 $\left(\frac{d_G(C)}{2m}\right)^2$  : expected fraction of edges within cluster C

### Modularity - weighted graphs

Given a weight function  $w: E(G) \to \mathbb{R}$  on the edges of a graph, we can define the **strength** of a vertex  $i \in V(G)$  as

$$s_G(i) := \sum_{j \in V(G)} w(i,j).$$

We can then write for the modularity of a clustering  ${\mathcal C}$  for some weighted graph G

$$Q_{m_w}(G,\mathcal{C}) = \frac{1}{2\sum_{e \in E(G)} w(e)} \sum_{C \in \mathcal{C}} \sum_{i,j \in C} \left( w(i,j) - \frac{s_G(i)s_G(j)}{2\sum_{e \in E(G)} w(e)} \right).$$

### Modularity - directed graphs

If G directed let  $a_{ij}$  denote the number of **directed** edges from vertex i to vertex j while  $d_G^+(i)$  and  $d_G^-(i)$  be in-degree and out-degree of vertex i, respectively. We will therefore have

$$d_G^+(i) = \sum_j a_{ji}, \ d_G^-(j) = \sum_i a_{ij}.$$

In order to generalize modularity for directed graphs, it is enough to construct a random directed graph without any community structure for where the expected in-degree and out-degree sequence will be the same as in G. The modularity of a clustering  $\mathcal C$  in a directed graph G is given by the following

$$Q_{m_d}(G,\mathcal{C}) = \frac{1}{m} \sum_{C \in \mathcal{C}} \sum_{i,j \in C} \left( a_{ij} - \frac{d_G^-(i)d_G^+(j)}{m} \right).$$

# Modularity - weighted directed graphs

Generalizing the strength of a vertex  $i \in V(G)$  into **in-strength** and **out-strength** for a weighted directed graph G as follows,

$$s_{G}^{-}(i) = \sum_{j \in V(G)} w(i, j), \quad s_{G}^{+}(i) := \sum_{j \in V(G)} w(j, i), \tag{6}$$

we can combine the expressions for  $Q_{m_d}$  and  $Q_{m_w}$  to derive the an expression for modularity for weighted directed graphs

$$Q_{m_{w,d}}(G,C) = \frac{1}{\sum_{i,j \in V(G)} (w(i,j) + w(j,i))} \sum_{C \in C} \sum_{i,j \in C} \left( w(i,j) - \frac{s_G^-(i)s_G^+(j)}{\sum_{i,j \in V(G)} (w(i,j) + w(j,i))} \right).$$

### Modularity maximization - IP Formulation

Define  $n^2$  binary variables  $x_{ij}$  for each pair of nodes  $i, j \in V(G)$  as

$$x_{ij} := \begin{cases} 1, & \text{if vertices } i \text{ and } j \text{ belong in the same cluster,} \\ 0, & \text{otherwise.} \end{cases}$$

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This results in the following  $\{0, 1\}$  program

max 
$$\frac{1}{2m} \sum_{i,j \in V(G)} \left( a_{ij} - \frac{d_G(i)d_G(j)}{2m} \right) x_{ij}$$
s.t. 
$$x_{ii} = 1, \quad \forall i \in V(G)$$

$$x_{ij} = x_{ji}, \quad \forall i, j \in V(G)$$

$$x_{ij} + x_{jk} \le 2x_{ik} + 1, \quad \forall i, j, k \in V(G)$$

$$x_{ij} \in 0, 1, \quad \forall i, j \in V(G)$$

# Modularity properties

#### Theorem (Gevezes, Kehagias and Pitsoulis, 2013)

The modularity function is **not**:

- monotone
- connected
- convex
- complementary
- resolution-limit free

so it seems that modularity fails in almost all theoretical properties, but is the most widely used!

# Anti-modularity

Based on the same random model as modularity, but instead of maximizing intra-cluster edge density it **minimizes extra-cluster edge density**.

$$Q_{anti-m}(G,C) = -\sum_{\substack{C_1,C_2 \in C \\ C_1 \neq C_2}} \left[ \frac{m_{C_1 \leftrightarrow C_2}}{m} - \left( \frac{d_G(C_1)d_G(C_2)}{4m^2} \right) \right]$$

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- similar behavior as modularity
- performs better in unbalanced community structure
- open problem: has not been examined yet w.r.t. properties

#### Components quality function

#### Definition

A graph is connected if for any  $v, w \in V(G)$  there exists a v - w path. The number of connected components of a graph G will be denoted by  $k_G$ .

The **components quality function** takes the value of 1 for clusterings which identify with the connected components of the graph and 0 elsewhere. It is defined as follows

$$Q_{coco} = \begin{cases} 1 & \text{if the members of } \mathcal{C} \text{ are the connected components of } G, \\ 0 & \text{otherwise,} \end{cases}$$
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# Theorem (Gevezes, Kehagias and Pitsoulis, 2013)

 $Q_{coco}$  is isomorphishm invariant, scale invariant, rich, connected, monotone, complementary and perfect.

# Higher connectivity

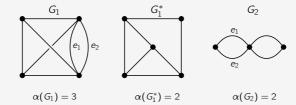
# Definition (edge connectivity)

- For  $k \in \mathbb{N}$  we say that a graph G is k-edge-connected, if |E(G)| > k and  $G \setminus Y$  is connected for any  $Y \subseteq E(G)$  with |Y| < k.
- Equivalently G is k-edge-connected if k is the minimum number of edges that you can delete and make G disconnected or the trivial graph  $K_1$ .
- We will write  $\alpha(G)$  for the edge connectivity number of a graph.

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# Edge connectivity quality function

Using the same random graph H definition as in modularity we define the edge connectivity quality function as

$$Q_{\alpha}(G, \mathcal{C}) = \sum_{C \in \mathcal{C}} \left[ \frac{\alpha(G[C])}{\alpha(G)} - \frac{mincut(H[C])}{mincut(H)} \right]$$

where G[C] and H[C] are the induced subgraphs of G and H by the set of vertices C, and

 $\frac{\alpha(G[C])}{\alpha(G)}$  : relative edge connectivity of cluster C

 $\frac{mincut(H[C])}{mincut(H)}$  : expected edge connectivity of cluster C

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- other variations using Tutte-connectivity and vertex connectivity
- computationally not attractive
- open problem: is it monotone, rich, etc. ?

# Local density

These functions are based on the **densities** of intra-cluster and extra-cluster edges. We are given a graph G and a clustering  $C = \{C_1, \ldots, C_k\}$ . Let

 $E_C$ : the edges of G with both end-vertices in cluster C

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The **local density** quality function is defined as

$$Q_{ld}(G,C) := \frac{1}{2k} \sum_{C \in C} \left[ \frac{|E_C|}{|C| \cdot (|C| - 1)/2} + \left( 1 - \frac{|E_C'|}{|C| \cdot |V(G) - C|} \right) \right]$$

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 $\frac{|E_C|}{|C| \cdot (|C| - 1)/2}$  : density of intra-cluster edges of cluster C

 $\frac{|E'_C|}{|C| \cdot |V(G) - C|}$  : density of extra-cluster edges of cluster C

 $Q_{Id}(G, C)$  : average of cluster densities

# Global density

The global density quality function as

$$Q_{gd}(G, \mathcal{C}) := \frac{1}{2} \left[ \frac{\sum_{C \in \mathcal{C}} |E_C|}{\sum_{C \in \mathcal{C}} |C| \cdot (|C| - 1)/2} + \left( 1 - \frac{\sum_{C \in \mathcal{C}} |E_C'|}{\sum_{C \in \mathcal{C}} |C| \cdot |V(G) - C|} \right) \right]$$

where

 $\frac{\sum_{C \in \mathcal{C}} |E_C|}{\sum_{C \in \mathcal{C}} |C| \cdot (|C| - 1)/2}$ : density of **all** intra-cluster edges

 $\frac{\sum_{C \in \mathcal{C}} |E'_C|}{\sum_{C \in \mathcal{C}} |C| \cdot |V(G) - C|} : \text{ density of all extra-cluster edges}$ 

 $Q_{gd}(G, C)$  : average of cluster densities

# Density based quality functions

# Theorem (Gevezes, Kehagias and Pitsoulis, 2013)

 $Q_{ld}$  and  $Q_{gd}$  are isomorphishm invariant, scale invariant, monotone, complementary and perfect.

- Let graph G, its complement  $\overline{G}$  and a clustering C of V(G).
- Since the range of both functions  $Q_{ld}$  and  $Q_{qd}$  is [0, 1] scaling will not be necessary.

We will first prove the statement for  $Q_{ld}$ 

- For some  $C \in \mathcal{C}$  let

$$m_C = |E_C| + |\bar{E}_C|$$
 : number of possible edges with both end-vertices in  $G[C]$  (8)

$$m'_C = |E'_C| + |\bar{E}'_C|$$
 : number of possible edges with one end-vertex in  $G[C]$  (9)

It follows that

$$\frac{|E_C|}{|C| \cdot (|C| - 1)/2} = \frac{|E_C|}{m_C} = 1 - \frac{|\bar{E}_C|}{m_C},$$

$$\frac{|E'_C|}{|C| \cdot |V(G) - C|} = \frac{|E'_C|}{m'_C} = 1 - \frac{|\bar{E}'_C|}{m'_C}.$$

Letting

$$a_C = \frac{|E_C|}{m_C}, \bar{a}_C = \frac{|\bar{E}_C|}{m_C},\tag{10}$$

and

$$e_C = \frac{|E'_C|}{m'_C}, \bar{e}_C = \frac{|\bar{E}'_C|}{m'_C},$$
 (11)

we have that

$$a_C = 1 - \bar{a}_C$$
,  $e_C = 1 - \bar{e}_C$ 

Substituting (10) and (11) in the expression for  $Q_{ld}(G, \mathcal{C})$  we get

$$Q_{ld}(G,C) = \frac{1}{2k} \sum_{C \in C} [a_C + (1 - e_C)]$$

$$= \frac{1}{2k} \sum_{C \in C} [(1 - \bar{a}_C) + 1 - (1 - \bar{e}_C)]$$

$$= \frac{1}{2} - \frac{1}{2k} \sum_{C \in C} (\bar{a}_C - \bar{e}_C)$$

$$= 1 - Q_{ld}(\bar{G},C).$$

For  $Q_{gd}$  we extend the analysis by summing up the values of (8) and (9)

Let

$$m = \sum_{C \in \mathcal{C}} m_C$$
,  $m' = \sum_{C \in \mathcal{C}} m'_C$ 

and

$$a = \frac{\sum_{C \in \mathcal{C}} |E_C|}{m}, \, \bar{a} = \frac{\sum_{C \in \mathcal{C}} |\bar{E}_C|}{m}, \tag{12}$$

$$e = \frac{\sum_{C \in \mathcal{C}} |E'_C|}{m}, \bar{e} = \frac{\sum_{C \in \mathcal{C}} |E'_C|}{m}, \tag{13}$$

while it follows that

$$a=1-\bar{a}, \ e=1-\bar{e}.$$

-Substituting (12) and (13) in the expression for  $Q_{qd}(G,\mathcal{C})$  we get

$$Q_{gd}(G,C) = \frac{1}{2}[a+1-e]$$

$$= \frac{1}{2}[(1-\bar{a})-(1-\bar{e})] + \frac{1}{2}$$

$$= 1 - Q_{gd}(\bar{G},C)$$

#### Definition

Given a graph G(V, E) we define the following:

- v w walk is an alternating sequence of vertices and edges, begining with vertex v and ending with vertex w
- trail is a walk with distinct edges
- **path** is a walk with distinct vertices
- shortest path between two vertices is a path with the smallest number of edges (may not be unique)

# Definition (adjacency matrix)

The adjacency matrix of a graph G(V, E), is a  $n \times n$  matrix  $A_G$  defined as

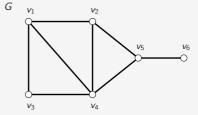
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$$A_{G} = \begin{bmatrix} v_{1} & v_{2} & v_{3} & v_{4} & v_{5} & v_{6} \\ v_{2} & 0 & 1 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 1 & 0 \\ v_{5} & 0 & 1 & 0 & 1 & 0 & 1 \\ v_{6} & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$



It is well know that by taking the powers of the adjacency matrix  $A_G^k$  we have

$$A_G^k$$
 = is the number of  $v_i - v_j$  walks

So we have for our example

$$A_{G}^{2} = \begin{bmatrix} v_{1} & v_{2} & v_{3} & v_{4} & v_{5} & v_{6} \\ v_{2} & 3 & 1 & 1 & 2 & 2 & 0 \\ 1 & 3 & 2 & 2 & 1 & 1 \\ 1 & 2 & 2 & 1 & 1 & 0 \\ 2 & 2 & 1 & 4 & 1 & 1 \\ v_{5} & v_{6} & 0 & 1 & 0 & 1 & 0 & 1 \end{bmatrix}$$

and the diagonal of  $A_G^2$  corresponds to the degrees of the vertices in G (if the graph is simple).

# Distance matrix

#### Definition

The **distance matrix** of a graph G(V, E) is a  $n \times n$  matrix  $D_V$ 

$$D_V = \min\{k : A_G^k(i,j) \neq 0\}$$

and it contains the distances between pairs of vertices. If only a subset of the vertices  $U \subseteq V$  is used we write  $D_U(i,j)$  to denote the distance of vertices  $v_i$  and  $v_j$  in G[U].

- the **diameter** of G(V, E) is  $diam(G) = \max\{D_V(i, j) : \forall i, j \in V\}$
- for  $C \subseteq W \subseteq V$  we denote  $D_W(C) = \sum_{i,j \in C} D_W(i,j)$ .
- so for  $C \subseteq V$  by  $D_V(C)$  we mean the sum of distances of vertex pairs in C using all vertices of the graph, while
- **by**  $D_C(C)$  we mean the sum of distances of vertex pairs in C in the subgraph G[C].

#### Paths matrix

#### Definition

The **paths matrix** of a graph G(V, E) is defined as an  $n \times n$  matrix  $P_V$ 

$$P_V(i,j) = A_G^I(i,j)$$
 where  $I = \min\{k : A_G^k(i,j) \neq 0\}$ 

and it contains number of different shortest paths between pairs of vertices. If only a subset of the vertices  $U \subseteq V$  is used we write  $P_U(i,j)$  to denote the number of shortest paths between vertices  $v_i$  and  $v_i$  in G[U].

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and it contains number of different shortest paths between pairs of vertices. If only a subset of the vertices  $U \subseteq V$  is used we write  $P_U(i,j)$  to denote the number of shortest paths between vertices  $v_i$  and  $v_j$  in G[U].

So the distance and paths matrices for our example:

# Generalized degree

### Definition (generalized degree)

The k-degree of a vertex v denoted by  $d_k(v)$  is the number of shortest paths of length k that this vertex participates as a source vertex.

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- we have  $d_k(v) = \sum \{P_V(v, i) : D_V(v, i) = k\}$
- given a graph G(V, E) the total number of shortest paths of length  $k \leq diam(G)$  is

$$m_k(G) = \frac{1}{2} \sum_{v \in V(G)} d_k(v)$$

• for k = 1 we have the degree of a vertex and the familiar  $m_1(G) = |E(G)|$ 

# Distance quality function

we are now ready to formulate the distance quality function using a random graph

 $\blacksquare$  the probability that vertices i, j are joined by a path of length k

$$Pr[i,j,k] = \frac{d_k(i)}{2m_k(G)} \frac{d_k(j)}{2m_k(G)}$$

expected distance between vertices i, j

$$\overline{D_V(i,j)} = \sum_{k=1}^{diam(G)} kPr[i,j,k]$$

■ sum of expected pairwise distances in cluster C

$$\overline{D_V(C)} = \frac{1}{2} \sum_{i,j \in C} \overline{D_V(i,j)}$$

given a cluster of vertices *C* we want to have the smallest sum of pairwise distances w.r.t. a random model

$$Q_d(G,C) = \sum_{C \in C} \left( \overline{D_V(C)} - D_V(C) \right)$$

# Outline of the talk

- 1 Preliminaries
- 2 Axioms for distance based clustering
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### Resolution limit: underestimation of clusters

■ Resolution limit in community detection, S. Fortunato and M. Barthelemy, Proceedings of the National Academy of Sciences, Vol. 104, pp. 36-41 (2007).

We have n cliques  $K_m$ 

$$Q_m = 1 - \frac{2}{m(m-2)+2} - \frac{1}{n}$$

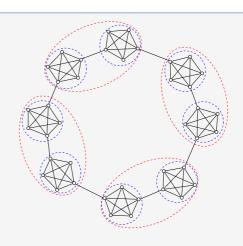
$$Q_m = 1 - \frac{1}{m(m-2)+2} - \frac{2}{n}$$

so  $Q_m > Q_m$  only if

$$m(m-1)+2>n$$

So for 
$$m = 5$$
,  $n = 30$ 

$$Q_m = 0.876 < 0.888 = Q_m$$



For a clustering  $C = \{C_1, \ldots, C_K\}$  we can decompose modularity

$$Q_m(\mathcal{C}, G) = \underbrace{\sum_{C \in \mathcal{C}} \frac{m_C}{m}}_{Q_f(C, G)} - \underbrace{\sum_{C \in \mathcal{C}} \left(\frac{d_G(C)}{2m}\right)^2}_{Q_0(C, G)}$$

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 $\blacksquare$   $Q_f(C, G)$  gets maximized at K = 1.

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- $ightharpoonup Q_0(\mathcal{C}, G)$  gets minimized at K = n.

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- $\mathbb{Q}_0(\mathcal{C}, G)$  gets minimized at K = n.
- $\blacksquare$   $Q_f$  term favors clusterings with few extra-cluster edges.

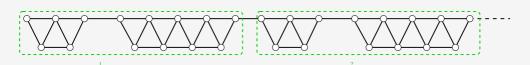
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- $lue{Q}_0$  term favors clusterings with *balanced* clusters.

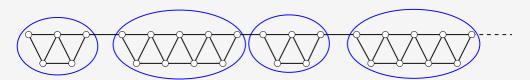
#### Consider the following family of graphs

 $\blacksquare$  family  $H_{k,n_1,n_2}$  of graphs



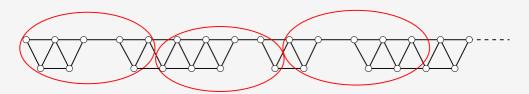
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#### Consider the following family of graphs

- $\blacksquare$  family  $H_{k,n_1,n_2}$  of graphs
- **natural** clustering  $C_N$
- **balanced** clustering  $C_B(J)$  for J=8



### Theorem (Kehagias and Pitsoulis (EPJ 2013))

For every  $k \in \mathbb{N}$  and  $\epsilon \in (0, \frac{1}{2k})$  there exist  $n_1, n_2, J$  such that

$$Q(\mathcal{C}_N, H_{k,n_1,n_2}) < 1 - \epsilon < Q(\mathcal{C}_B(J), H_{k,n_1,n_2})$$

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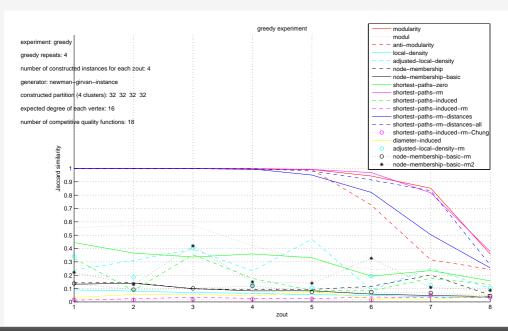
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- ⇒ natural clustering can be arbitrarily different than balanced clustering.
- ⇒ modularity maximization can **overestimate** the number of clusters.

### Outline of the talk

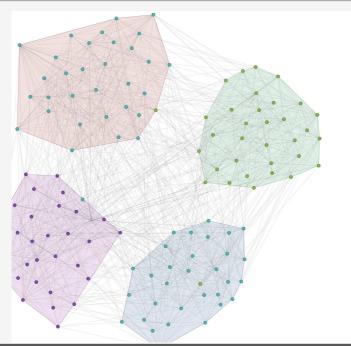
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# Girvan-Newman artificial graphs

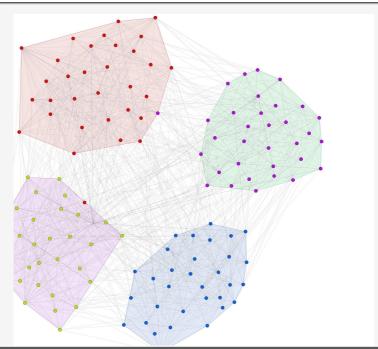
- preliminary results with the GN graphs
- $\blacksquare$  n=128, 4 communities with 32 vertices each
- expected degree of each vertex = 16
- $\blacksquare$   $p_{in}$ ,  $p_{out}$ : probabilities for an intra-cluster and extra-cluster edge respectively
- more tests with benchmark instances with heterogeneous cluster sizes and degree distributions
  - A. Lancichinetti, S. Fortunato and F. Radicchi (2008). "Benchmark graphs for testing community detection algorithms". Phys. Rev. E 78 (4): 046110.



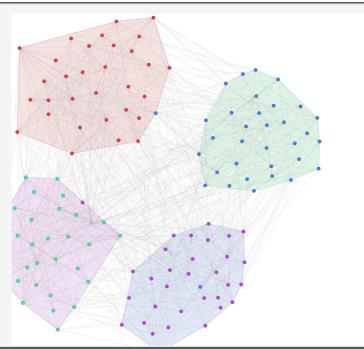
 ${32, 32, 32, 32}, z_{out} = 6$ , antimodularity



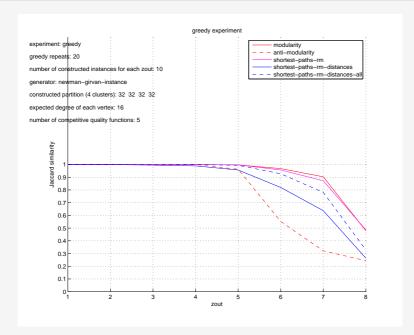
 $\{32, 32, 32, 32\}, z_{out} = 6 \text{ modularity}$ 

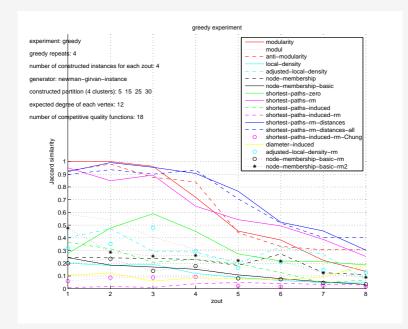


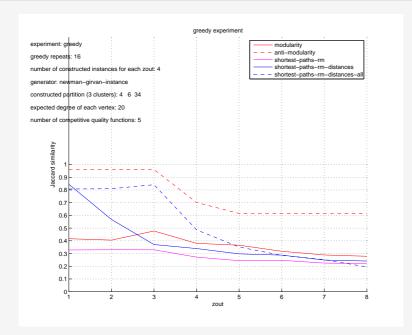
 $\{32, 32, 32, 32\}, z_{out} = 6 \text{ distance}$ 



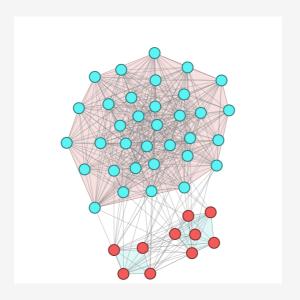
{32, 32, 32, 32}



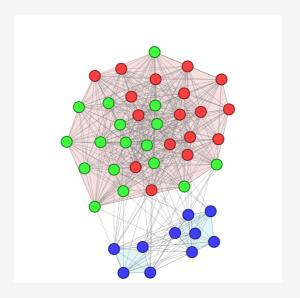




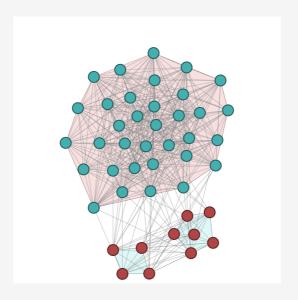
# {4, 6, 34} antimodularity



# {4, 6, 34} modularity



# {4, 6, 34} distance



### resolution limit

bash			bash									
	20.	and distance of		0.0750	0.00	1 0	0.0121					
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		modul	y :	0.3924			-0.0288					
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		NM Dasic III		0.8248			0.3763		good -			
		NM basic rm2		1.9267			-0.0267		good			
		LD adjstd rm		0.0165			0.0011		good -			
		LD ddj3td 1111		0.0165			0.0011		good -			
		SP rm dist all		4478.2019			-5036.0951		good			
		SP rm		1592.8626			-1013.8844					
		SP rm dist		4483.3091			-5039.7694					
		SP indcd rm di	st:	150.0000			456.7966		good -			
		SP indcd rm Ch	un:	2.1658			2.3241		good -			
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		SP inf		2.1658	-0.158	3 [	2.3241	j	good -			
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J -	32.	anti modularit		0.3935			-0.0142					
		modul	.y .	0.3935			-0.0298					
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		NM		0.8232			0.3766		good -			
		NM basic rm2		1.9312			-0.0313		good			
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		SP inf		2.3102			2.4790		good -			
		SP induced		_128.0000:	> -272.000	IA I	144.0000		annd -	_	_	

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#### Definition (Community in the Strong Sense)

Given a graph G(V, E) some  $C \subseteq V(G)$  is a community in the **strong sense** if

$$d_{in}(v) > d_{out}(v), \ \forall v \in C$$

where  $d_{in}(v)$  and  $d_{out}(v)$  are the incident intra-cluster and extra-cluster edges respectively.

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Consider a GN graph with no fixed expected degree, k clusters each with size n and

 $p_{in}$ : probability of intra-cluster edge

 $p_{out}$  : probability of extra-cluster edge

#### Then we have the following:

 $\blacksquare$  probability that a vertex is incident to  $m_{in}$  intra-cluster edges

$$\pi^+(m_i) = \binom{n}{m_i} p_{in}^{m_i} (1 - p_{in})^{n-m_i}$$

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 $\blacksquare$  probability that a vertex is incident to  $m_{in}$  intra-cluster and  $m_{out}$  extra-cluster edges

$$\pi(m_i, m_o) = \pi^+(m_i)\pi^-(m_o)$$

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$$\pi(m_i, m_o) = \pi^+(m_i)\pi^-(m_o)$$

 probability that a vertex satisfies the strong condition, assuming independence between the events of having different degrees

$$Pr[i \text{ is strong}] = \sum_{m_o < m_i} \pi(m_i, m_o)$$

 $\blacksquare$  probability that a cluster with n vertices satisfies the strong condition

$$Pr[C \text{ is strong}] = (Pr[i \text{ is strong}])^n$$

 $\blacksquare$  probability that a clustering with k clusters of size n satisfies the strong condition

$$(Pr[i \text{ is strong}])^{nk} = \left(\sum_{m_o < m_i} \pi(m_i, m_o)\right)^{nk}$$

Thank You!