Large-scale structure of complex networks (Part 2)

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2018-01-06

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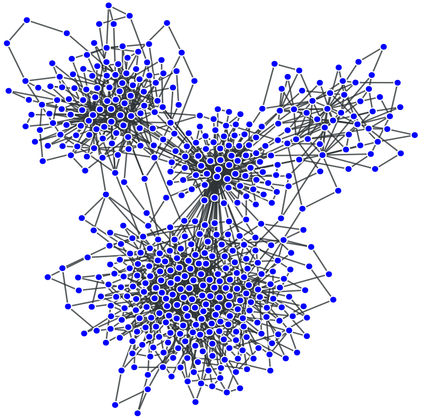
Hello

Community structure in networks



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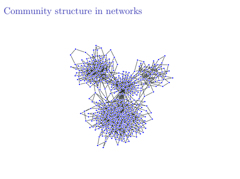
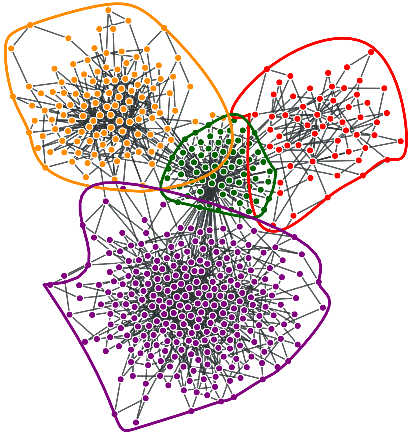


Community structure in networks



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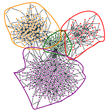

Community structure in networks

What are communities?

- **Traditional definition**: Groups of nodes with a high internal link density
- **Modern definition**: Nodes with similar connection probabilities to the rest of the network

Community structure in networks

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Communities in the real-world networks

- **Social networks**:
  - Friend-circles
  - Research communities
  - Co-workers
- **World Wide Web**:
  - Pages with similar contents
  - Webpages under the same domain (e.g. Wikipedia)
- **Biological networks**:
  - Proteins with similar roles in protein interaction networks
  - Chemicals together taking part in chemical reactions in metabolic networks
  - Communities in neuronal networks

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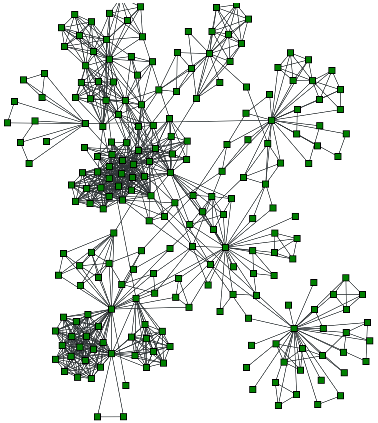
Community detection



Detecting communities is important!

- Communities are building blocks of networks
- Communities allow us to see “the big picture”
- Functional/Autonomous units
- Non-trivial effects on the processes on networks

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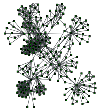

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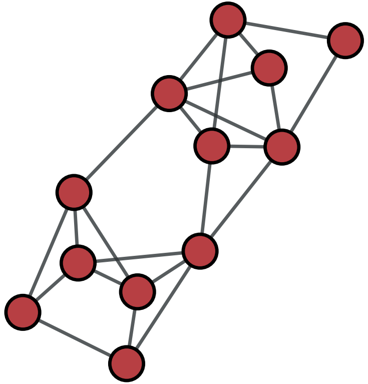
Graph partitioning

Problem of dividing a graph in a given number of groups of given sizes such that the number of links between the groups (**cut size**) is minimized



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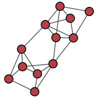

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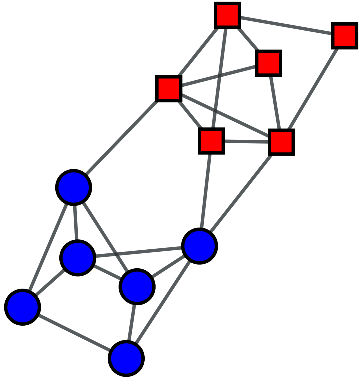

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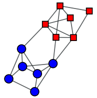

Partitioning is hard!

- Graph with n vertices
- Find two groups with sizes n_1 and n_2 such that the cut size is minimum
- Number of ways: $\frac{n!}{n_1!n_2!} \approx \frac{2^{n+1}}{\sqrt{n}}$

Heuristics are needed!

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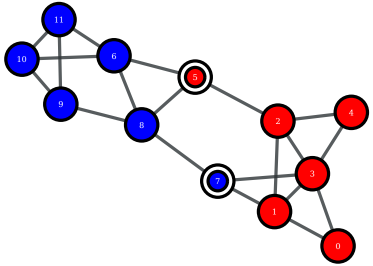
Kernighan-Lin algorithm

cut size $= 4$



- Divide the vertices into two groups of the required sizes and calculate the cut size

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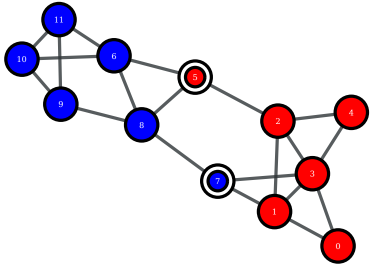

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- Find a pair of nodes which when switched, will reduce the cut size most and switch them

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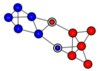

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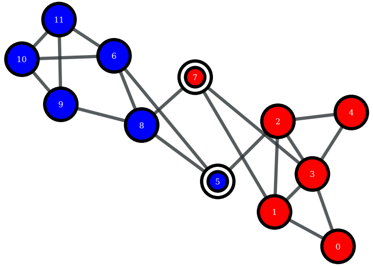

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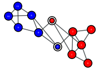

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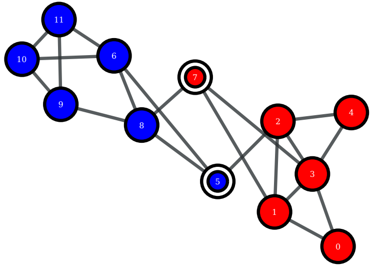

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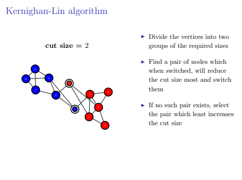

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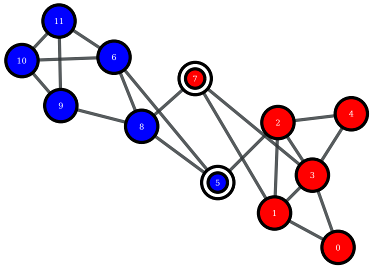

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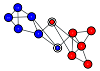

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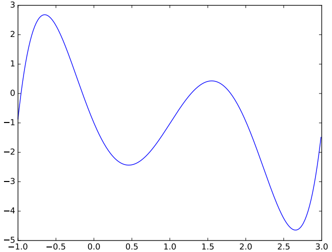
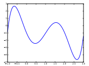


- Go through all the states and select the one with the least cut size
- Start with this state and repeat the whole procedure
- Continue till the cut size no longer becomes smaller
- Starting with many random initial conditions is better

Kernighan-Lin algorithm



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Group sizes remain constant

Spectral partitioning

- Faster algorithm than Kernighan-Lin
- Uses properties of the graph Laplacian
- More complex to implement than Kernighan-Lin

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Spectral partitioning

Cut size:

$$R = \frac{1}{2} \sum_{\substack{i,j \text{ in} \\ \text{different} \\ \text{groups}}} A_{ij}$$

Define

$$s_i = \begin{cases} +1 & \text{if vertex } i \text{ belongs to group 1} \\ -1 & \text{if vertex } i \text{ belongs to group 2} \end{cases}$$

Then

$$\frac{1}{2}(1 - s_i s_j) = \begin{cases} 1 & \text{if } i \text{ and } j \text{ are in different groups,} \\ 0 & \text{if } i \text{ and } j \text{ are in the same group} \end{cases}$$

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$$R = \frac{1}{4} \sum_{ij} A_{ij}(1 - s_i s_j)$$

First term,

$$\sum_{ij} A_{ij} = \sum_i k_i = \sum_i k_i s_i^2 = \sum_{ij} k_i \delta_{ij} s_i s_j$$

$$R = \frac{1}{4} \sum_{ij} (k_i \delta_{ij} - A_{ij}) s_i s_j = \frac{1}{4} \sum_{ij} L_{ij} s_i s_j$$

$$R = \frac{1}{4} \mathbf{s}^T \mathbf{L} \mathbf{s}$$

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L is so imp that we have a name for it! Laplacian

.

s is a columnvector

.

L: structure, s: division

.

find s that minimizes R

.

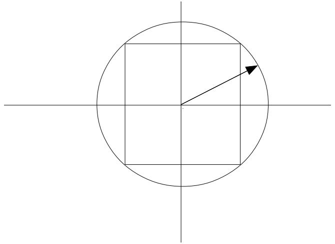
Problem is hard, s takes only integer values

.

Relaxation method

Two constraints:

- s_i can be only ± 1
- $\sum_i s_i = n_1 - n_2 \Rightarrow \mathbf{1}^T\mathbf{s} = n_1 - n_2$



Relax the first constraint

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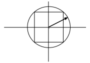

hypercube

.

continuous s, differentiate

Spectral partitioning

Minimization with constraints $\Rightarrow$ Lagrange multipliers

$$\frac{\partial}{\partial s_i}\left[\sum_{jk} L_{jk} s_j s_k + \lambda\left(n - \sum_j s_j^2\right) + 2\mu\left((n_1 - n_2) - \sum_j s_j\right)\right] = 0$$

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$$\mathbf{L}\mathbf{s} = \lambda\mathbf{s} + \mu\mathbf{1} = \lambda\left(\mathbf{s} + \frac{\mu}{\lambda}\mathbf{1}\right)$$

$$\mathbf{L}\left(\mathbf{s} + \frac{\mu}{\lambda}\mathbf{1}\right) = \lambda\left(\mathbf{s} + \frac{\mu}{\lambda}\mathbf{1}\right)$$

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Spectral partitioning

$\mathbf{x}$ is an eigenvector of the Laplacian with eigenvalue λ

Which eigenvector to choose?

$$\mathbf{x} \text{ cannot be the eigenvector } \mathbf{1} = \begin{pmatrix} 1 \\ 1 \\ . \\ . \\ 1 \end{pmatrix}$$

$$\mathbf{1}^T\mathbf{x} = \mathbf{1}\left(\mathbf{s} + \frac{\mu}{\lambda}\mathbf{1}\right) = (n_1 - n_2) + \frac{\mu}{\lambda}n = 0$$

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x is orthogonal to 1

.

x is eigenvector but not 1

Spectral partitioning

Which eigenvector to choose?

$$R = \frac{1}{4}\mathbf{s}^T\mathbf{L}\mathbf{s} = \frac{1}{4}\mathbf{x}^T\mathbf{x} = \frac{n_1 n_2}{n}\lambda$$

Choose the eigenvector with smallest possible eigenvalue!

Eigenvalues of the Laplacian are non-negative and smallest is always 0

$\mathbf{v}_1 = \mathbf{1}$ is ruled out already. So choose $\mathbf{v}_2$ with the smallest positive eigenvalue

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$$\mathbf{s} = x + \frac{n_1 - n_2}{n}\mathbf{1}$$

OR

$$s_i = x_i + \frac{n_1 - n_2}{n}$$

But s_i can be only ± 1

Thus, we want $\mathbf{x}$ to be as close as possible to $\mathbf{s}$

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Maximize:

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Equivalently, maximize:

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Simply put the n_1 vertices with most positive elements in group 1 and the rest ones in group 2

Group assignments are arbitrary

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Choose the assignment with the smaller cut size

Spectral partitioning

- Calculate $\mathbf{v}_2$ of the Laplacian
- Put vertices corresponding to largest n_1 elements in group 1 and others in group 2. Calculate the cut size
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Community detection is harder!

- **Graph partitioning**
  - well defined
  - Number of groups is fixed
  - Sizes of the groups are fixed
  - Divide even if no good division exists
- **Community detection**
  - ill-defined
  - Number of groups depends on the structure of the network
  - Sizes of the groups depend on the structure of the network
  - Discover natural fault lines

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Many definitions.. many algorithms!

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- Kernighan-Lin-Newman algorithm
- Spectral decomposition
- Clique-percolation
- Radom walk methods
- Statistical inference
- Label propagation
- Hierarchical clustering

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I can go on.. These algorithms use different definitions/views of communities

Broad classification

- **Agglomerative algorithms:**
  - Hierarchical clustering
  - Louvain method
  - CNM algorithm
- **Divisive algorithms:**
  - Girvan-Newman algorithm
  - Radichhi algorithm
- **Assignment algorithms:**
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"The" simplest community detection problem

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- Minimum cut size?
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  - Needs ad hoc specification of sizes

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Empty group

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A different measure of the quality of division is required..

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Different measure

Quantification of community structure

- Fewer than expected edges between the groups

Quantification of community structure

- Fewer than expected edges between the groups

few edges = expected edges = not a good division

Quantification of community structure

- Fewer than expected edges between the groups
- Equivalently, more than expected edges inside the groups

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Remember assortativity

Quantification of community structure

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- Assortativity mixing and modularity

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Divide network using modularity

Quantification of community structure

- Fewer than expected edges between the groups
- Equivalently, more than expected edges inside the groups
- Assortativity mixing and modularity
- Look for divisions with high modularity

Quantification of community structure

- Fewer than expected edges between the groups
- Equivalently, more than expected edges inside the groups
- Assortativity mixing and modularity
- Look for divisions with high modularity

Heuristics are needed

Modularity

How to find the division which maximizes the modularity?

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Kernighan-Lin-Newman algorithm

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Variation of KL algorithm

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Sizes of the groups are not fixed

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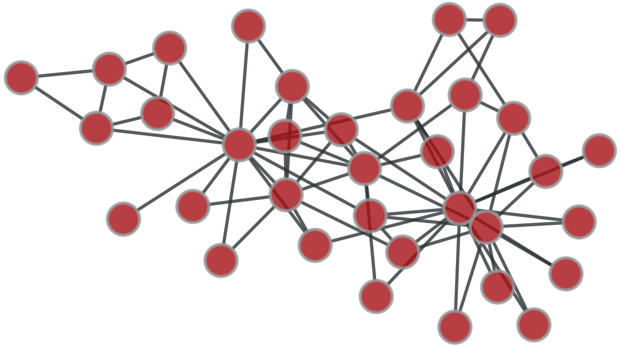
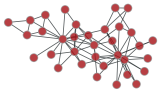


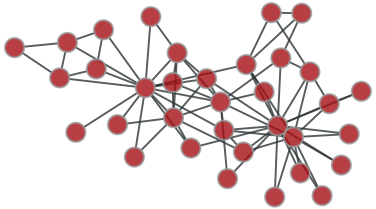
2018-01-06

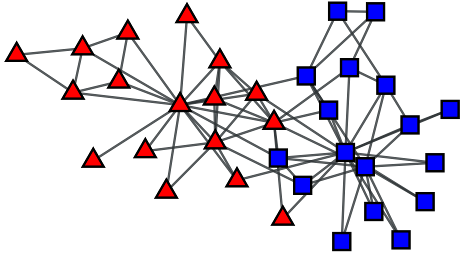
Large-scale structure of complex networks (Part 2)

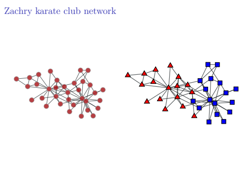


Does somebody know this network?

Zachry karate club network

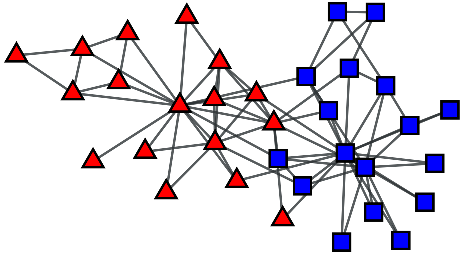






Application to Zachry karate club

Actual division



Application to Zachry karate club
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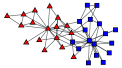

Application to Zachry karate club

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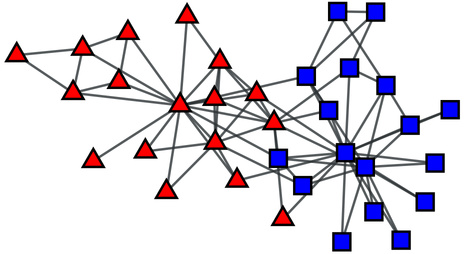
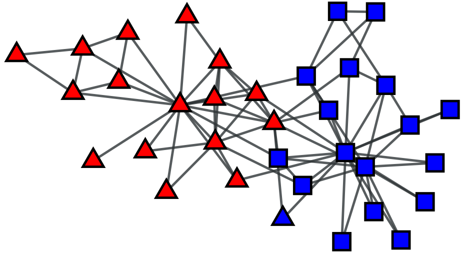
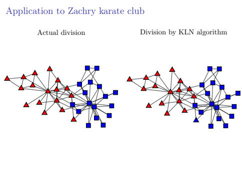


Division by KLN algorithm





Spectral modularity maximization

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

Note that:

$$\sum_j B_j = \sum_j A_{ij} - \frac{k_i}{2m}\sum_j k_j = k_i - \frac{k_i}{2m}2m = 0$$

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spectral partitioning: cut size
.
analogous algorithm exists

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

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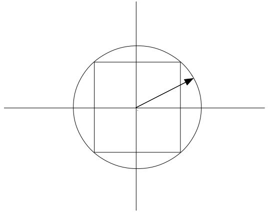
Spectral modularity maximization

Relaxation method

- Numbers of elements with values $+1$ and -1 are not fixed
- Only constraint: $\mathbf{s}^T\mathbf{s} = \sum_i s_i^2 = n$



$$\frac{\partial}{\partial s_i}\left[\sum_{ij} B_{jk} s_j s_k + \beta\left(n - \sum_j s_j^2\right)\right] = 0$$

$$\sum_j B_{ij} s_j = \beta s_i$$

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Spectral modularity maximization
Relaxation method
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s is eigenvector of modularity matrix

Spectral modularity maximization

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Thus, choose $\mathbf{s}$ to be the eigenvector $\mathbf{u}_1$ corresponding to the largest eigenvalue of the modularity matrix

Maximize:

$$\mathbf{s}^T \mathbf{u}_1 = \sum_i s_i u_{1i}$$

Maximum is achieved when each term is non-negative $\Rightarrow$ Use signs of u_{1i}!

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- Calculate the modularity matrix
- Calculate its eigenvector corresponding to the largest eigenvalue
- Assign nodes to communities based on the signs of elements

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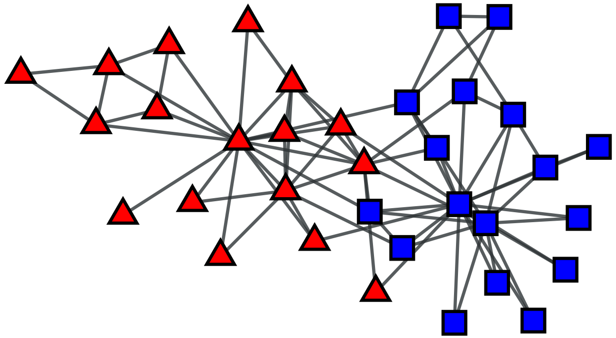
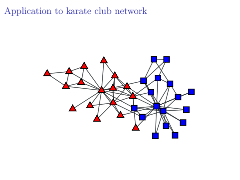
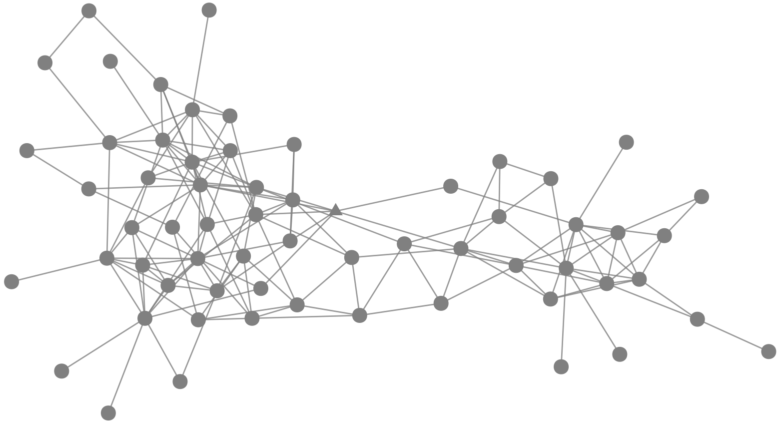
Application to karate club network





Bottlenose dolphins



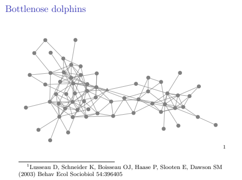
[1]

[1]Lusseau D, Schneider K, Boisseau OJ, Haase P, Slooten E, Dawson SM (2003) Behav Ecol Sociobiol 54:396405

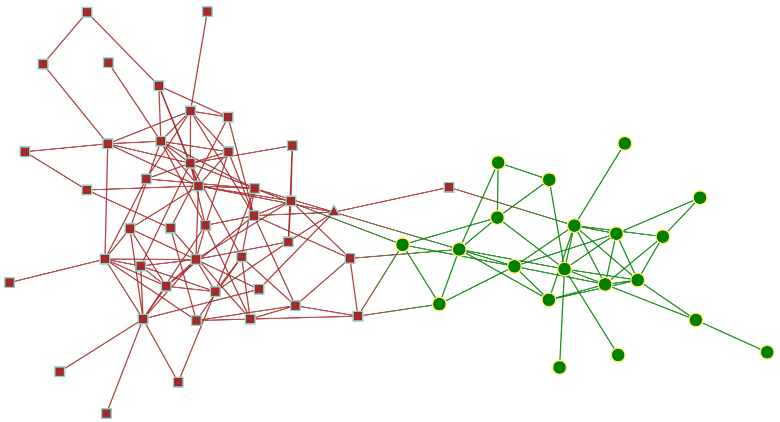
2018-01-06

Large-scale structure of complex networks (Part 2)

└─Bottlenose dolphins



Bottlenose dolphins



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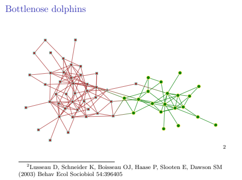

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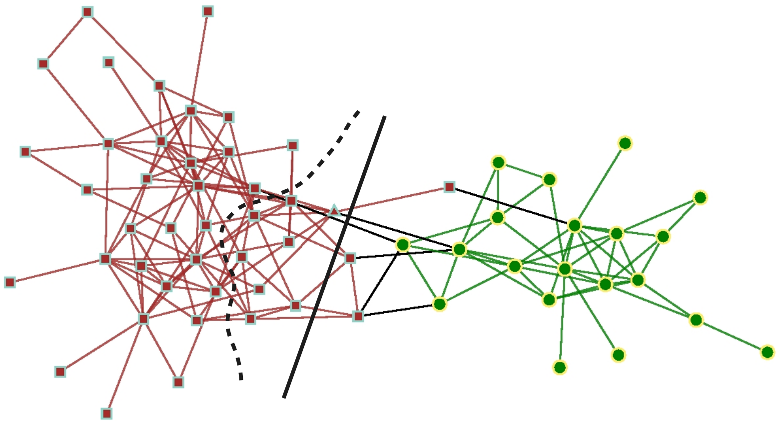

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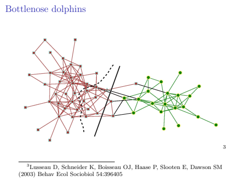

Newman-Girvan algorithm

- Look for edges between the communities
- Edge betweenness

Newman-Girvan algorithm

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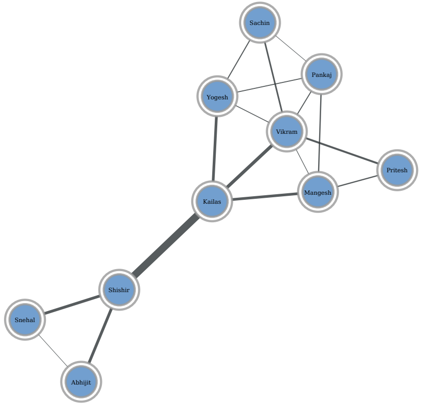
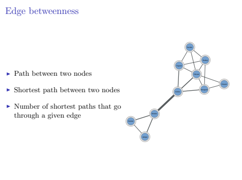
- Edge betweenness

Let's have a look at the edge betweenness

Edge betweenness

- Path between two nodes
- Shortest path between two nodes
- Number of shortest paths that go through a given edge





The algorithm

- Calculate betweenness for all edges
- Remove the edge with the highest betweenness
- Recalculate betweenness for all edges
- Repeat

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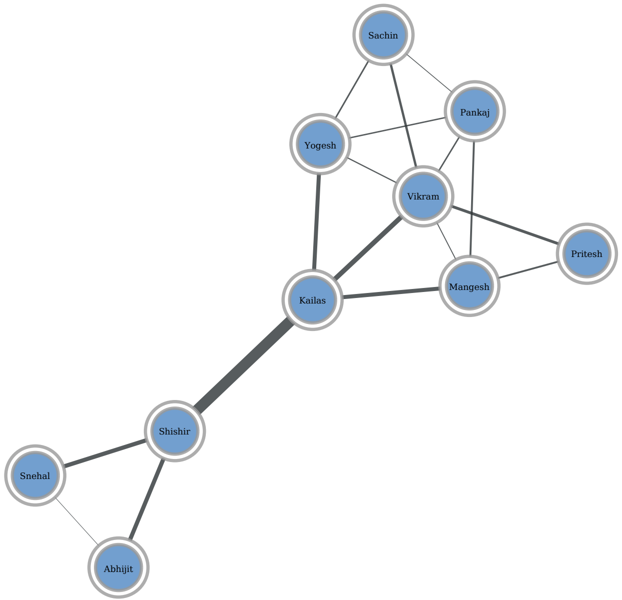
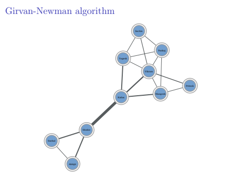
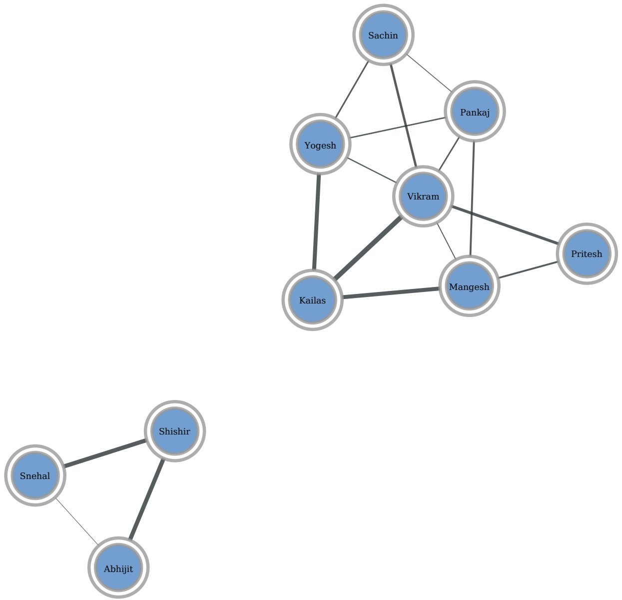
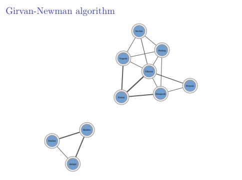
Girvan-Newman algorithm





Girvan-Newman algorithm





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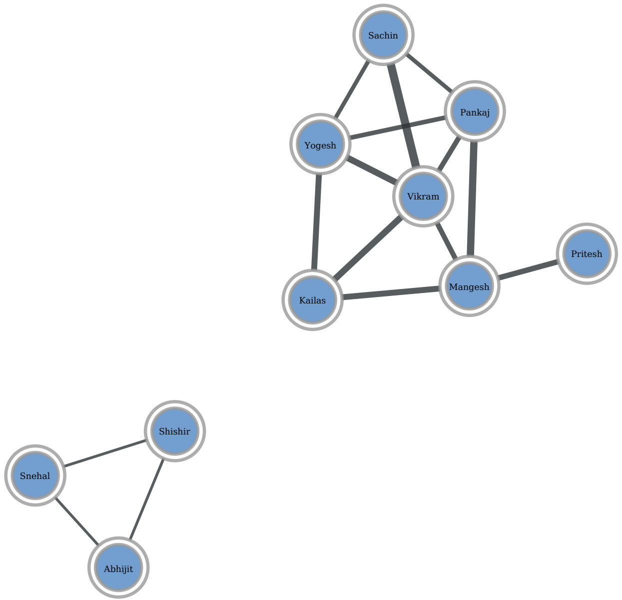

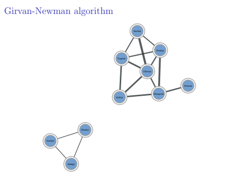

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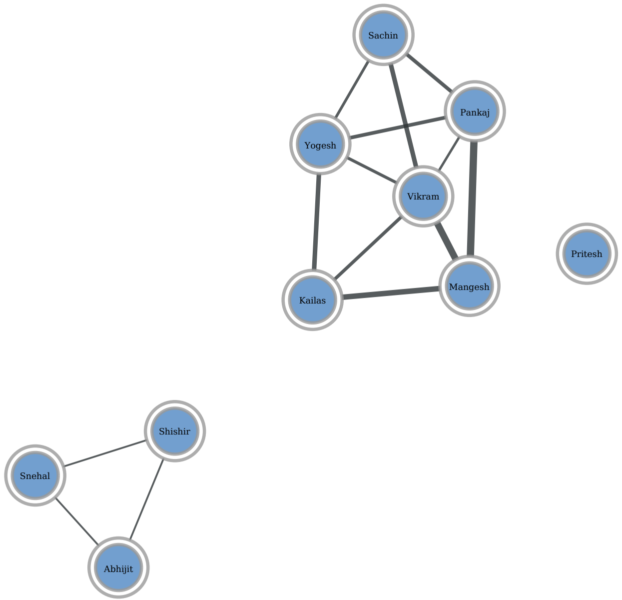

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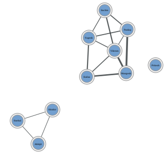

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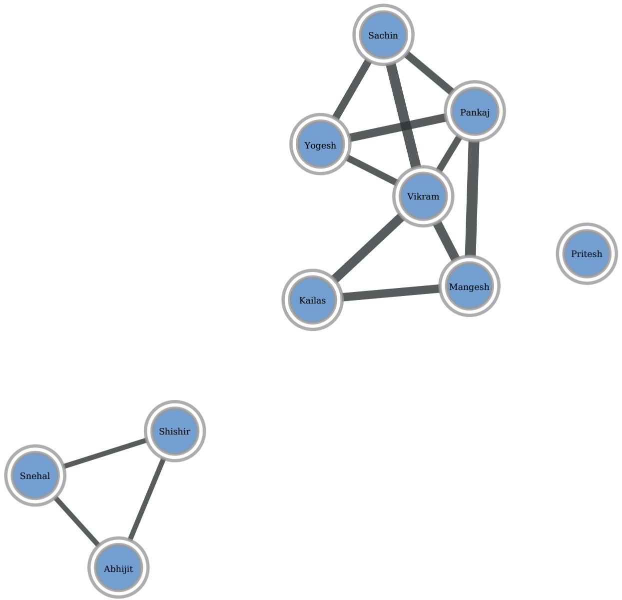

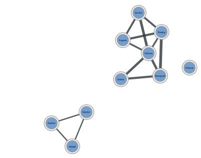

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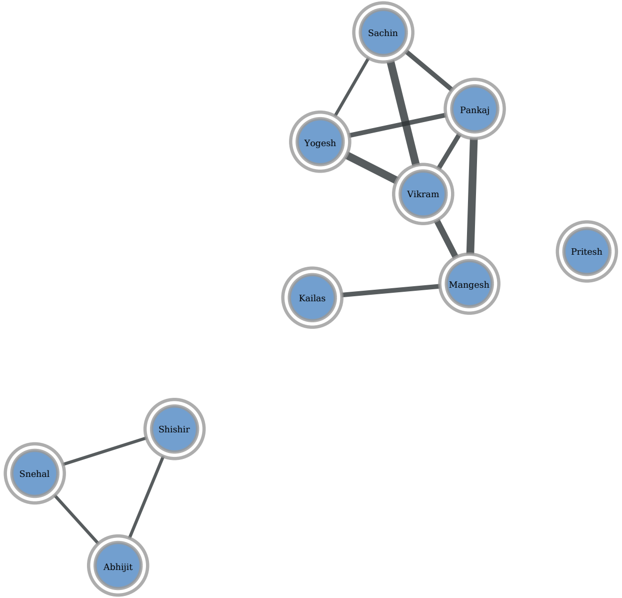

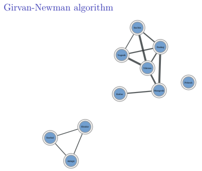

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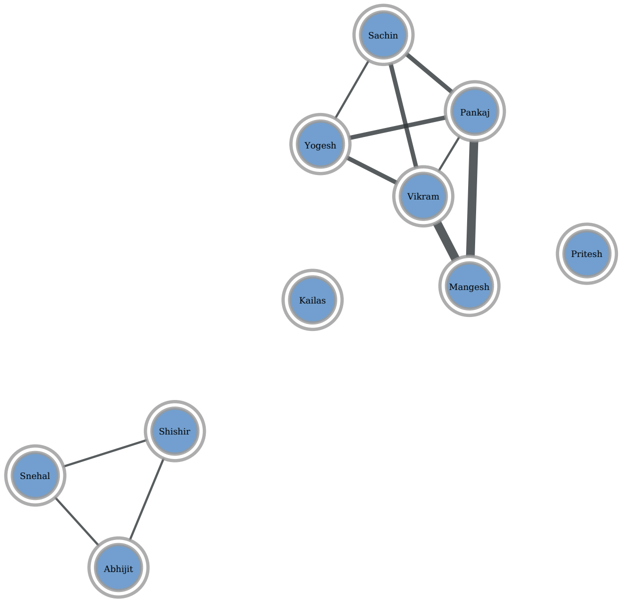
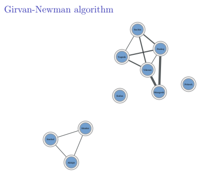
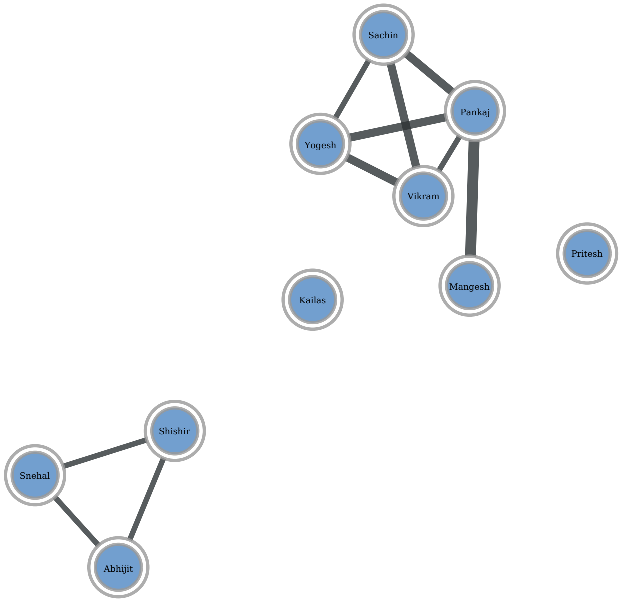




Girvan-Newman algorithm



2018-01-06

Large-scale structure of complex networks (Part 2)

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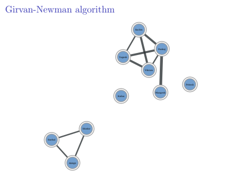

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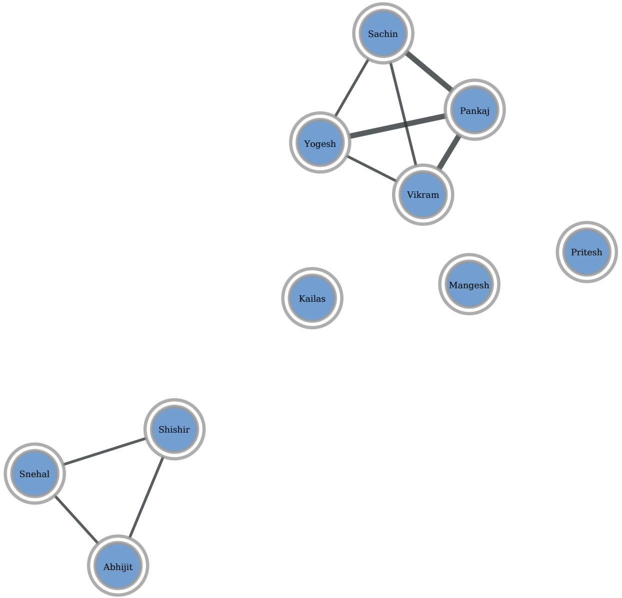

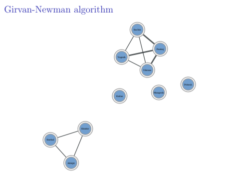

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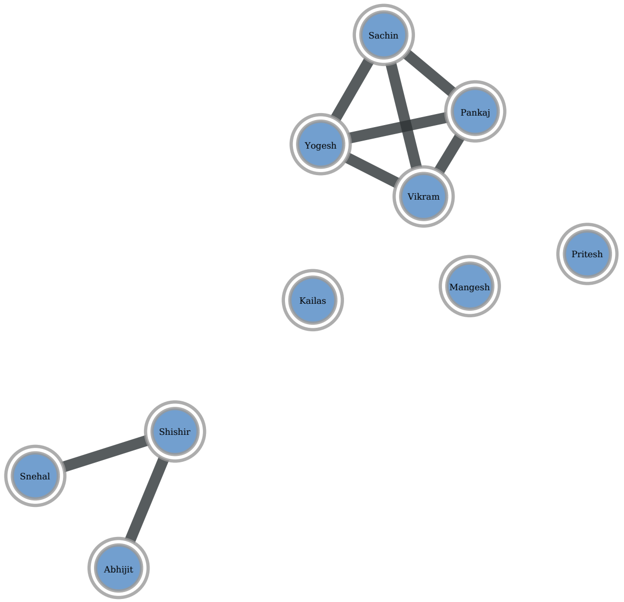

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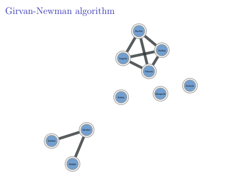

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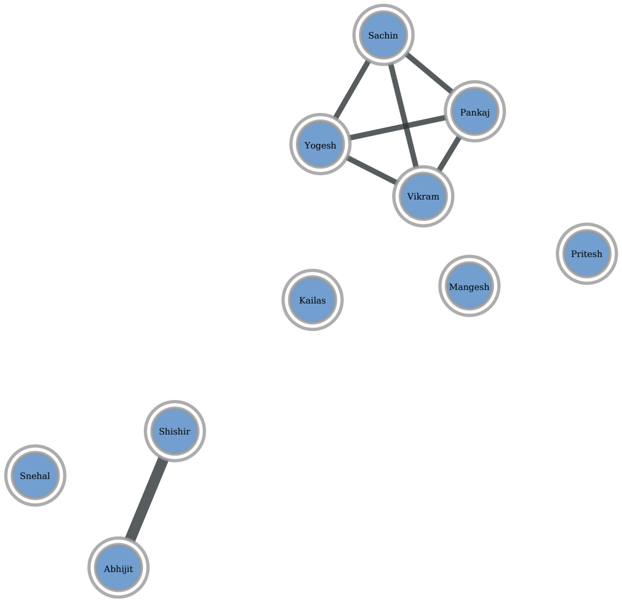

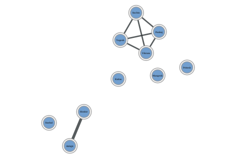
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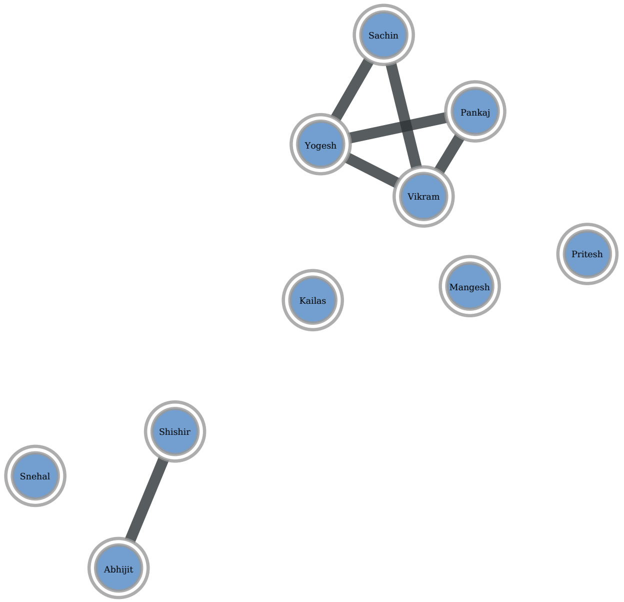

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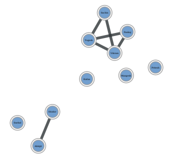

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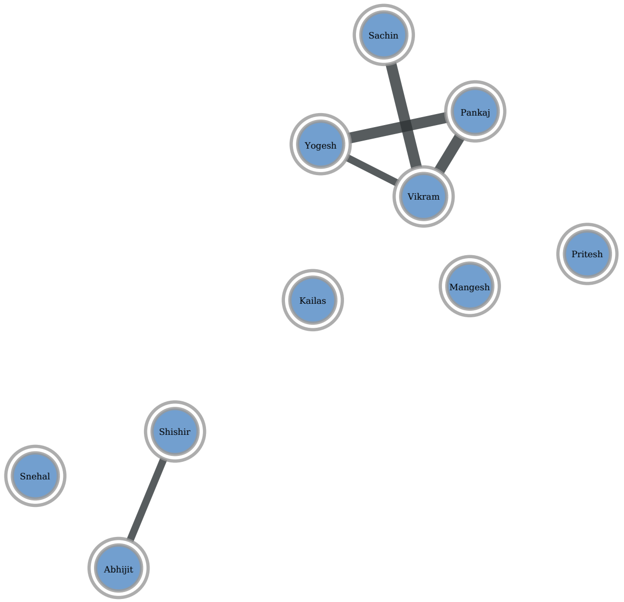

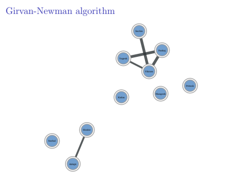

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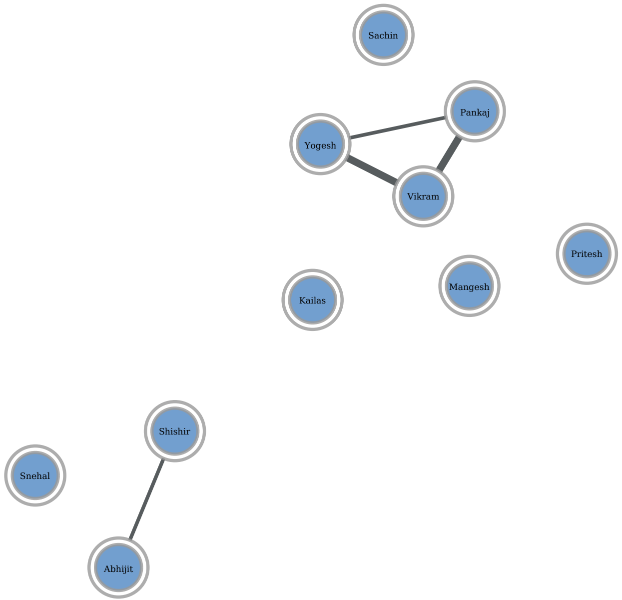

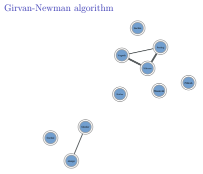

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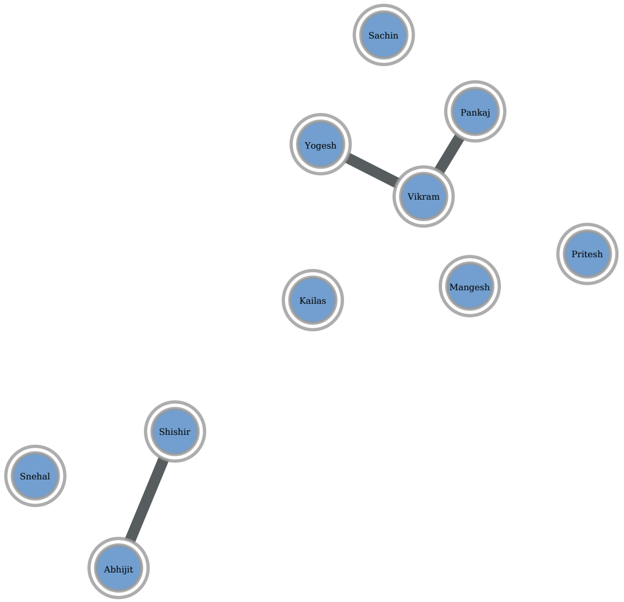

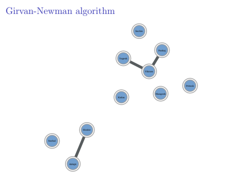

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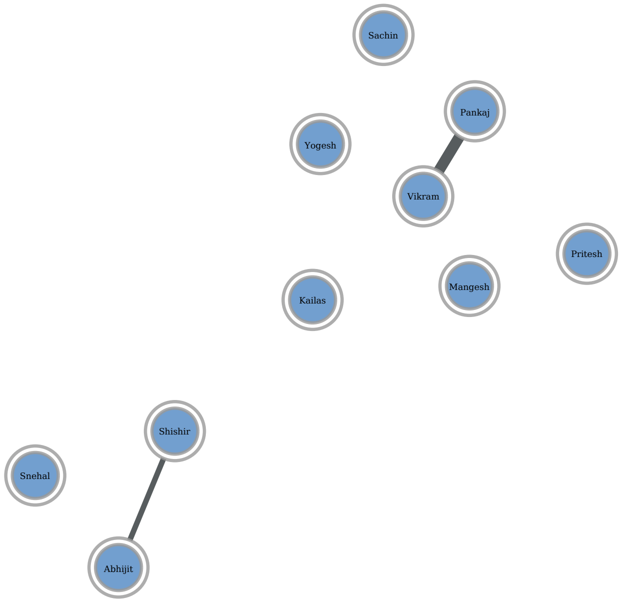

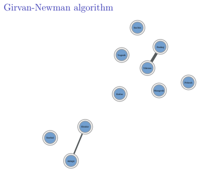

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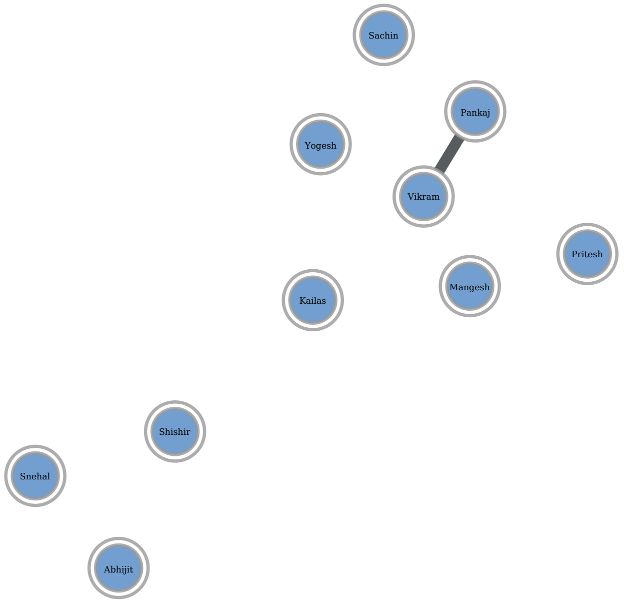

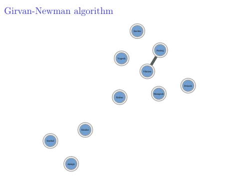

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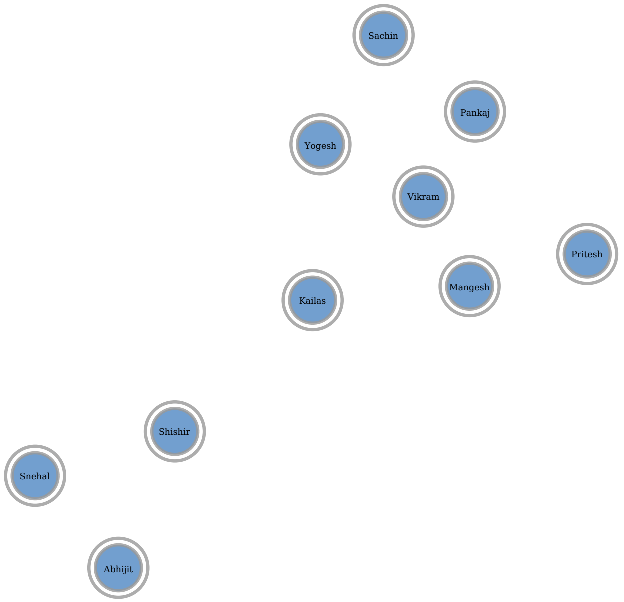

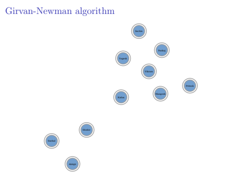

Problems with traditional community detection algorithms

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- Resolution limit
- Structure vs Noise

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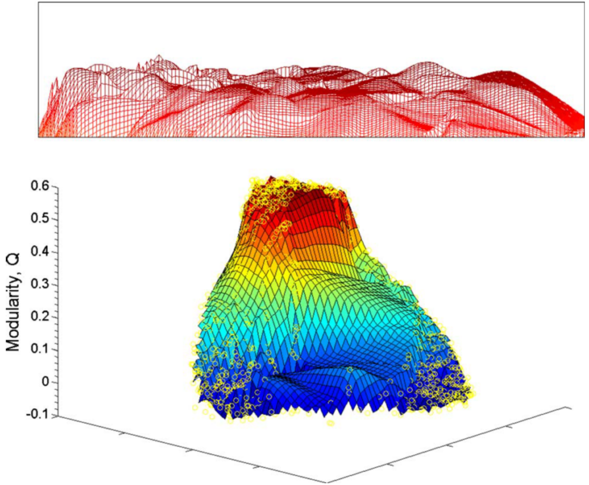

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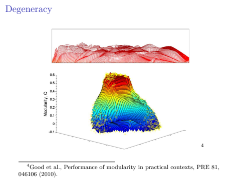
[4] Good et al., Performance of modularity in practical contexts, PRE 81, 046106 (2010).



Resolution limit

- Maximizing the modularity can fail to resolve small sized modules
- Modular structures like cliques can be hidden in the larger groups of nodes with higher modularity score
- Peak of the modularity function may not coincide with divisions that identify such modular structures

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

Contribution of the group s,

$$Q_s = \frac{1}{2m} \sum_{ij} \left(A_{ij} - \frac{k_i k_j}{2m} \right) \delta(c_i, s)\delta(c_j, s) = \frac{e_s}{m} - \left(\frac{d_s}{2m} \right)^2$$

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e_s: Number of links inside module s

.

d_s: sum of the degrees inside s

Resolution limit

The group s is a module whenever $Q_s > 0 \Rightarrow \frac{e_s}{m} > \left(\frac{d_s}{2m}\right)^2$

Consider two modules s_1 and s_2 with $e_{s_1 s_2}$ edges between them
The change in modularity if we merge these:

$$\triangle Q_{s_1 s_2} = \frac{e_{s_1 s_2}}{m} - 2\left(\frac{d_{s_1}}{2m}\right)\left(\frac{d_{s_2}}{2m}\right) > 0$$

whenever:

$$e_{s_1 s_2} > \frac{d_{s_1} d_{s_2}}{2m} \to 0$$

Thus, modules would be merged even when the number of links $e_{s_1 s_2}$ between them is small! [5]

[5] Fortunato, Barthelemy, Resolution limit in community detection, PNAS, (2006)

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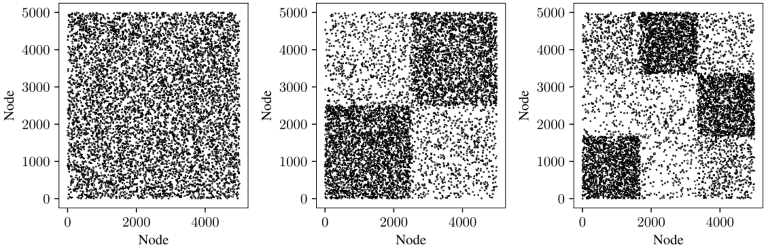
High wavelength light

Structure vs Noise



[6]

[6] Tiago Peixoto, Bayesian stochastic blockmodeling

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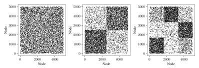

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Conclusions

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