

# Simulations in Statistical Physics

## Course for MSc physics students

Janos Török

Department of Theoretical Physics

December 1, 2015

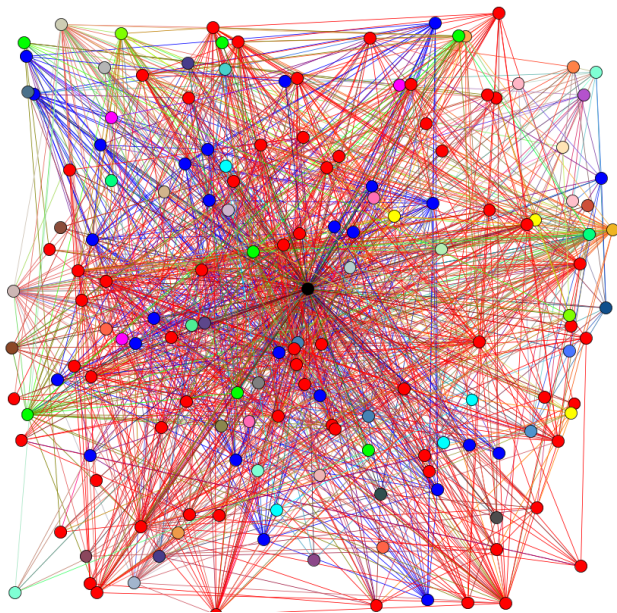
# Clustering, modularity, community detection



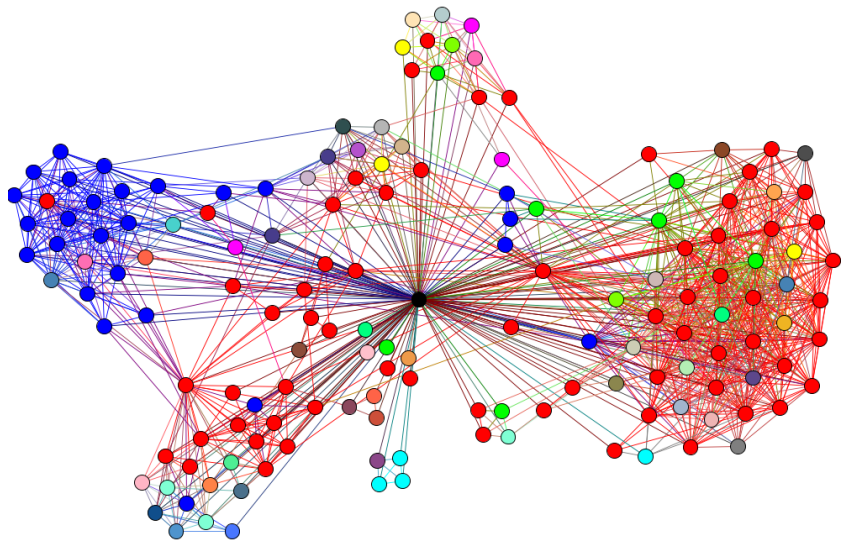
# Patterns in complex network

- ▶ Natural networks are not homogeneous
- ▶ There are natural groups
- ▶ These groups are more densely connected internally then externally
- ▶ Nodes in groups are more similar
- ▶ Exact mathematical definition is lacking
- ▶ These groups are called *communities*
- ▶ *Clustering*: group similar items together

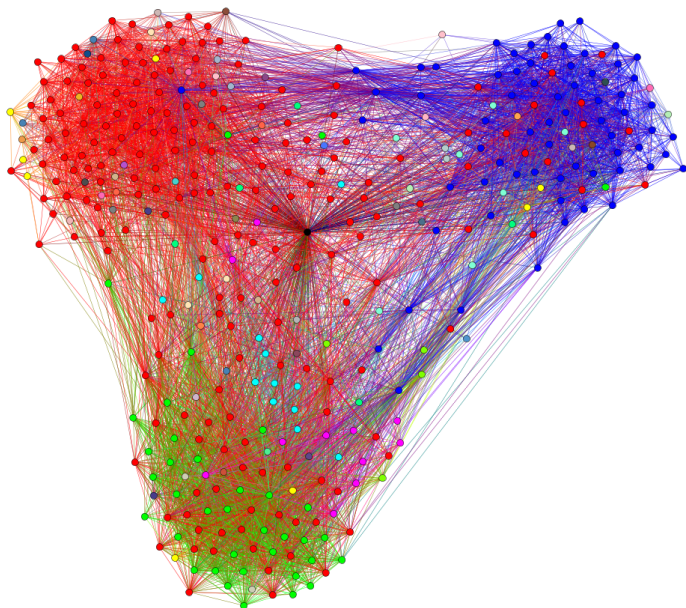
## Egocentric network on iwiw



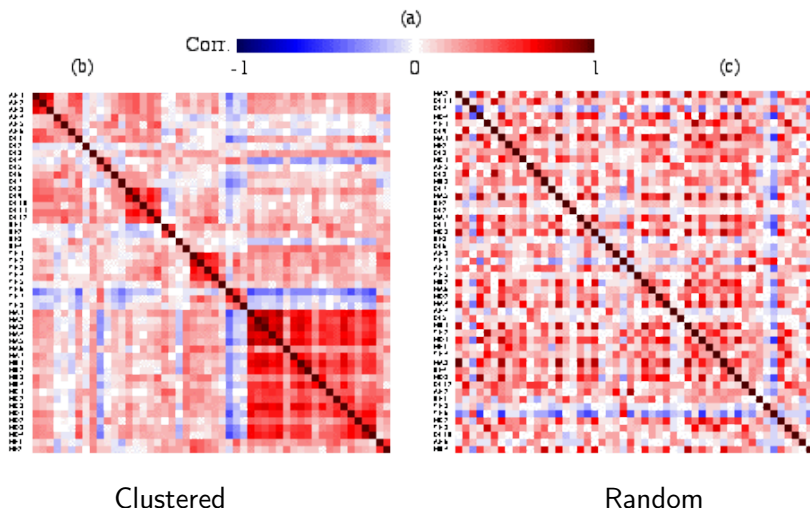
## Egocentric network on iwiw



## Egocentric network on iwiw

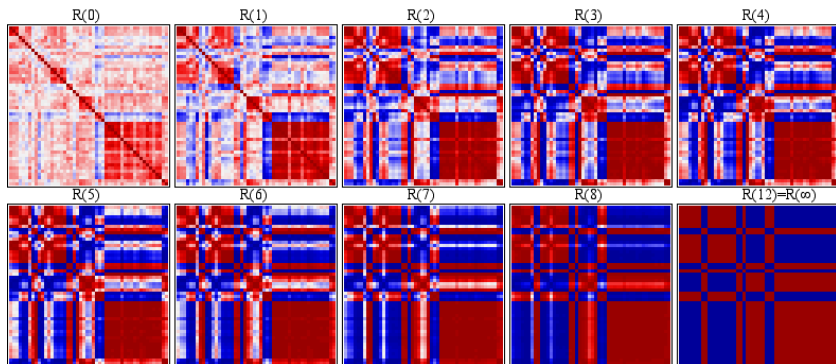


# Clustering example: Correlation between 50 symptoms

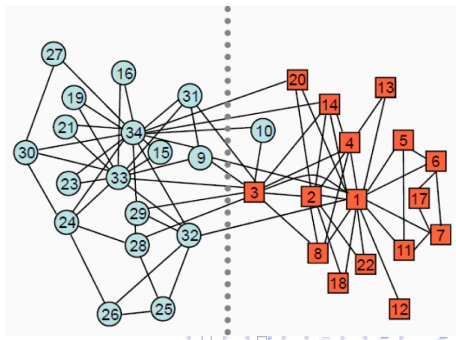
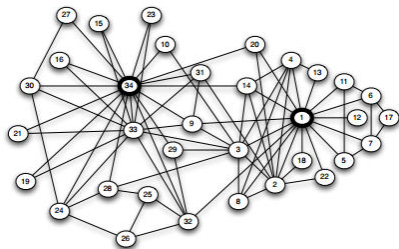


# Clustering example: Correlation between 50 symptoms

## Community detection



# Zachary karate club

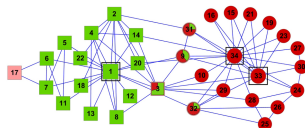


## Cluster, Community definition:

- ▶ Group which is more connected to itself than to the rest
- ▶ Group of items which are more similar to each other than to the rest of the system.

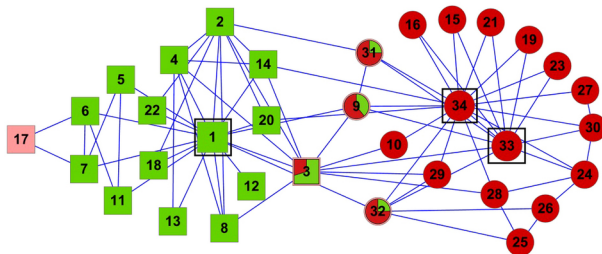
### Communities, Partitioning:

- ▶ Strict partitioning clustering: each object belongs to exactly one cluster
- ▶ Overlapping clustering: each object may belong to more clusters
- ▶ Hierarchical clustering: objects that belong to a child cluster also belong to the parent cluster
- ▶ Outliers: which do not conform to an expected pattern



# Communities, Partitioning

- ▶ Strict partitioning clustering: each object belongs to exactly one cluster
- ▶ Overlapping clustering: each object may belong to more clusters
- ▶ Hierarchical clustering: objects that belong to a child cluster also belong to the parent cluster
- ▶ Outliers: which do not conform to an expected pattern



# Communities, Partitioning, definitions:

- ▶ Local:
  - ▶ (Strong) Each node has more neighbors inside than outside
  - ▶ (Weak) Total degree within the community is larger than the total degree out of it.
  - ▶ Modularity by local definition (above)
  - ▶ Clique-percolation
- ▶ Global: The community structure found is optimal in a global sense
  - ▶ Modularity
  - ▶ k-means clustering
  - ▶ Agglomerative hierarchical clustering

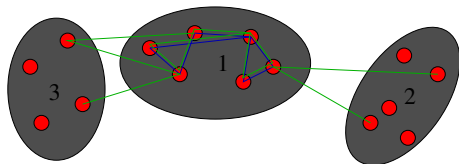
# Communities, Partitioning, definitions:

- ▶ Hundreds of different algorithms, definitions
- ▶ Starting point: *adjacency matrix*  $A_{ij}$ , the strength of the link between nodes  $i$  and  $j$
- ▶ Nodes as vectors (e.g. rows of adjacency matrix)
- ▶ Metric between nodes:  $\|a - b\|$ :
  - ▶ Euclidean distance:  $\|a - b\|_2 = \sqrt{\sum_i (a_i - b_i)^2}$
  - ▶ Maximum distance:  $\|a - b\|_\infty = \max_i |a_i - b_i|$
  - ▶ Cosine similarity:  $\|a - b\|_c = \frac{a \cdot b}{\|a\| \|b\|}$
  - ▶ Hamming distance: number of different coordinates

# Modularity

## Global method

- ▶  $e_{ij}$  percentage of edges in module (cluster)  $i$   
probability edge is in module  $i$
- ▶  $a_i$  percentage of edges with at least 1 end in module  $i$   
probability a random edge would fall into module  $i$



- ▶ Modularity is

$$Q = \sum_{i=1}^k (e_{ii} - a_i^2)$$

- ▶ Try to maximize  $Q$

# Modularity algorithm

- ▶ Rewrite  $Q$ :

$$Q = \frac{1}{2m} \sum_{i,j} \left[ A_{ij} - \frac{k_i k_j}{2m} \right]$$

$$2m = \sum_i k_i$$

- ▶ Only two modules
- ▶  $s_i = \pm 1$ : 1 if node  $i$  is in module 1; -1 otherwise

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

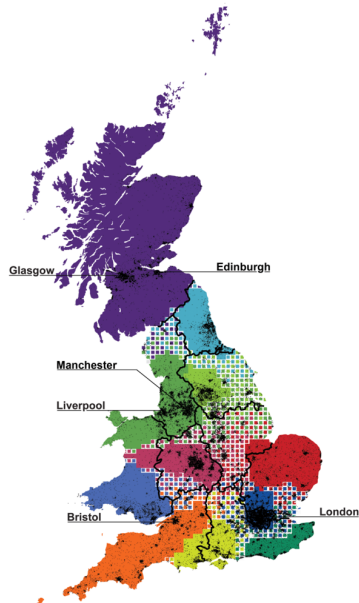
- ▶ +1 is a constant can be omitted
- ▶ Change the vector  $s_i$  to maximize  $Q$

# Modularity algorithm

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

- ▶ Try to find  $\pm 1$  vector  $s_i$  that maximizes the modularity.
- ▶ Start with two groups
- ▶ Then split one of the two groups using the same technique
- ▶ Very similar to spin glass Hamiltonian
- ▶ Generally a np-complete problem, we can use the same techniques.
- ▶ Often steepest descent is used, (greedy method): change the site that would increase the modularity the most.

# Modularity: human interactions between cities



# Problems with modularity

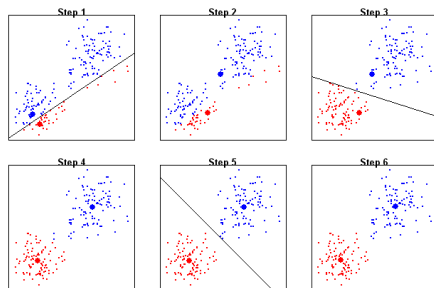
## Resolution

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

- ▶ On large networks normalization factor  $m$  can be very large
- ▶ (It relies on random network model)
- ▶ The expected edge between modules decreases and drops below 1
- ▶ A single link is a strong connection.
- ▶ Small modules will not be found

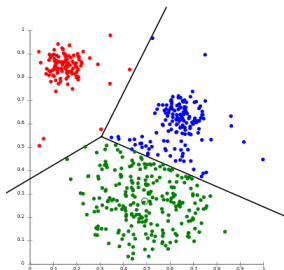
## k-means clustering

- ▶ Cut the system into exactly  $k$  parts
- ▶ Let  $\mu_i$  be the mean of each cluster (using a metric)
- ▶ The cluster  $i$  is the set of points which are closer to  $\mu_i$  than to any other  $\mu_j$
- ▶ The result is a partitioning of the data space into Voronoi cells



## k-means clustering, standard algorithm:

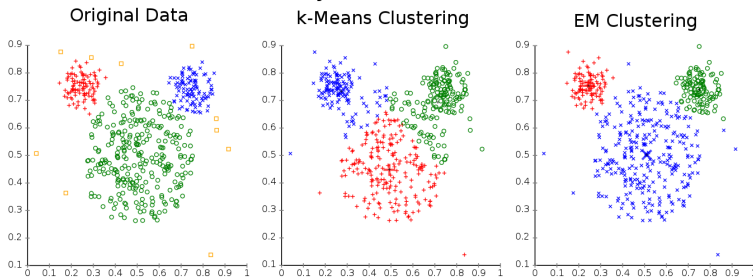
- ▶ Define a norm between nodes
- ▶ Give initial positions of the means  $m_i$
- ▶ **Assignment step:** Assign each node to cluster whose mean  $m_i$  is the closest to node.
- ▶ **Update step:** Calculate the new means of the clusters
- ▶ Go to Assignment step.



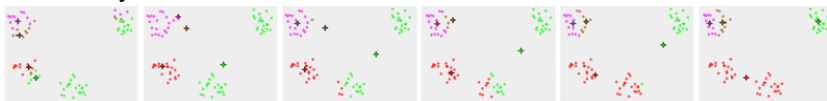
# k-means clustering, problems:

- ▶  $k$  has to be fixed beforehand
- ▶ Favors equal sized clusters:

Different cluster analysis results on "mouse" data set:



- ▶ Very sensitive on initial conditions:



- ▶ No guarantee that it converges

# Hierarchical clustering

1. Define a norm between nodes  $d(a, b)$
2. At the beginning each node is a separate cluster
3. Merge the two closest cluster into one
4. Repeat 3.

Norm between clusters  $||A - B||$

- ▶ Maximum or complete linkage clustering:

$$\max\{d(a, b) : a \in A, b \in B\}$$

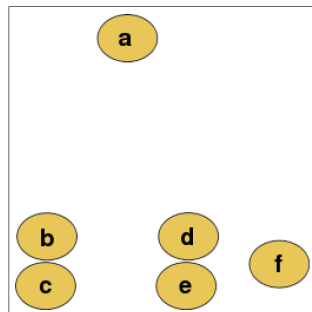
- ▶ Minimum or single-linkage clustering:

$$\min\{d(a, b) : a \in A, b \in B\}$$

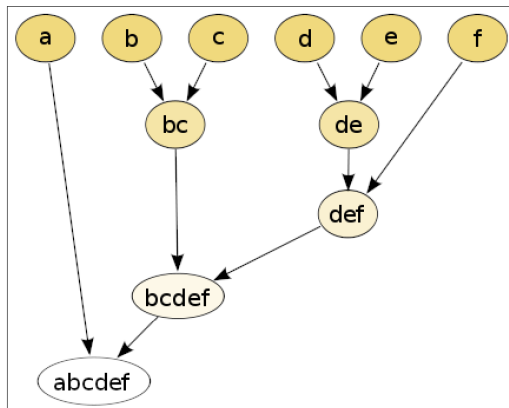
- ▶ Mean or average linkage clustering:

$$\frac{1}{||A|| ||B||} \sum_{a \in A} \sum_{b \in B} d(a, b)$$

# Hierarchical clustering

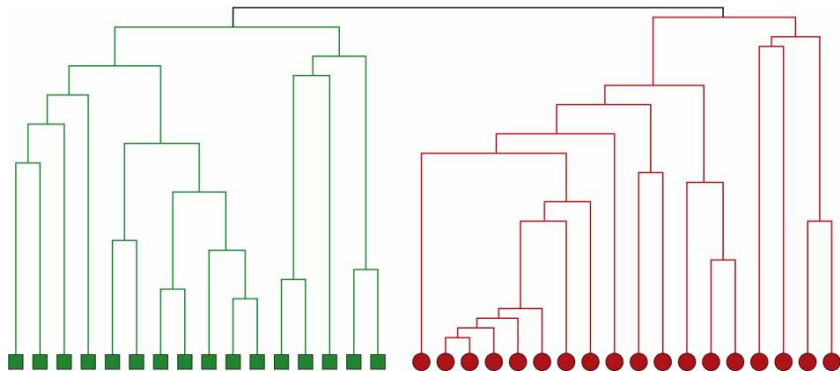


Original



Dendrogram

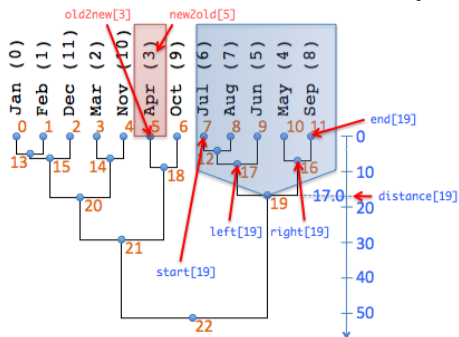
# Dendrogram of the Zachary karate club



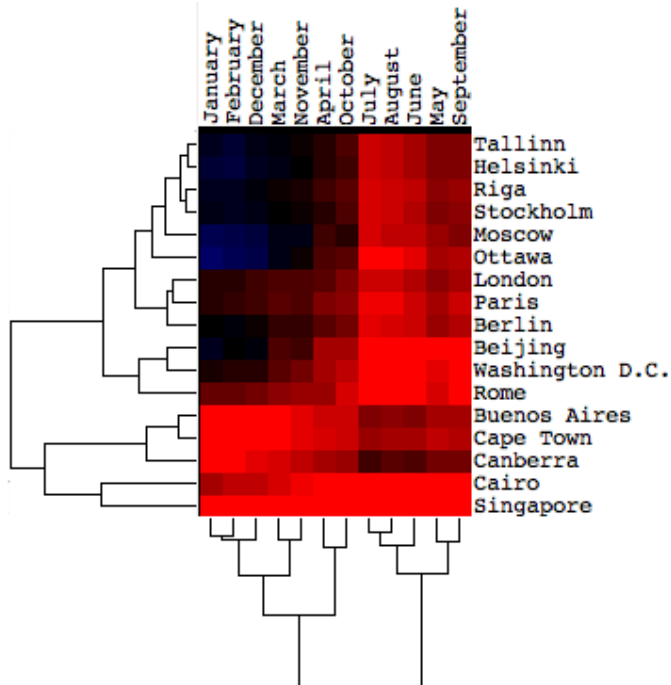
## Example: Temperatures in capitals

	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
Tallinn	-3	-5	-1	3	10	13	16	15	10	6	1	-2
Beijing	-3	0	6	13	20	24	26	25	20	13	5	-1
Berlin	0	-1	4	7	12	16	18	17	14	9	4	1
Buenos Aires	23	22	20	16	13	10	10	11	13	16	18	22
Cairo	13	15	17	21	25	27	28	27	26	23	19	15
Canberra	20	20	17	13	9	6	5	7	9	12	15	18
Cape Town	21	21	20	17	15	13	12	13	14	16	18	20
Helsinki	-5	-6	-2	3	10	13	16	15	10	5	0	-3
London	3	3	6	7	11	14	16	16	13	10	6	5
Moscow	-8	-7	-2	5	12	15	17	15	10	3	-2	-6
Ottawa	-10	-8	-2	6	13	18	21	20	14	7	1	-7
Paris	3	4	7	10	13	16	19	19	16	11	6	5
Riga	-3	-3	1	5	11	15	17	16	12	7	2	-1
Rome	8	8	11	12	17	20	23	23	21	17	12	9
Singapore	27	27	28	28	28	28	28	28	27	27	27	26
Stockholm	-2	-3	0	3	10	14	17	16	11	6	1	-2
Washington D.C.	2	3	7	13	18	23	26	25	21	15	9	3

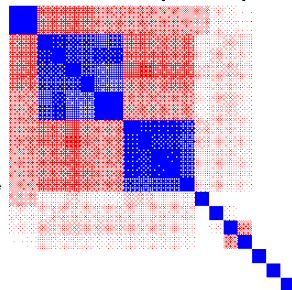
	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
Tallinn	-3	-5	-1	3	10	13	16	15	10	6	1	-2
Beijing	-3	0	6	13	20	24	26	25	20	13	5	-1
Berlin	0	-1	4	7	12	16	18	17	14	9	4	1
Buenos Aires	23	22	20	16	13	10	10	11	13	16	18	22
Cairo	13	15	17	21	25	27	28	27	26	23	19	15
Canberra	20	20	17	13	9	6	5	7	9	12	15	18
Cape Town	21	21	20	17	15	13	12	13	14	16	18	20
Helsinki	-5	-6	-2	3	10	13	16	15	10	5	0	-3
London	3	3	6	7	11	14	16	16	13	10	6	5
Moscow	-8	-7	-2	5	12	15	17	15	10	3	-2	-6
Ottawa	-10	-8	-2	6	13	18	21	20	14	7	1	-7
Paris	3	4	7	10	13	16	19	19	16	11	6	5
Riga	-3	-3	1	5	11	15	17	16	12	7	2	-1
Rome	8	8	11	12	17	20	23	23	21	17	12	9
Singapore	27	27	28	28	28	28	28	28	27	27	27	26
Stockholm	-2	-3	0	3	10	14	17	16	11	6	1	-2
Washington D.C.	2	3	7	13	18	23	26	25	21	15	9	3



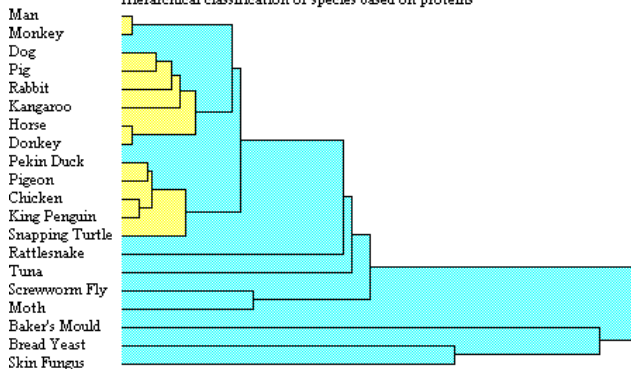
Euclidean distance



Man  
Monkey  
Dog  
Pig  
Rabbit  
Kangaroo  
Horse  
Donkey  
Pekin Duck  
Pigeon  
Chicken  
King Penguin  
Snapping Turtle  
Rattlesnake  
Tuna  
Screwworm Fly  
Moth  
Baker's Mould  
Bread Yeast  
Skin Fungus



Hierarchical classification of species based on proteins



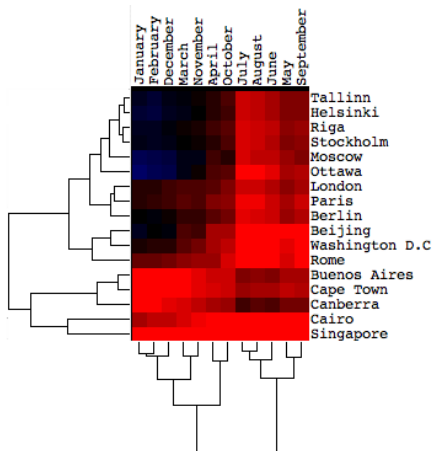
# Hierarchical clustering: problems

## ► Advantages

- Simple
- Fast
- Number of clusters can be controlled
- Hierarchical relationship

## ► Disadvantages

- No a priori cutting level
- Meaning of clusters unclear
- Important links may be missed
- Different result if one item omitted



# Ahn method: Hierarchical clustering of edges

- Partition density:

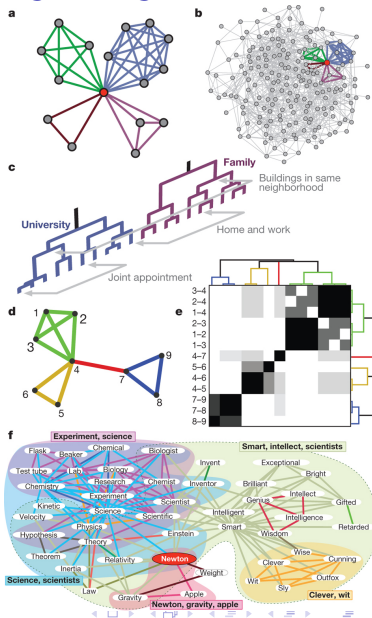
$$D_c = \frac{m_c - (n_c - 1)}{n(n_c - 1)/2 - (n_c - 1)}$$

$m_c$  # of links in subset  $c$

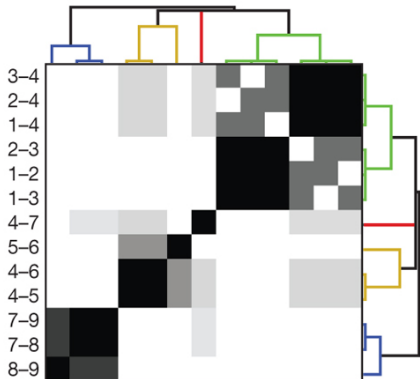
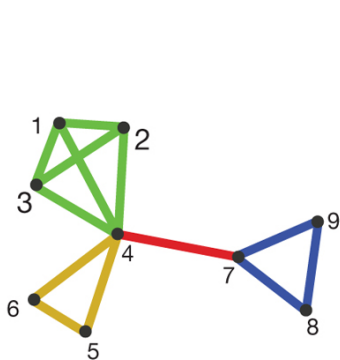
$n_c$  # of nodes in subset  $c$

$$D = \frac{2}{M} \sum m_c D_c$$

- Cutting at the max of  $D$
- Overlapping communities



# Ahn method: Example



## LFK method

- ▶ Try to use definition: more links in than out in cluster

$$f_G = \frac{k_{in}^G}{(k_{in}^G + k_{out}^G)^\alpha}$$

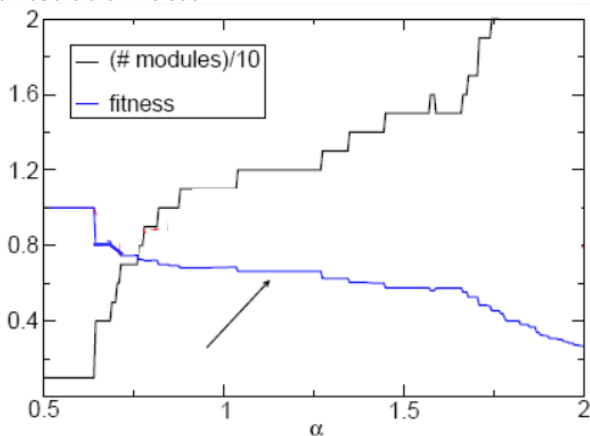
- ▶ Try to maximize fitness:
  - ▶ Add node if it increases fitness
  - ▶ Check all others whether they decrease it
- ▶ Algorithm:
  1. Loop for all neighboring nodes of  $G$  not included in  $G$
  2. The neighbor with the largest fitness is added to  $G$ , yielding a larger subgraph  $G'$
  3. The fitness of each node of  $G'$  is recalculated
  4. If a node turns out to have negative fitness change, it is removed from  $G'$ , yielding a new subgraph  $G''$
  5. if 4 occurs go to 3 than repeat from 1 with  $G''$

---

<sup>1</sup>Andrea Lancichinetti, Santo Fortunato and János Kertész New J. Phys. 11 033015, 2009.

# LFK method

- ▶  $\alpha$  resolution factor



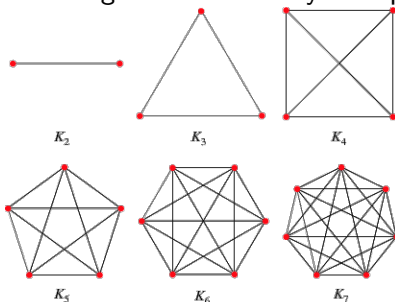
- ▶ Long plateaus indicate stable structure, (as e.g. hierarchical)

# LFK method: problems

- ▶ Advantages
  - ▶ Resolution can be controlled
  - ▶ Close to most trivial definition
  - ▶ Can be extended to overlapping clusters
- ▶ Disadvantages
  - ▶ Code runs for ages
  - ▶ Heuristic cutting

# Clique percolation

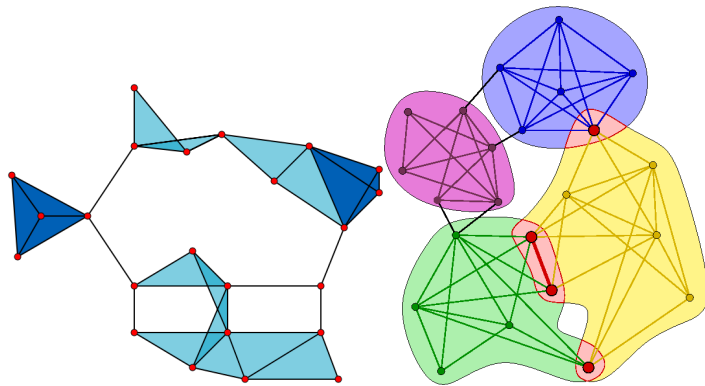
- ▶ Motivation: clusters are formed with at least triangles
- ▶ Can be generalized to any  $k$ -clique



- ▶  $k = 2$  normal percolation

# Clique percolation

- ▶ It will definitely lead to overlapping communities, but overlap is limited to  $k - 1$  nodes
- ▶  $k$ -clusters are included in  $k - 1$  clusters



# Clique percolation

- ▶ Algorithm
  - ▶ Similar to normal percolation on networks but with multiple loops
- ▶ Advantages
  - ▶ Different level of clusters
  - ▶ Clusters are generally relevant
  - ▶ No heuristics
- ▶ Disadvantages
  - ▶ Running time cannot be guessed (finding the maximal clique is an np-complete problem)
  - ▶ Code may run for ages