



# Modules

Analysis of complex interconnected data



Slides mostly based on  
newman's book



# Outline

- Quick Notes
- Quick Recap of Centrality Measures
- Modules
  - Real graphs are modular
  - Spectral clustering
  - Objectives for quality of a module
  - TopLeaders
  - Using Betweenness Centrality
  - Modularity Optimization, FastModularity & Louvain
  - Resolution limits of Modularity
  - Link clustering
  - Evaluating clustering results

# Quick Notes

- Reminder second assignment is out, due on Oct 4th
  - [http://www.reirab.com/Teaching/NS20/Assignment\\_2.pdf](http://www.reirab.com/Teaching/NS20/Assignment_2.pdf)
  - Submit single entry as a Group (pairs or two or individual) in Mycourses
- Use slack for easier communications
- Any questions?

## Deadlines

- assignment 1 due on Sep. 20th
- assignment 2 due on Oct. 4th
- assignment 3 due on Oct. 18th
- project proposal slides due on Oct. 25th
- project proposal due on Nov. 1th
- Reviews (first round) due on Nov. 8th
- project progress report due on Nov. 22nd
- Reviews (second round) due on Nov. 29th
- project final report slides due on Dec. 1st
- project final report due on Dec. 6th
- Reviews (third round) due on Dec. 13th
- project revised report and rebuttal due on Dec. 20th
- note: dates are tentative, please check them for the updated deadlines

# Quick Recap of Centrality Measures

$$x_i = \sum_{j \in N(i)} 1$$

$$x_i = c \sum_{j \in N(i)} x_j, \quad c = \frac{1}{\lambda^*(A)}$$

$$x_i = c \sum_{j \in N(i)} x_j + 1, \quad c < \frac{1}{\lambda^*(A)}$$

$$x_i = c \sum_{j \in N(i)} \frac{x_j}{\sum_k x_{kj}} + 1, \quad c < \frac{1}{\lambda^*(AD^{-1})}$$

$$x_i = c \sum_{j \in N(i)} y_j, \quad y_i = c' \sum_{j \in N(i)} x_j, \quad cc' = \frac{1}{\lambda^*(AA^T)}$$

$$x_i = \frac{1}{n-1} \sum_j \frac{1}{s_{ij}}, \quad s_{ij}: \text{length of shortest path from } i \text{ to } j$$

$$x_i = \frac{1}{n^2} \sum_{jk} \frac{|i \in s_{jk}|}{|s_{jk}|} \quad s_{ij}: \text{set of shortest paths from } i \text{ to } j$$

$N(i) = \{j | A_{ij} = 1\}$ ,  $\lambda^*(A)$ : largest eigenvalue of  $A$

- Degree Centrality
  - count the number of neighbours, ignores their importance
- Eigenvalue Centrality
  - consider importance of connections, gives zero to nodes not in scc or its out component, in extreme case of an acyclic networks, e.g. citation networks, all nodes get zero score
- Katz Centrality
  - avoid zeros by giving everyone a basic importance
- PageRank
  - divide importance on how many connections it is passed over to
- HITS
  - consider two types of importance, hubs and authorities
- Closeness centrality
  - average how close you are to the rest
- Betweenness centrality
  - count what fraction of shortest paths pass through you

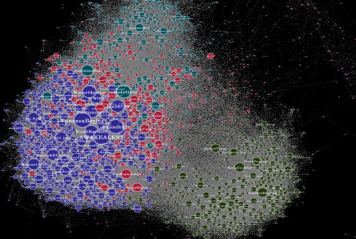


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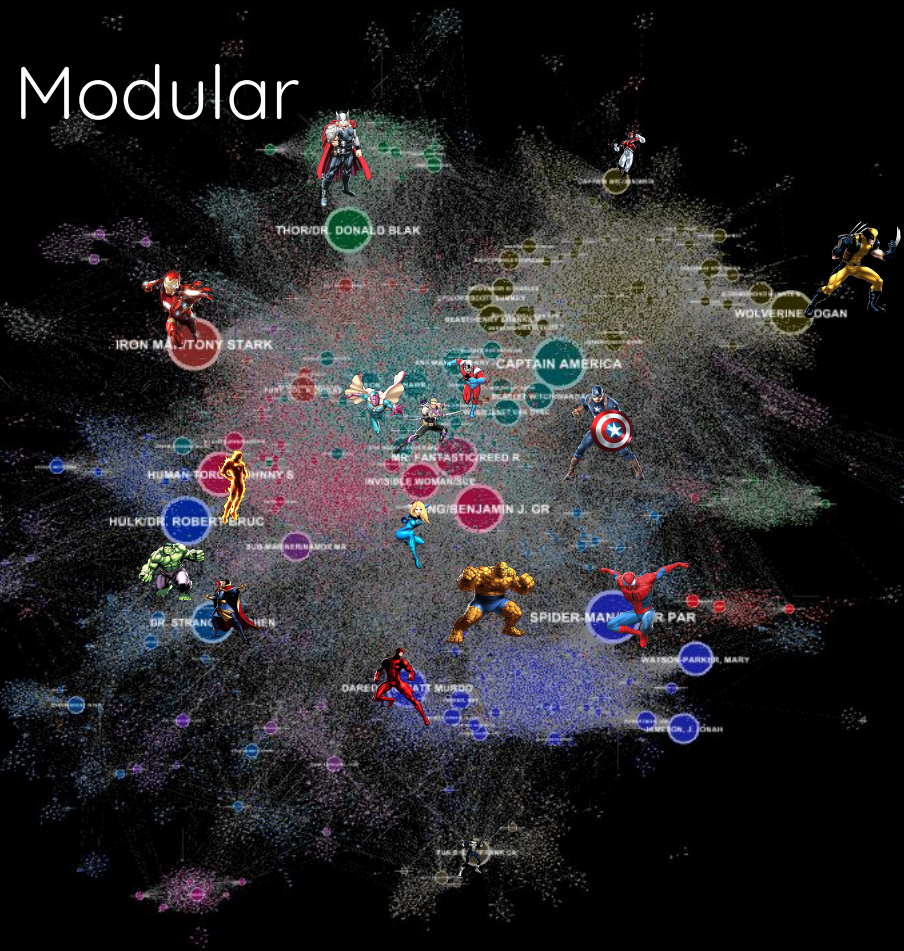
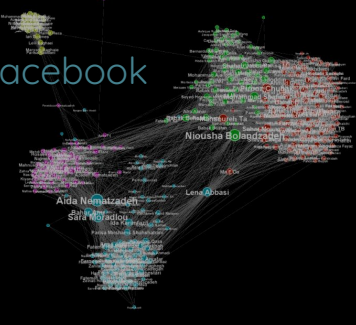
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# Network are Modular

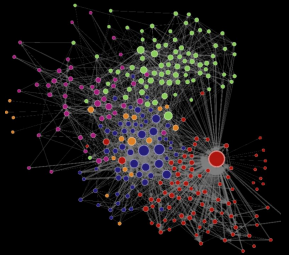
Twitter



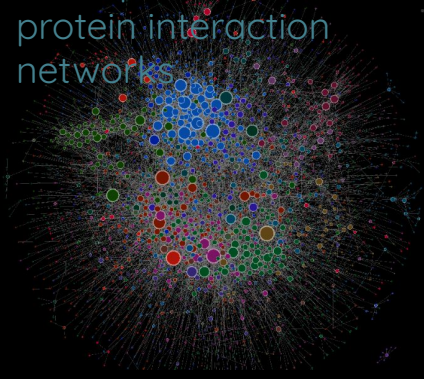
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C. elegans neural network



Yeast protein protein interaction networks

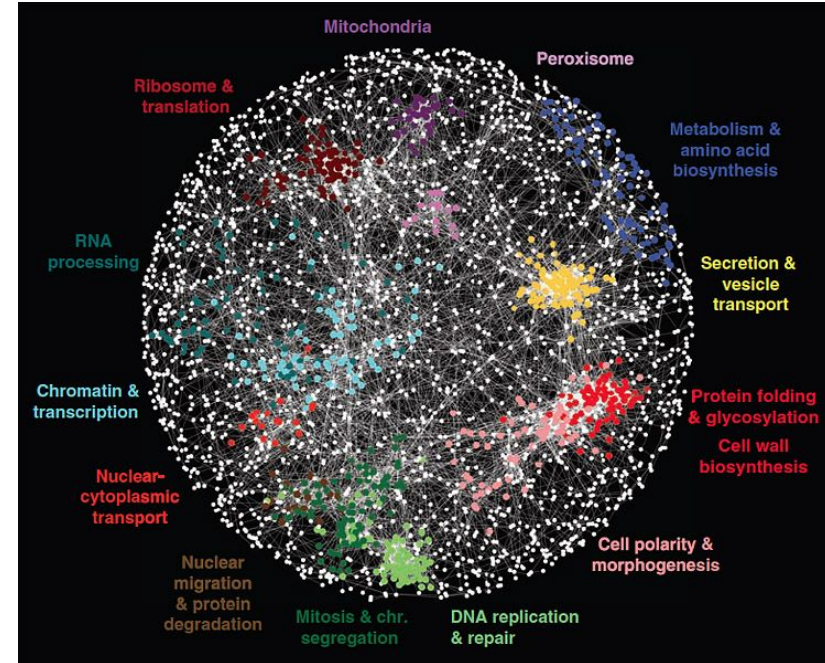


# Example Applications



## Module identification in biological networks

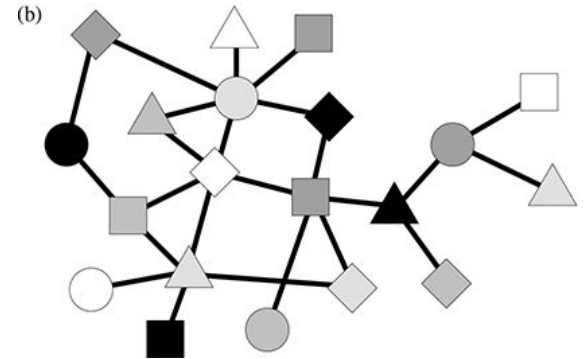
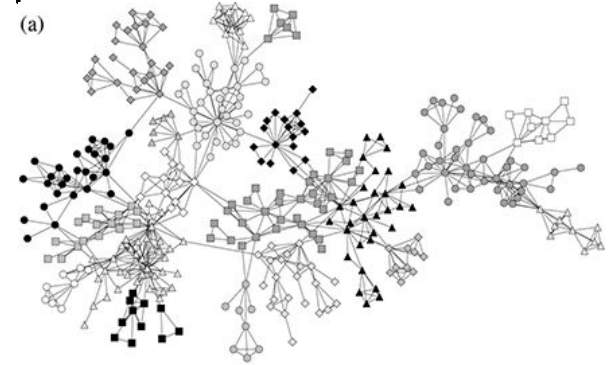
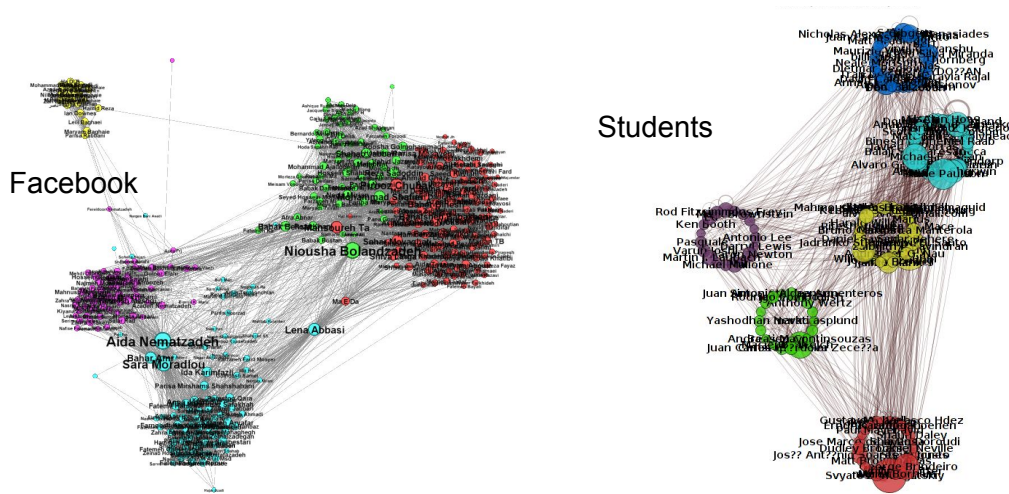
- Protein complexes and functional modules in PPI networks (Spirin & Mirny, PNAS 2003)
  - protein complexes: proteins that interact to carry out a task as a single complex unit, e.g., RNA splicing
  - functional units: proteins that bind at different time to participate in a cellular process, e.g., communicating a signal from the surface of the cell to the nucleus
- Representation of the metabolic networks (R Guimerà & Amaral, Nature 2005)
  - ultra-peripheral metabolites (that have all their connections inside their modules) have the highest evolutionary loss rate, whereas connector hubs (that connect to most of the other modules) are the most conserved across the species



# Modules as Coarse Representation

Modules give a coarse-grained representation of the structure

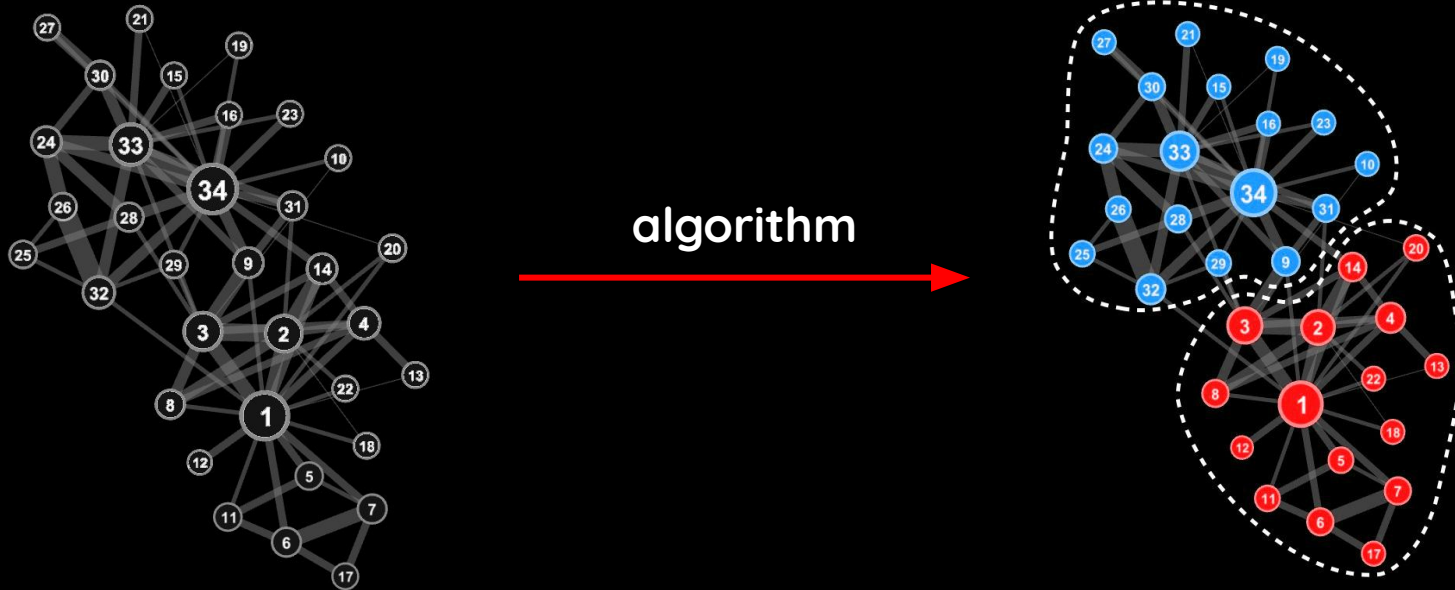
Also referred to as meso-scale, cluster, communities, etc.





# Clustering a.k.a Community Detection

Given a graph, how to cluster the nodes into modules?



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# Spectral clustering

Uses the relation between connectivity & Laplacian matrix

Recall:

$$\text{Laplacian Matrix: } \mathbf{L} = \mathbf{D} - \mathbf{A}$$

**A**: adjacency matrix

**D**: diagonal matrix of degrees

```
[[ 3 -1 -1 -1 0]
 [-1 3 -1 0 -1]
 [-1 -1 4 -1 -1]
 [-1 0 -1 2 0]
 [0 -1 -1 0 2]]
```

**L**

example

```
[[3 0 0 0 0]
 [0 3 0 0 0]
 [0 0 4 0 0]
 [0 0 0 2 0]
 [0 0 0 0 2]]
```

**D**

```
[[0 1 1 1 0]
 [1 0 1 0 1]
 [1 1 0 1 1]
 [1 0 1 0 0]
 [0 1 1 0 0]]
```

**A**

# Spectral clustering

Uses the relation between connectivity & Laplacian matrix

## Recall the Spectral Spectrum

- $\mathbf{L}\mathbf{u} = \lambda\mathbf{u}$  : Eigenvalues of Laplacian Matrix
- We have  $n$  eigenvalues which we call **Laplacian Spectrum**:  
$$0 = \lambda_0 \leq \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$$
- $\lambda_0$  is always zero since we have  $\mathbf{L}(\mathbf{1}, \mathbf{1}, \dots, \mathbf{1}) = \mathbf{0}$
- $\lambda_0 = \lambda_1 = \dots = \lambda_k = 0 \Rightarrow k$  is number of connected components
- Largest is bounded by twice the maximum degree in  $G$
- $E = \frac{1}{2} \sum d_i = \frac{1}{2} \text{Tr}(\mathbf{L}) = \frac{1}{2} \sum \lambda_i$
- Spectral gap: smallest nonzero eigenvalue
- Fiedler vector: eigenvector corresponding to the spectral gap
- Spectral ordering: Fiedler vector sorted
- Laplacian Spectrum relates to graph connectivity & clustering

# Laplacian Matrix & Smoothness

- $\mathbf{f} = (f_1, \dots, f_n)$  function on Graph
  - $\mathbf{f} \in \mathbb{R}^n \Rightarrow \mathbf{f}^T \mathbf{L} \mathbf{f} = \frac{1}{2} \sum_{ij} A_{ij} (f_i - f_j)^2$

Measures how much the value of  $f$  is smooth over edges, i.e. the difference of values for connecting nodes

How to find modules?

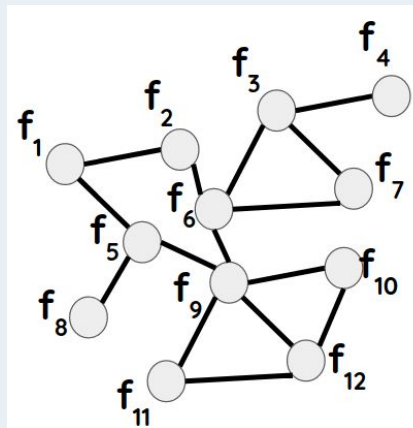
$$\mathbf{f}^T \mathbf{L} \mathbf{f} = \mathbf{f}^T \mathbf{D} \mathbf{f} - \mathbf{f}^T \mathbf{A} \mathbf{f} = \sum_i d_i f_i^2 - \sum_{ij} f_i f_j A_{ij}$$

$$= \frac{1}{2} [ \sum_i d_i f_i^2 - 2 \sum_{ij} f_i f_j A_{ij} + \sum_i d_i f_i^2 ]$$

$$= \frac{1}{2} \sum_{ij} A_{ij} (f_i - f_j)^2$$

See [this](#) for more details.

Consider function  $\mathbf{f}$  that maps vertices to a value



# Laplacian Matrix & Smoothness

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Measures how much the value of  $f$  is smooth over edges, i.e. the difference of values for connecting nodes

How to find modules? Find  $f$  that give smoothest results, i.e. minimizes this

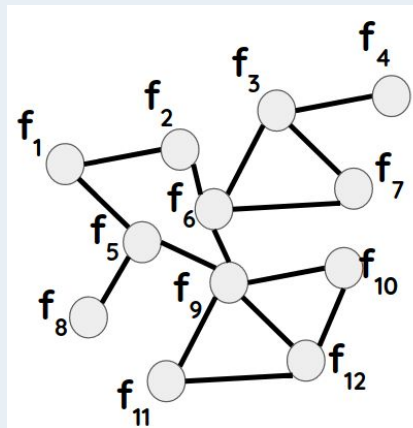
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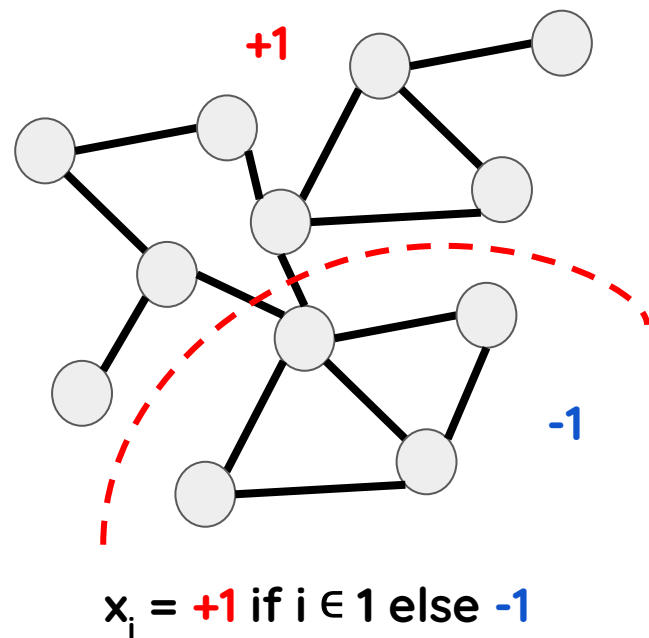
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Consider function  $\mathbf{f}$  that maps vertices to a value



# Spectral Clustering

- $\mathbf{f} = (f_1, \dots, f_n)$  function on Graph
  - $\mathbf{f} \in \mathbb{R}^n \Rightarrow \mathbf{f}^T \mathbf{L} \mathbf{f} = \frac{1}{2} \sum_{ij} A_{ij} (f_i - f_j)^2$
- Cut edges =  $\frac{1}{4} \mathbf{x}^T \mathbf{L} \mathbf{x}$
- Find best **balanced** cut
  - Minimize given  $\mathbf{x}_i \in \{+1, -1\}$  &  $\sum_i x_i = 0$
  - What does it mean?
- $\mathbf{x}_i \in \{+1, -1\} \Rightarrow \mathbf{x}_i \in \mathbb{R} \text{ \& } \sum_i x_i^2 = n \text{ (} \mathbf{x}^T \mathbf{x} = n \text{)}$ 
  - $\text{Min } \frac{1}{4} \mathbf{x}^T \mathbf{L} \mathbf{x} = \frac{1}{4} n \mathbf{v}_1^T \mathbf{L} \mathbf{v}_1 = \frac{1}{4} n \lambda_1$   
Courant Fisher Minmax Theorem
- Second smallest **eigenvalue**  
 $\Rightarrow$  **sparsest cut**
- Signs of corresponding **eigenvector**



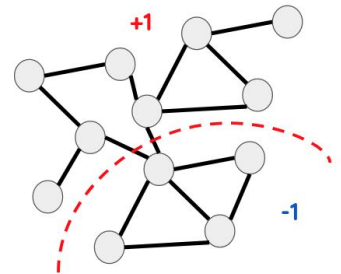
# Normalized Graph Laplacian

- **Symmetric normalization** {used for spectral clustering by Ng, Jordan, and Weiss (2002)}
  - $L_{\text{sym}} = D^{-1/2} L D^{-1/2} = I - D^{-1/2} A D^{-1/2}$
- **Random walk normalization** {used for spectral clustering by Shi and Malik (2000)}
  - $L_{\text{rw}} = D^{-1} L = I - D^{-1} A$
  - $\Rightarrow$  **Normalized cut (Ncut)**, by the number of **edges** in the clusters

**K Clusters?** Use k-means on top k eigenvectors (each node is represented with k features)

Many successful applications including image segmentation but not the best choice for finding modules in real world graph.

How can we define a better objective for finding modules in real world graph ?



$$x_i = +1 \text{ if } i \in 1 \text{ else } -1$$

$$\text{Cut} = 2 \\ \text{NCut} = 2 \left( \frac{1}{12} + \frac{1}{18} \right)$$

$$\text{Ncut}(A_1, \dots, A_k) = \sum_{i=1}^k \frac{\text{cut}(A_i, \bar{A}_i)}{\text{vol}(A_i)}$$
$$\text{vol}(A) := \sum_{i \in A} d_i$$

Further reading? [See this](#)

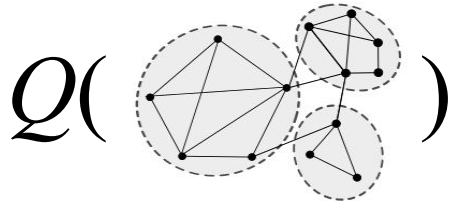


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$$f(S) = \frac{c_S}{2m_S + c_S} + \frac{c_S}{2(m - m_S) - c_S}$$

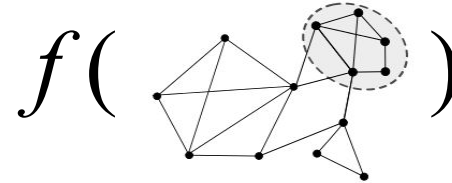
# Objectives for quality of a community



**Globally-defined** quality function to partition the whole network

- Q-modularity (Newman 2003)

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



**Locally defined** quality function for one subset of nodes in a network

- **Conductance** (Sinclair & Jerrum 1989)

$$f(S) = \frac{c_S}{2m_S + c_S}$$

- Normalized Cut (Shi & Malik 2000)

$$f(S) = \frac{c_S}{2m_S + c_S} + \frac{c_S}{2(m - m_S) - c_S}$$

In the example above

$$= 3/(2*7+3)$$

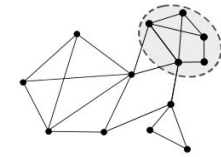
$$= 3/(2*7+3) + 3/(2*(12)+3)$$

$c_S$  = cut size: number of edges going out of module  
 $m_S$  = module size: number of edges inside module

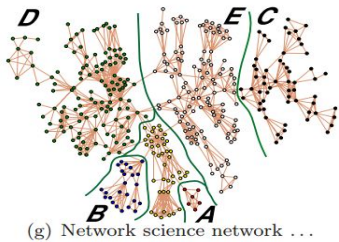
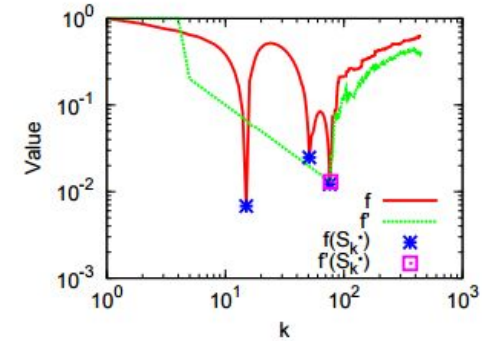


# Locally defined objectives

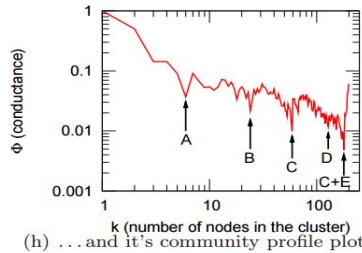
Defining and evaluating network communities based on ground-truth (Yang, J., Leskovec, J., Knowledge and Information Systems, 2015)



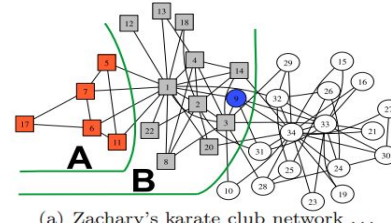
- Community detection from a seed node
  - Score proximity of nodes from seed using random walk
  - Expand from the closest node, and compute the objective
  - Local optima of objective correspond to detected communities



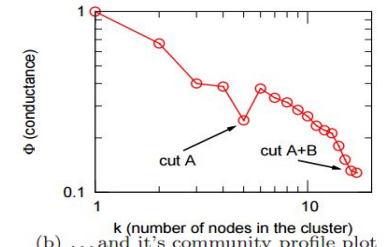
(g) Network science network ...



(h) ... and its community profile plot



(a) Zachary's karate club network ...

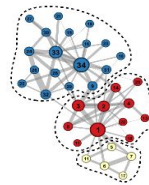


(b) ... and its community profile plot

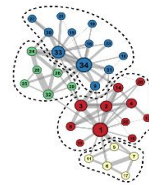


# Defining the Modular Structure of Networks

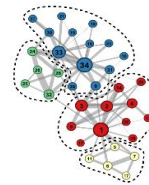
- **Number of links between them is more than chance**
  - Modularity  $Q$  (Newman & Grivan, Phys Rev E, 2004)
    - FastModularity (Clauset, Phys Rev E 2005); Louvain (Blondel et al., J Stat Mech Theory Exp, 2008)
- **Within them a random walk is more likely to trap**
  - Walktrap (Pons & Latapy, ISCI 2005)
- **Coding gives efficient compression of any random walk**
  - Infomap (Rosvall & Bergstrom, PNAS 2008; PloS One 2010)
- **Follow their closest leader**
  - TopLeader



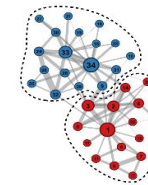
*FastModularity*  
 $Q = 0.434$



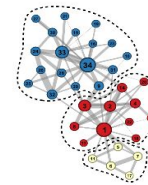
*Louvain*  
 $Q = 0.445$



*Walktrap*  
 $Q = 0.44$



*TopLeader(2)*  
 $Q = 0.403$



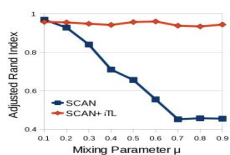
*Infomap*  
 $Q = .434$

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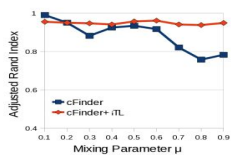
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# TopLeaders: K-medoid for graphs

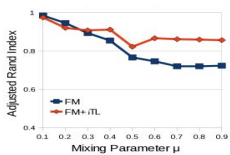
- Iteratively assigns nodes to leaders, selects leaders
  - Leader: central member in community
  - Community: set of followers surrounding a leader
  - Assigning followers to closest leader based on neighbourhoods
- Initialization requires  $k$  (central nodes with few neighbours in common)



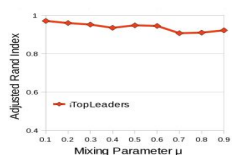
SCAN



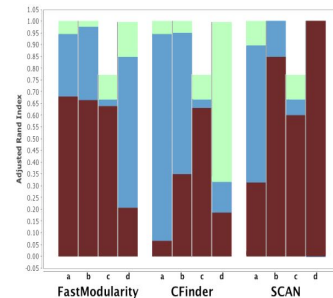
CFinder



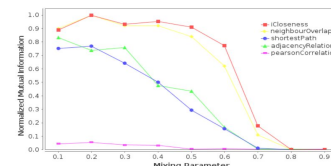
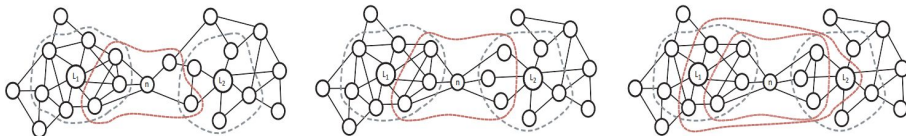
FastModularity



GroundTruth



- Also identifies outliers and hubs in the network
- Closeness measure based on diffusion of innovation



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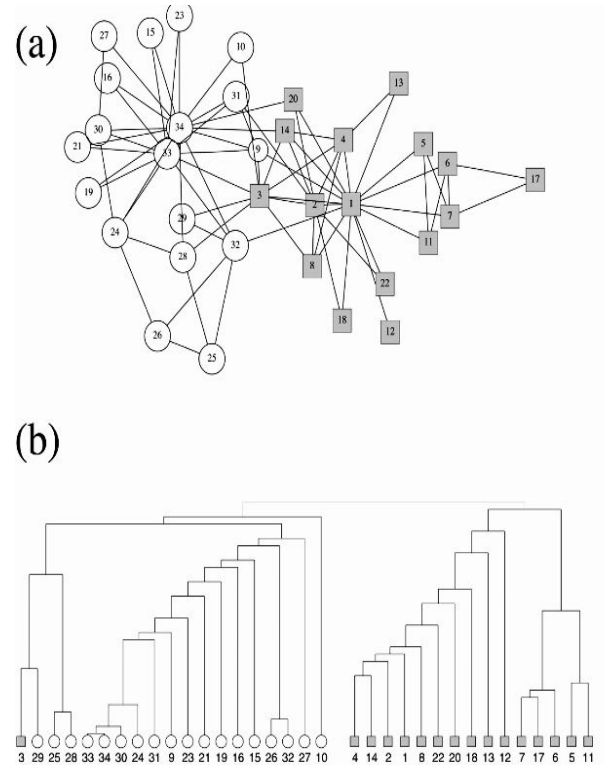
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# A divisive hierarchical clustering

(Girvan and Newman, PNAS 2002)

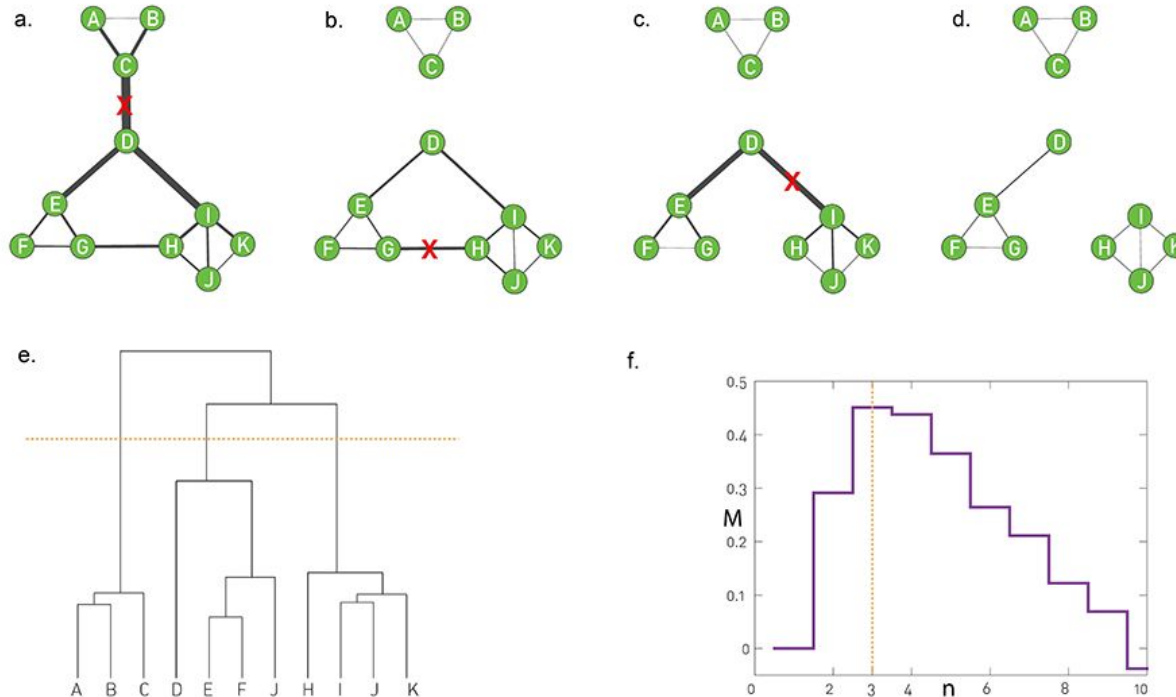
1. Calculate the betweenness for all edges in the network
2. Remove the edge with the highest betweenness
3. Recalculate betweennesses for all edges affected by the removal
4. Repeat from step 2 until no edges remain
5. Where to cut?

<https://networkkarate.tumblr.com/>





# A divisive hierarchical clustering



Recursively remove  
**bridges**, edges with  
high edge-betweenness

In the resulted  
dendrogram,  
evaluate  $M$  for flat  
modules obtained at  
different levels

How to define  $M$ ?

# How good is a clustering of a network?

Originally proposed to know where to cut the dendrogram, but we optimize this directly in practice

Measure the difference between the fraction of edges that are within the clusters and the expected such fraction if the edges were randomly distributed when degrees are fixed

Use configuration model as the null model

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

$k_i$  = degree of node  $i$

$M$  = total edges

Kronecker delta: 1 only if  $i$  &  $j$  are in the same cluster,  $C_i = C_j$

# Q-modularity

Sums over all pair of nodes in the same clusters

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

We can reformulate this to sum over clusters

$$Q = \sum_i (e_{ii} - a_i^2) = \text{Tr}[e] - \|e^2\|$$

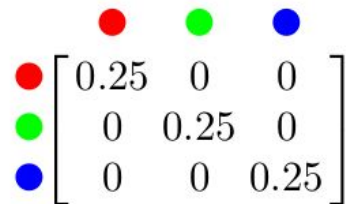
$e_{ij}$  : fraction of edges between cluster  $i$  and  $j$

$$a_i = e_i = \sum_j e_{ij}$$

$k_i$  = degree of node  $i$

$M$  = total edges

Kronecker delta: 1 only if  $i$  &  $j$  are in the same cluster,  $C_i = C_j$


$$\begin{matrix} & \bullet & \bullet & \bullet \\ \bullet & \begin{bmatrix} 0.25 & 0 & 0 \\ 0 & 0.25 & 0 \\ 0 & 0 & 0.25 \end{bmatrix} & & \\ \bullet & & & \\ \bullet & & & \end{matrix}$$

# Outline

- Quick Notes
- Quick Recap of Centrality Measures
- Modules
  - Real graphs are modular
  - Spectral clustering
  - Objectives for quality of a module
  - TopLeaders
  - Using Betweenness Centrality
  - **Modularity Optimization, FastModularity & Louvain**
  - Resolution limits of Modularity
  - Link clustering
  - Evaluating clustering results

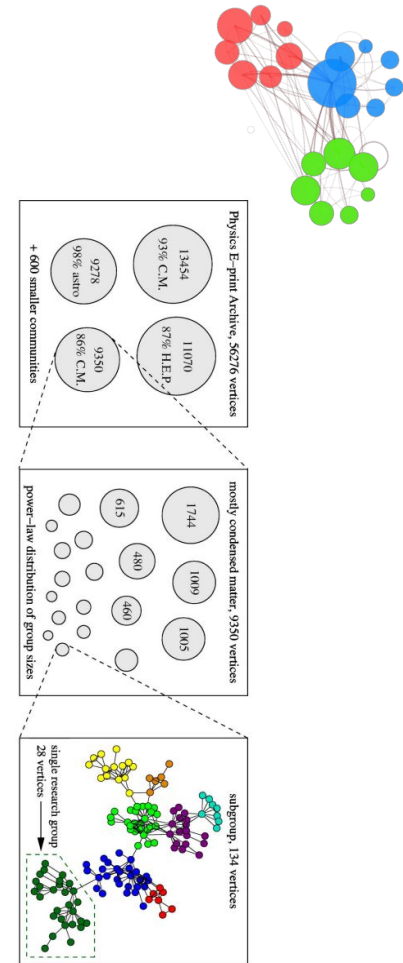
# An agglomerative hierarchical clustering

(Newman, Phys. Rev. E 2004)

1. Start from every node a cluster
2. Initialize  $e$  as the adjacency matrix
3. Merge two cluster that give the highest gain in  $Q$ :

$$\Delta Q = 2(e_{ij} - a_i a_j)$$

4. Update the  $e$  by adding together the rows and columns corresponding to the joined communities
5. Go to step 3 until no increase in  $Q$



# Modularity optimization

- Divisive hierarchical clustering (Girvan and Newman, PNAS 2002)
  - Removes the edge with highest betweenness
  - All pairs shortest paths: expensive to compute
  - can be approximated but still not scalable
- Agglomerative hierarchical clustering (Newman, Phys. Rev. E 2006)
  - Start from every node a cluster, and merge
  - $O(n(m+n))$  :  $n, m$ : number of nodes and edges
  - With heap based data structure  $\Rightarrow O(m \log n)$  (Clauset et al., 2004)  
 **$\Rightarrow$  FastModularity**

# Louvain, another agglomerative method

Agglomerative method tends to produce super-communities

$$Q = \sum_i (e_{ii} - a_i^2)$$

$$Q = \sum_i \sum_{u,v \in i} (w_{uv} - w_u \cdot w_v)$$

$w_{uv}$ : normalized weight of the edge from node  $u$  to node  $v$

Gain of adding node  $u$  to community  $i$  is:  $\Delta Q = 2 \sum_{v \in i} (w_{uv} - w_u \cdot w_v)$ .

Move nodes around (only through links), aggregate clusters, repeat

(Blondel et al. Journal of Statistical Mechanics, 2008)

$O(n \log n)$

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  - Evaluating clustering results



# Q problems

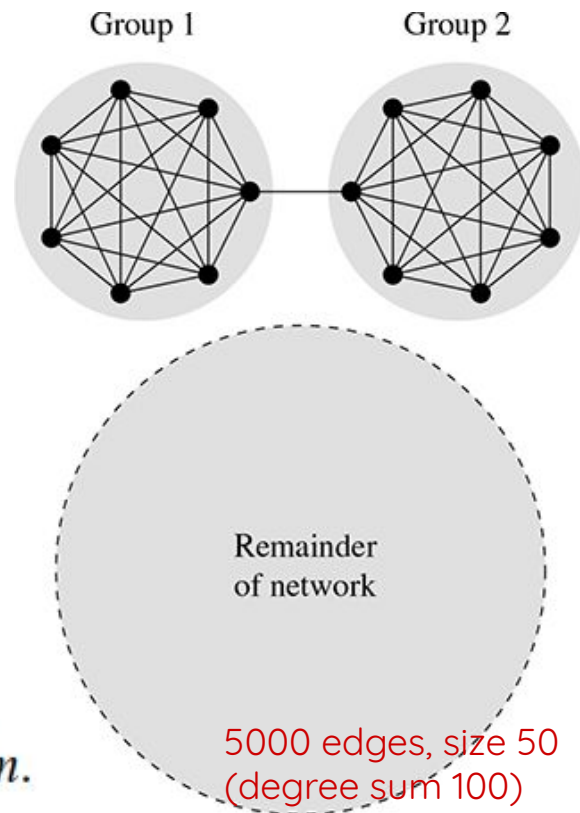
very different divisions of the network  
but same Q

resolution limit, the inability to see  
communities in a network if they are  
too small, relative to the size of the  
network as a whole

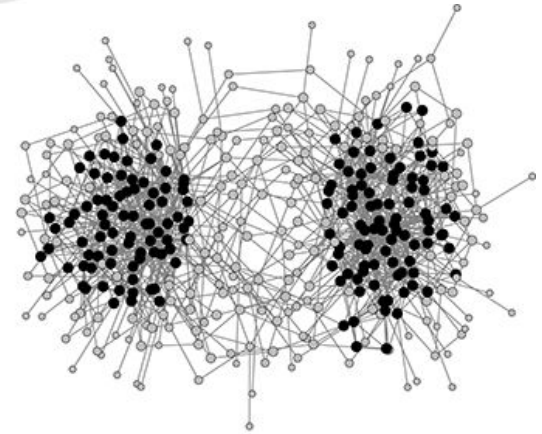
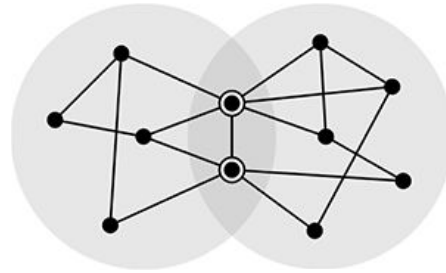
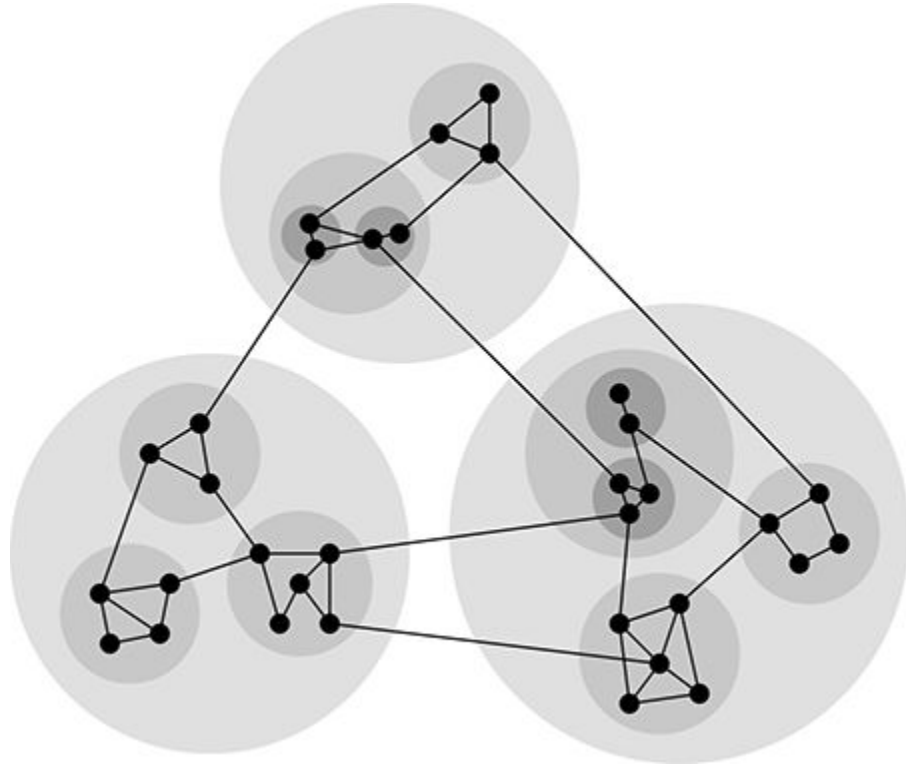
$$\Delta Q = \frac{1}{2m} \left( 1 - \frac{\kappa_1 \kappa_2}{2m} \right),$$

$\kappa_1$  and  $\kappa_2$  be the sums of the degrees  
of the nodes in each of the two groups

$$\kappa_1 \kappa_2 < 2m.$$



# Overlap, hierarchy, periphery



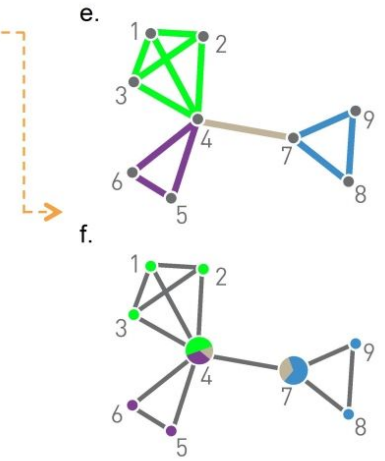
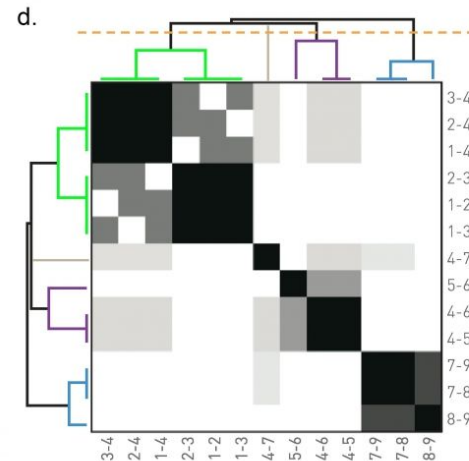
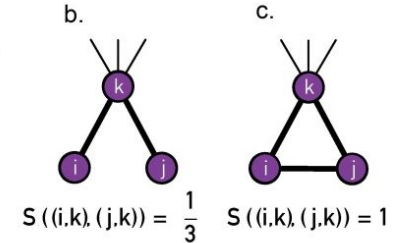
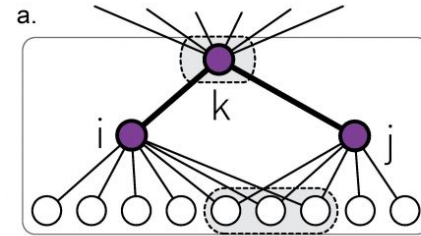
(b)



# Link Clustering

Find overlapping clusters naturally by clustering edges instead of nodes

The similarity of a link pair is determined by the neighborhood of the nodes connected by them.



Ahn YY, Bagrow JP, Lehmann S. Link communities reveal multiscale complexity in networks. *nature*. 2010 Aug;466(7307):761-4.

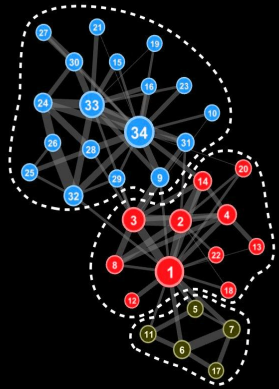
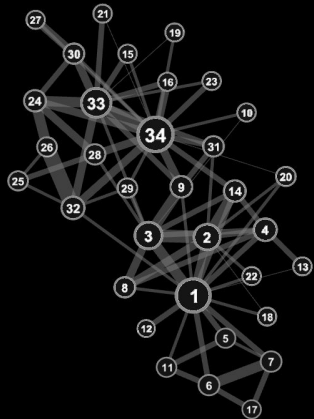


# Outline

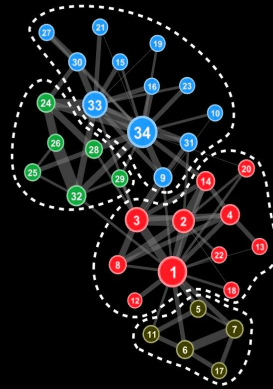
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  - **Evaluating clustering results**

# Evaluating the Modular Structure of Networks

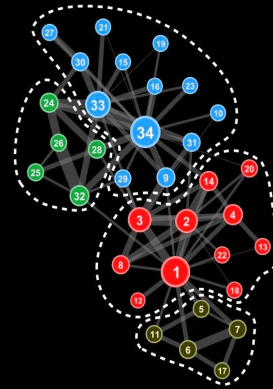
Given different algorithms **which one** is better?



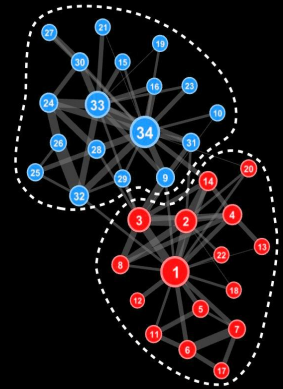
FastModularity



Louvain



Walktrap



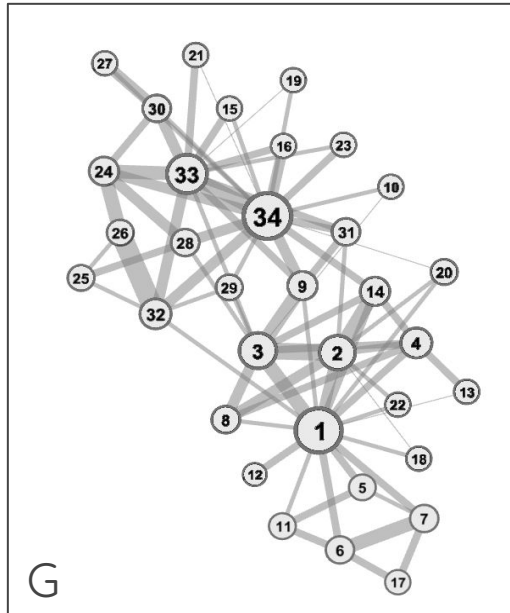
TopLeader

# Evaluation of Community Detection

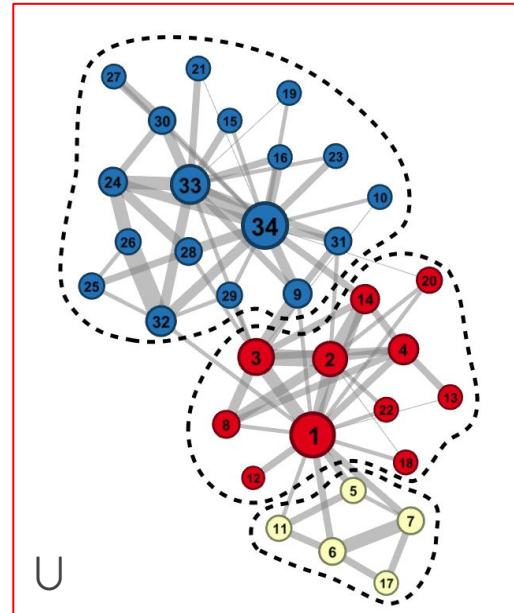
Validation on benchmarks for which we know the ground-truth, a common practice

$(G_1, U_1)$   
 $(G_2, U_2)$   
 $(G_3, U_3)$

•  
•  
•

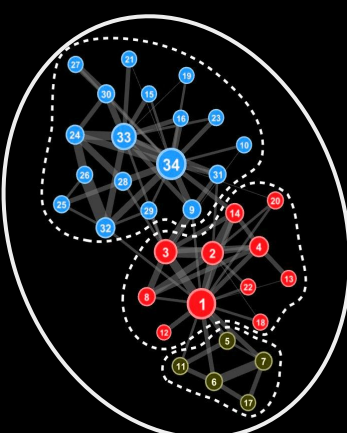
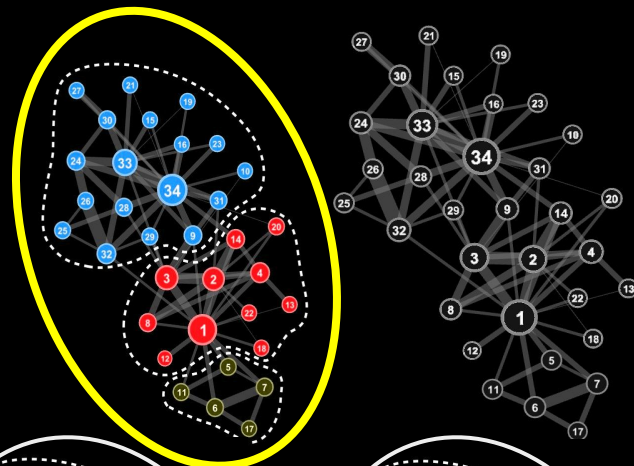


**Ground-Truth**

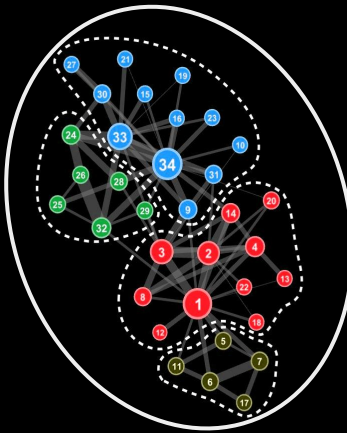


# Validation on Benchmarks

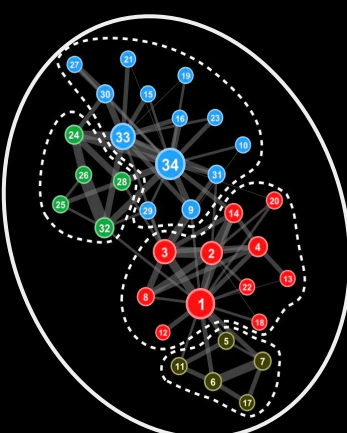
Compare with **ground-truth**



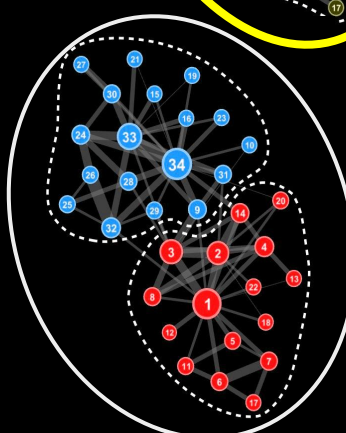
FastModularity



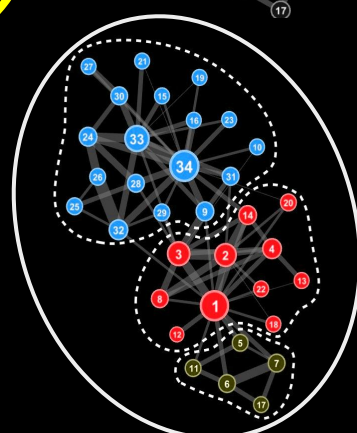
Louvain



Walktrap



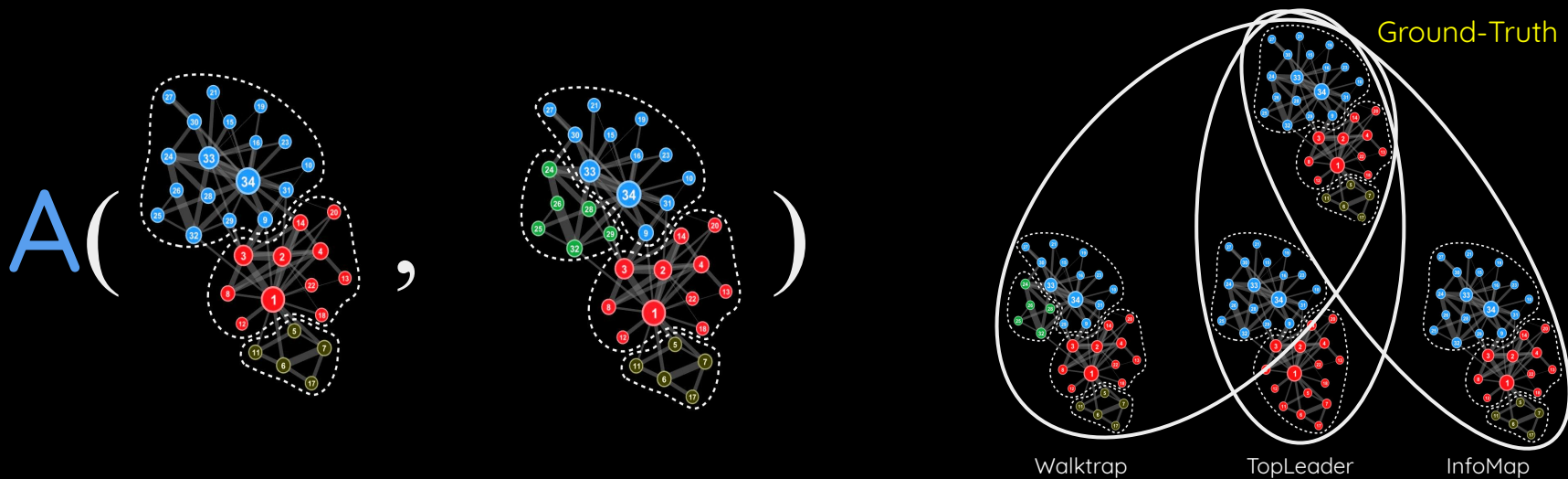
TopLeader



InfoMap

# Validation on Benchmarks

## Agreement measure

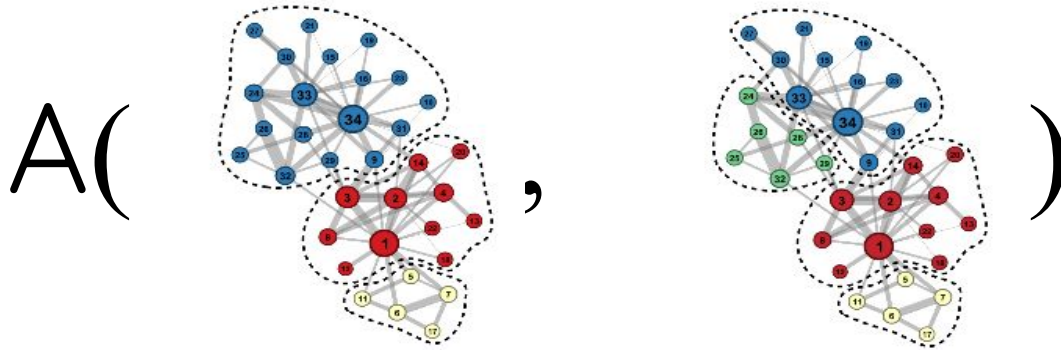




# Clusterings Agreement Measures

Current families, background

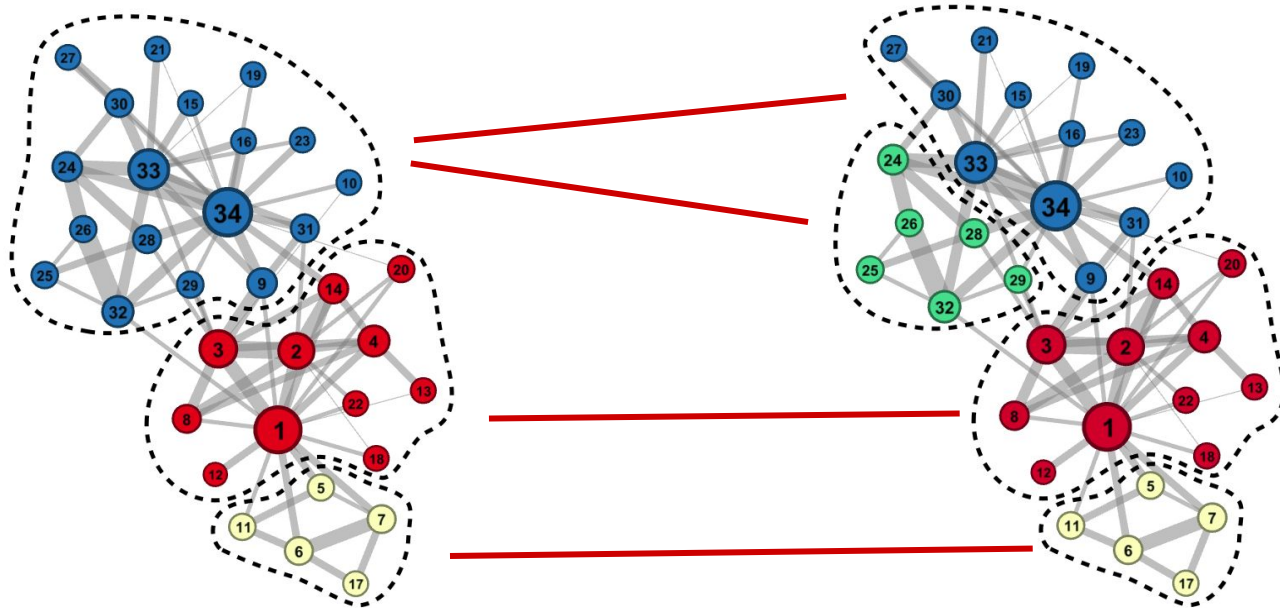
- Set matching
- Information theoretic
- Pair counting



# Clusterings Agreement Measures

Set matching, background

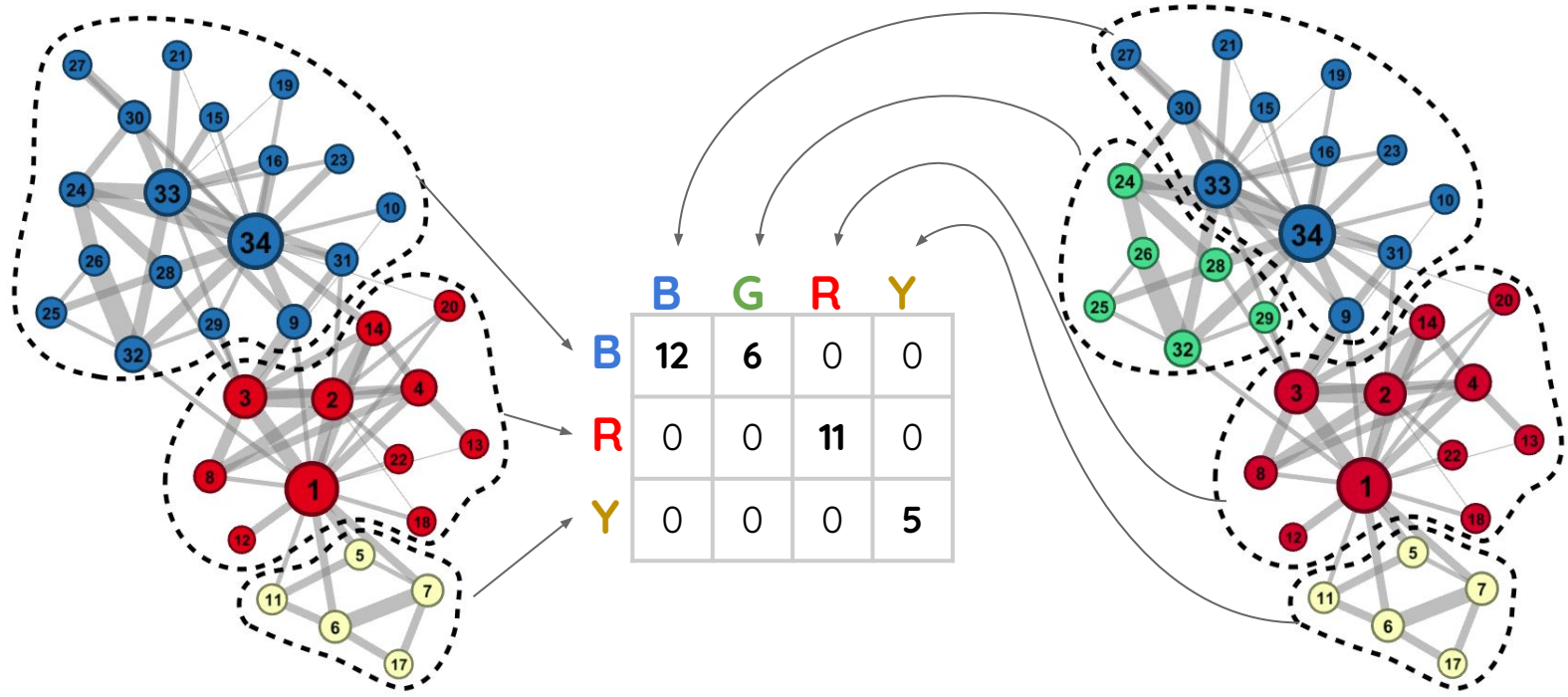
“problem of matching”



# Clusterings Agreement Measures

Information theoretic, background

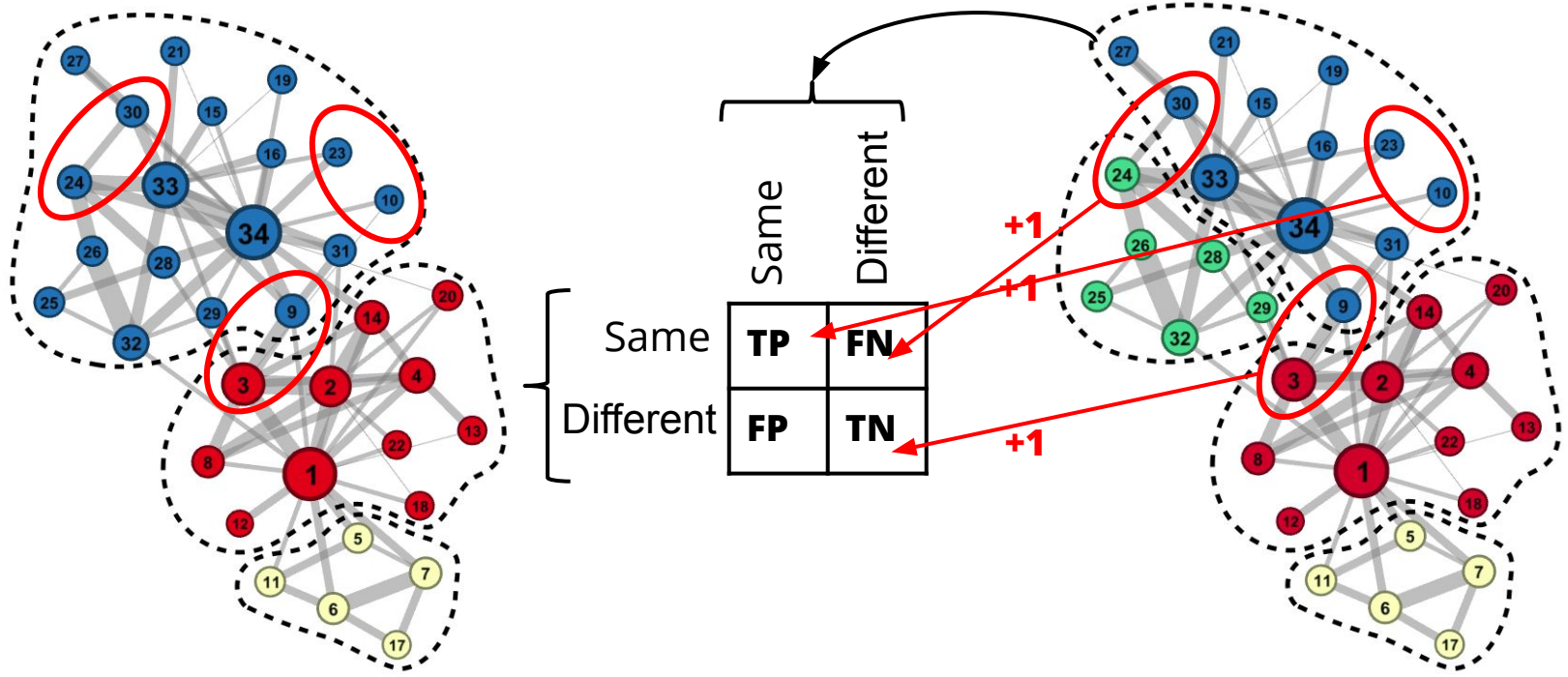
Examples: Variation of Information (VI), Normalized Mutual Information (NMI)



# Clusterings Agreement Measures

Pair counting, background

Examples: Jaccard, Rand Index, F-measure, Adjusted Rand Index (ARI)



# Generalization

## Linking the two families

- Pair counting
- Information theoretic

dispersion in the contingency table

	B	G	R	Y
B	12	6	0	0
R	0	0	11	0
Y	0	0	0	5

	Same	Different
Same	TP	FN
Different	FP	TN

$$TP = \binom{12}{2} + \binom{6}{2} + \binom{11}{2} + \binom{5}{2}$$

# Generalization

## Measuring dispersion

	B	G	R	Y	$\Sigma$
B	12	6	0	0	18
R	0	0	11	0	11
Y	0	0	0	5	5
$\Sigma$	12	6	11	5	34

$$\varphi(18) - \varphi(12) - \varphi(6)$$

$$\varphi(11) - \varphi(11)$$

$$\varphi(5) - \varphi(5)$$

$$\varphi(18) - \varphi(12) - \varphi(6)$$

---

$$\varphi(34)$$

# Generalization

Subsumes pair counting

	B	G	R	Y	$\Sigma$
B	12	6	0	0	18
R	0	0	11	0	11
Y	0	0	0	5	5
$\Sigma$	12	6	11	5	34

$$\varphi(x) = \binom{x}{2}$$

$$\frac{\varphi(18) - \varphi(12) - \varphi(6)}{\varphi(34)} = 1 - \underbrace{\frac{TP+TN}{TP+TN+FP+FN}}_{\text{Rand Index}}$$

# Generalization

Subsumes information theoretic

		V				
		B	G	R	Y	Σ
U {	B	12	6	0	0	18
	R	0	0	11	0	11
	Y	0	0	0	5	5
	Σ	12	6	11	5	34

$$\varphi(x) = x \log(x)$$

$$\frac{\varphi(18) - \varphi(12) - \varphi(6)}{\varphi(34)}$$

$$= \frac{H(U, V) - I(U, V)}{\log(34)}$$

**Variation of Information**



# Generalization

## Second normalization

	B	G	R	Y	$\Sigma$
B	12	6	0	0	18
R	0	0	11	0	11
Y	0	0	0	5	5
$\Sigma$	12	6	11	5	34

$$\frac{\varphi(18) - \varphi(12) - \varphi(6)}{\varphi(34)}$$

$$\frac{\varphi(18) - \varphi(12) - \varphi(6)}{\varphi\left(\frac{18}{34} \times \frac{12}{34}\right) + \varphi\left(\frac{18}{34} \times \frac{6}{34}\right) + \varphi\left(\frac{18}{34} \times \frac{11}{34}\right) + \dots}$$

➤  $\varphi(x) = x^2 \Rightarrow$  **ARI** (Adjusted Rand Index)

➤  $\varphi(x) = x \log x \Rightarrow$  **NMI** (Normalized Mutual Information)

# Generalization

Subsumes common measures

- Pair counting
- Information theoretic

A generalized distance with a plug-in function

➤  $\phi(x) = x^2 \Rightarrow \text{RI}$

➤  $\phi(x) = x^2 \Rightarrow \text{ARI}$

➤  $\phi(x) = x \log x \Rightarrow \text{VI}$

➤  $\phi(x) = x \log x \Rightarrow \text{NMI}$

Normalization 1

Normalization 2