Large-scale structure of complex networks (Part 2)

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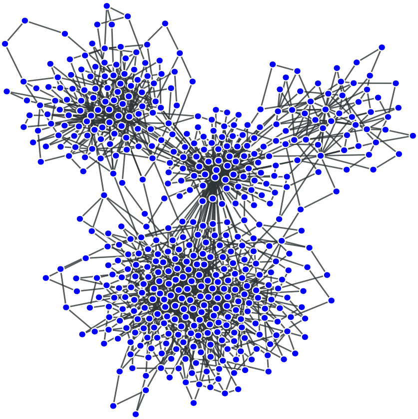
Community structure in networks



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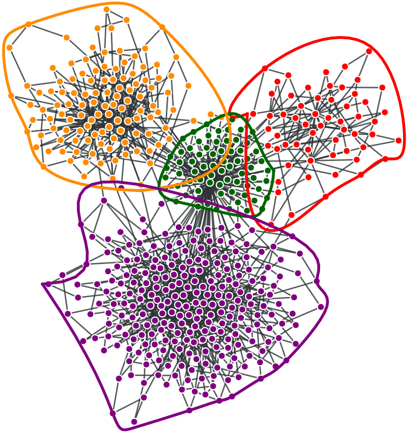


Community structure in networks

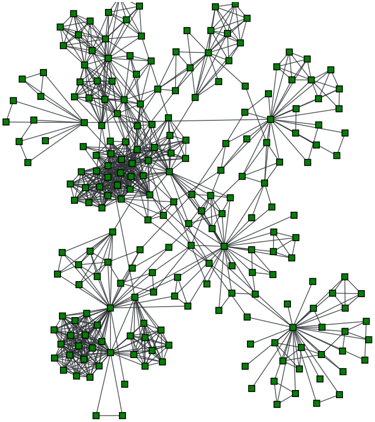
What are communities?

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

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

Community detection

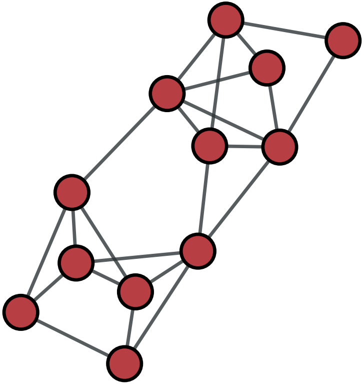


Detecting communities is important!

- 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

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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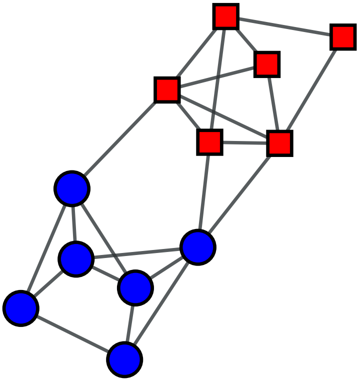


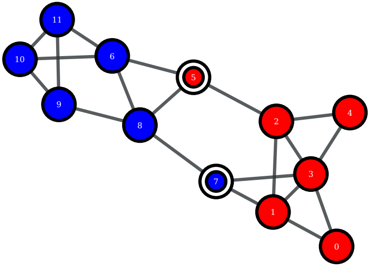
Partitioning is hard!

- 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!

Kernighan-Lin algorithm

cut size $= 4$



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

Kernighan-Lin algorithm

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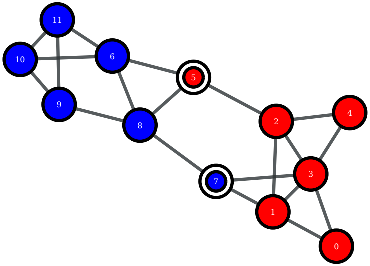
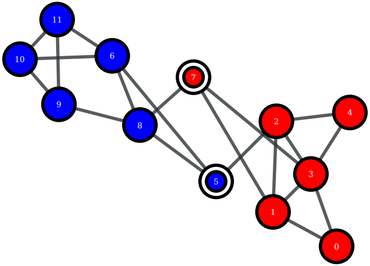


- Divide the vertices into two groups of the required sizes and calculate the cut size
- Find a pair of nodes which when switched, will reduce the cut size most and switch them

Kernighan-Lin algorithm

cut size $= 2$



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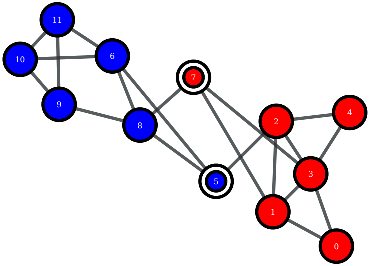

- Divide the vertices into two groups of the required sizes
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- If no such pair exists, select the pair which least increases the cut size

Kernighan-Lin algorithm

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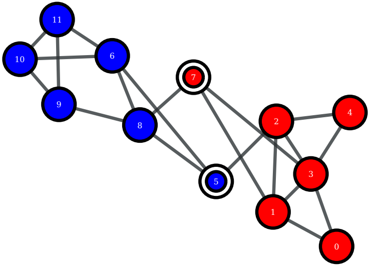
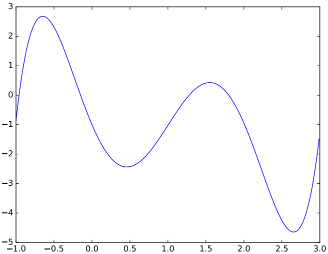


- Divide the vertices into two groups of the required sizes
- Find a pair of nodes which when switched, will reduce the cut size most and switch them
- If no such pair exists, select the pair which least increases the cut size
- Continue this such that the already switched pair is not switched again

Kernighan-Lin algorithm



- 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

Spectral partitioning

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

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

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

Spectral partitioning

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

First term,

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

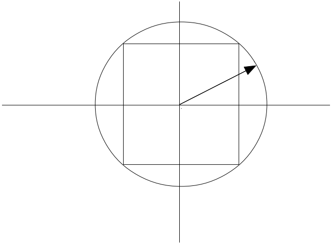
$$R = \frac{1}{4} \sum_{ij} (k_i \delta_{ij} - A_{ij}) s_i s_j = \frac{1}{4} \sum_{ij} L_{ij} s_i s_j$$

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

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

Spectral partitioning

Minimization with constraints ⇒ Lagrange multipliers

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

Spectral partitioning

Minimization with constraints $\Rightarrow$ Lagrange multipliers

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

$$\sum_j L_{ij} s_j = \lambda s_i + \mu$$

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

Spectral partitioning

Minimization with constraints $\Rightarrow$ Lagrange multipliers

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

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

$\mathbf{1}$ is an eigenvector of the Laplacian with eigenvalue 0

$$\mathbf{L}\mathbf{x} = \lambda \mathbf{x}$$

$$\mathbf{L}\mathbf{s} = \lambda\mathbf{s} + \mu\mathbf{1}$$

$$\mathbf{1}^T\mathbf{L}\mathbf{s} = \lambda\mathbf{1}^T\mathbf{s} + \mu\mathbf{1}^T\mathbf{1}$$

$$(\mathbf{L}\mathbf{1})^T\mathbf{s} = \lambda\mathbf{1}^T\mathbf{s} + \mu\mathbf{1}^T\mathbf{1}$$

$$0 = (n_1 - n_2)\lambda + \mu n$$

$$\mu = -\frac{n_1 - n_2}{n}\lambda$$

Spectral partitioning

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

Which eigenvector to choose?

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

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

Spectral partitioning

Which eigenvector to choose?

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

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

Spectral partitioning

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

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 $\mathbf{s}$

Spectral partitioning

Maximize:

$$\mathbf{s}^T \left(\mathbf{x} + \frac{n_1 - n_2}{n} \mathbf{1} \right) = \sum_i s_i \left(x_i + \frac{n_1 - n_2}{n} \right)$$

Equivalently, maximize:

$$\sum_i s_i x_i$$

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

Group assignments are arbitrary

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
- Put vertices corresponding to smallest n_1 elements in group 1 and others in group 2. Calculate the cut size
- Choose the division with the smallest cut size among the two

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

Many definitions.. many algorithms!

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

Broad classification

- **Agglomerative algorithms:**
  - Hierarchical clustering
  - Louvain method
  - CNM algorithm
- **Divisive algorithms:**
  - Girvan-Newman algorithm
  - Radichhi algorithm
- **Assignment algorithms:**
  - Label propagation
  - Spectral partitioning
  - Kernighan-Lin-Newman algorithm

“The” simplest community detection problem

- Bisecting a graph with n nodes
- Group sizes are not fixed
- Minimum cut size?
  - Trivial partition
  - Needs ad hoc specification of sizes

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

Quantification of community structure

- Fewer than expected edges between the groups

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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

Modularity

How to find the division which maximizes the modularity?

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- With a fast computer which checks 100 billion divisions per second: 3×10^{10} years!

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- Total possible divisions $= {}^{100}C_{50} > 10^{29}$
- With a fast computer which checks 100 billion divisions per second: 3×10^{10} years!
- Clever heuristics are required

Kernighan-Lin-Newman algorithm

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- Select a state with the highest modularity

Kernighan-Lin-Newman algorithm

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- Choose vertex whose shift makes maximum modularity change
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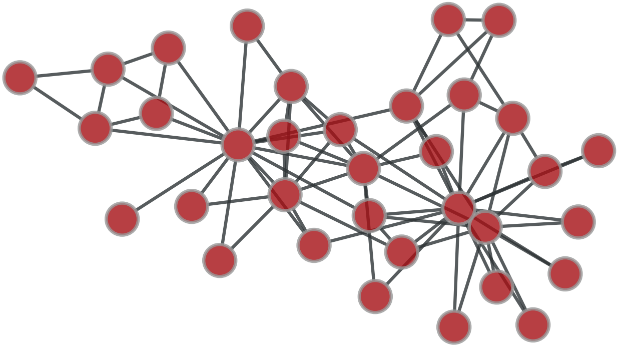
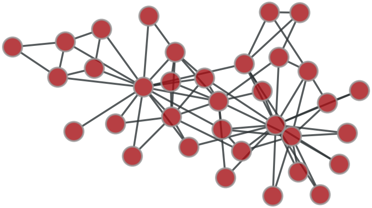
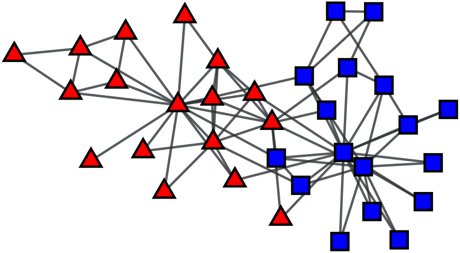
- Repeat so that the vertex once moved is not moved again
- Select a state with the highest modularity
- Repeat the whole process starting with this state till the modularity stabilizes



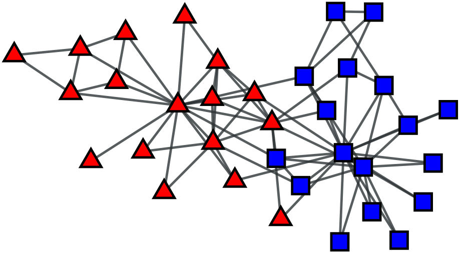
Zachry karate club network





Application to Zachry karate club

Actual division



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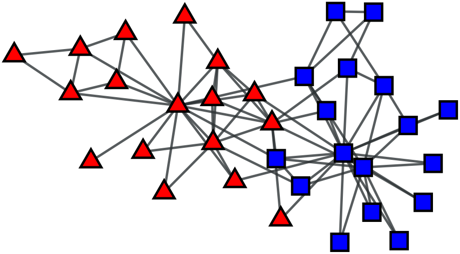
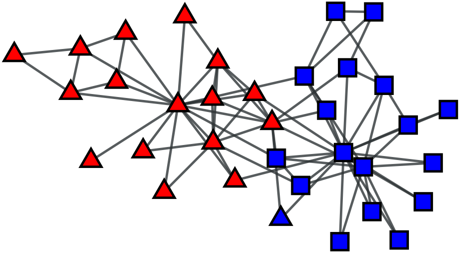


Division by KLN algorithm



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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$$\frac{1}{2}(1 + s_i s_j) = \begin{cases} 1 & \text{if } i \text{ and } j \text{ belong to the same group} \\ 0 & \text{Otherwise} \end{cases}$$

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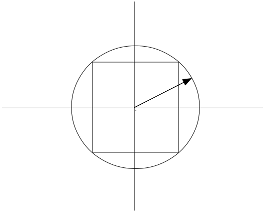
$$Q = \frac{1}{2m}\sum_{ij} B_{ij}\delta(c_i, c_j) = \frac{1}{4m}\sum_{ij} B_{ij}(1+s_i s_j) = \frac{1}{4m}\sum_{ij} B_{ij} s_i s_j$$

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

Spectral modularity maximization

Relaxation method

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



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

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

$$\mathbf{B}\mathbf{s} = \beta\mathbf{s}$$

Spectral modularity maximization

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

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

Maximize:

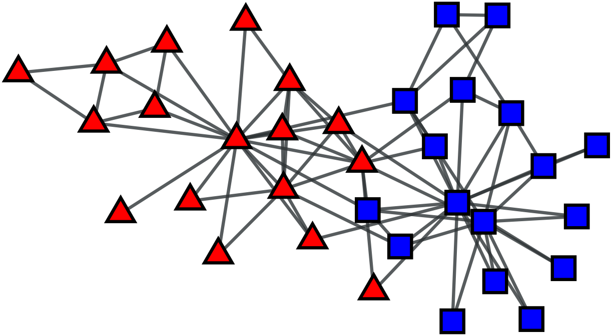
$$\mathbf{s}^T \mathbf{u}_1 = \sum_i s_i u_{1i}$$

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

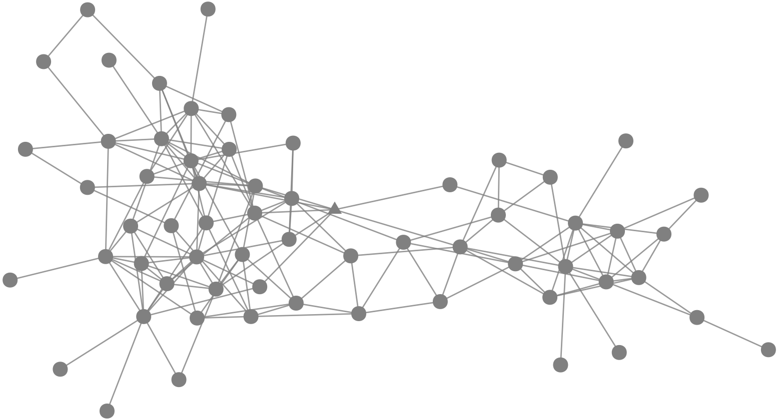
Spectral modularity maximization

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

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

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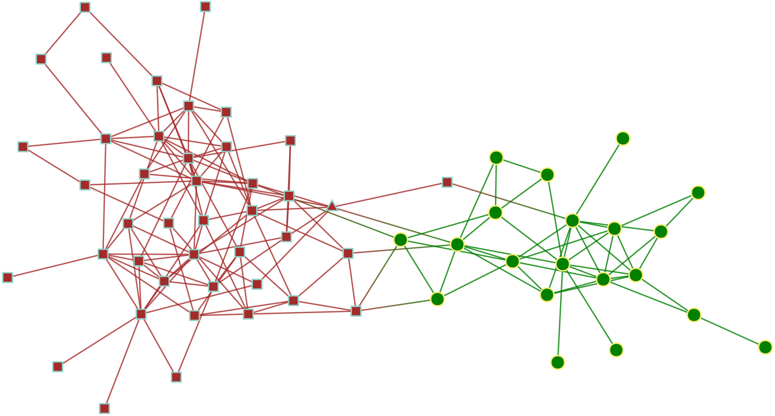

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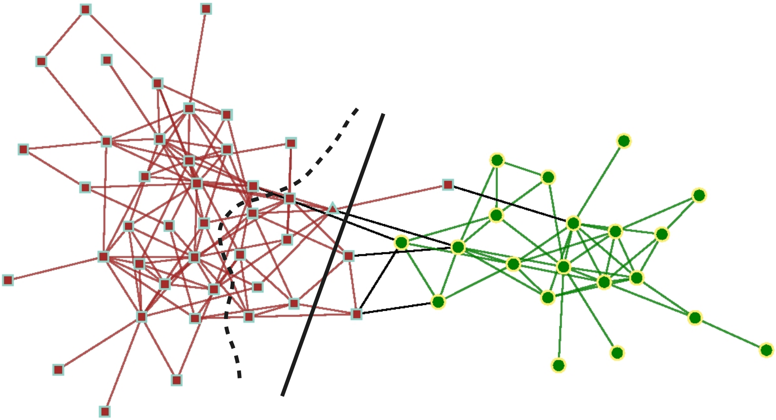


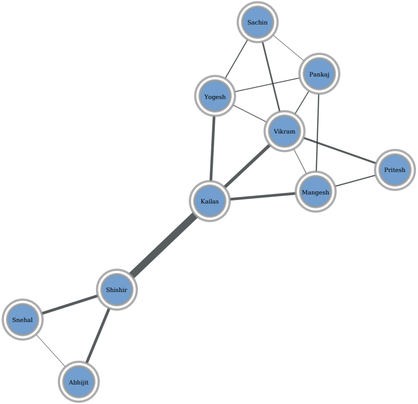
[3]Lusseau D, Schneider K, Boisseau OJ, Haase P, Slooten E, Dawson SM (2003) Behav Ecol Sociobiol 54:396405

Newman-Girvan algorithm

- Look for edges between the communities
- Edge betweenness

Edge betweenness

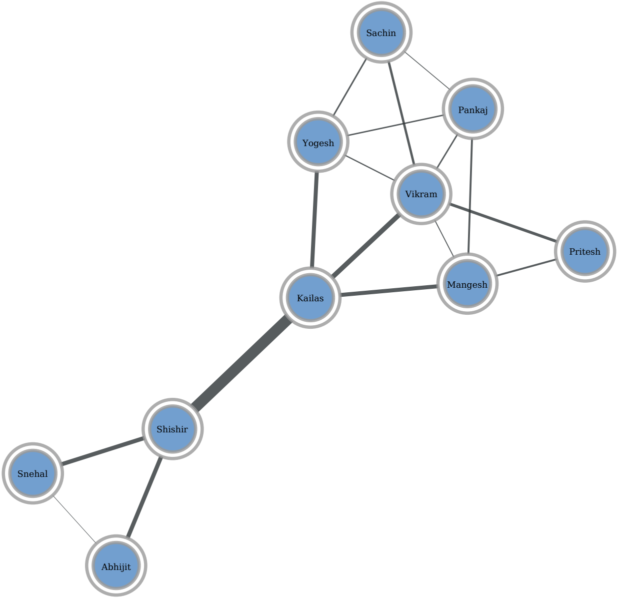
- Path between two nodes
- Shortest path between two nodes
- Number of shortest paths that go through a given edge



The algorithm

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

Girvan-Newman algorithm



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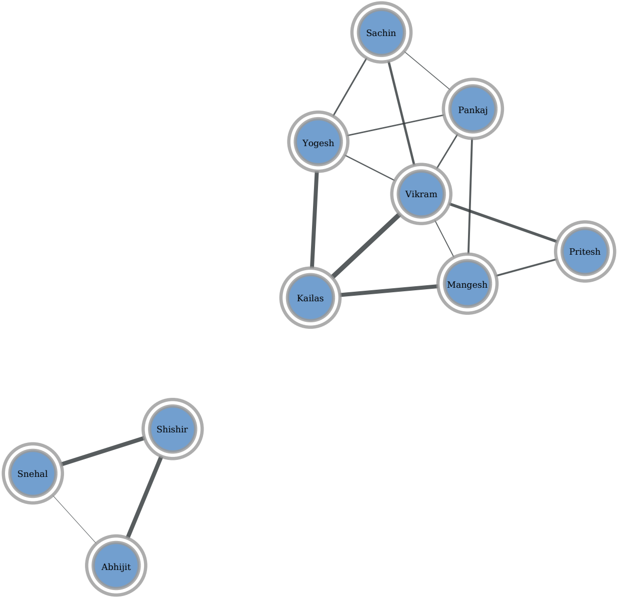

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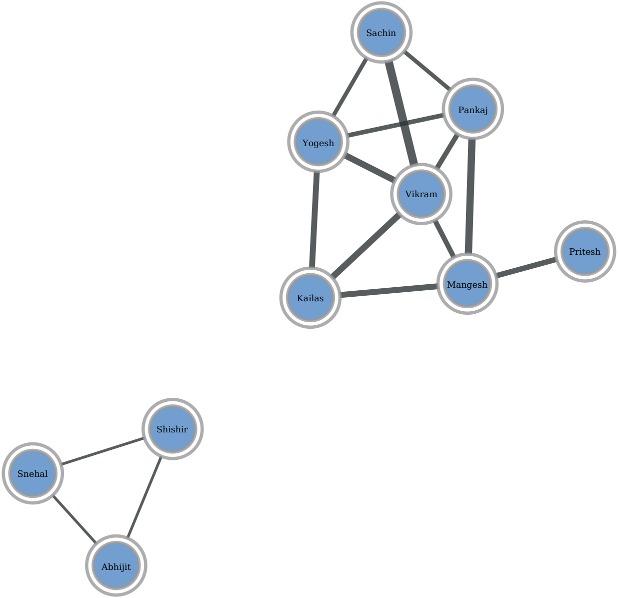
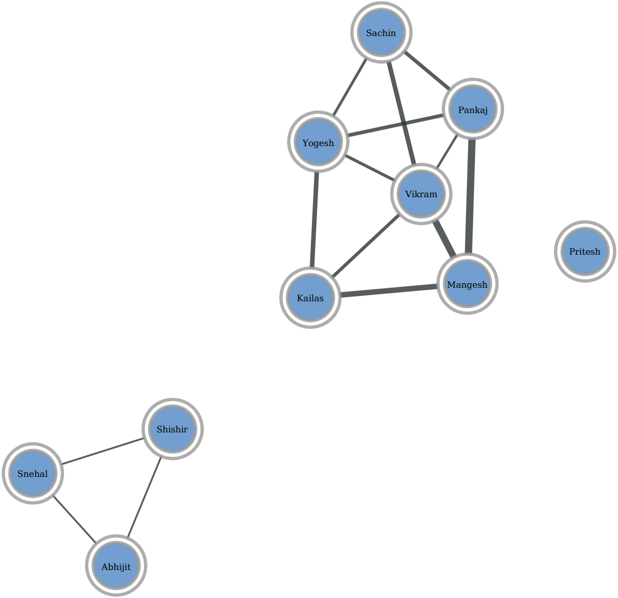
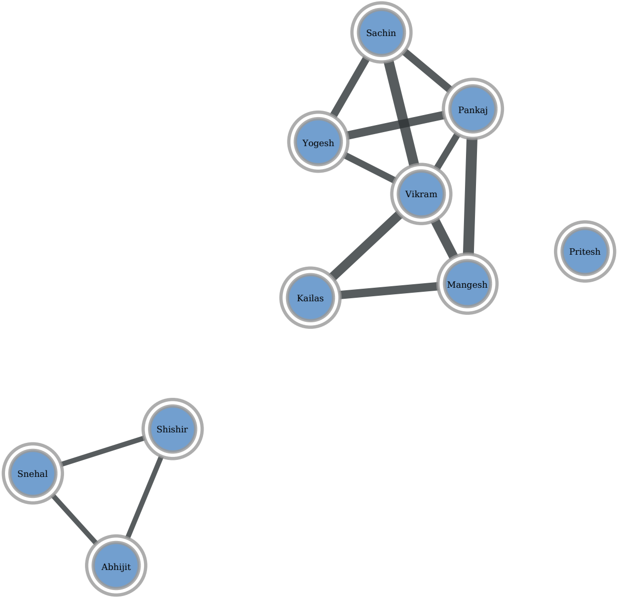


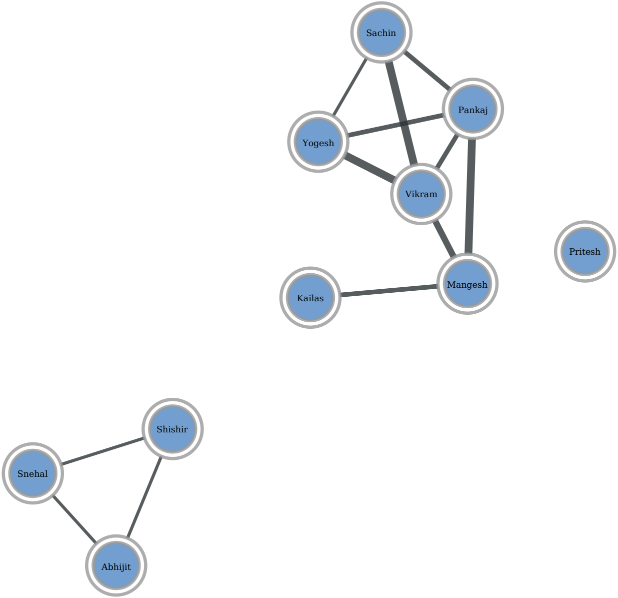
Girvan-Newman algorithm



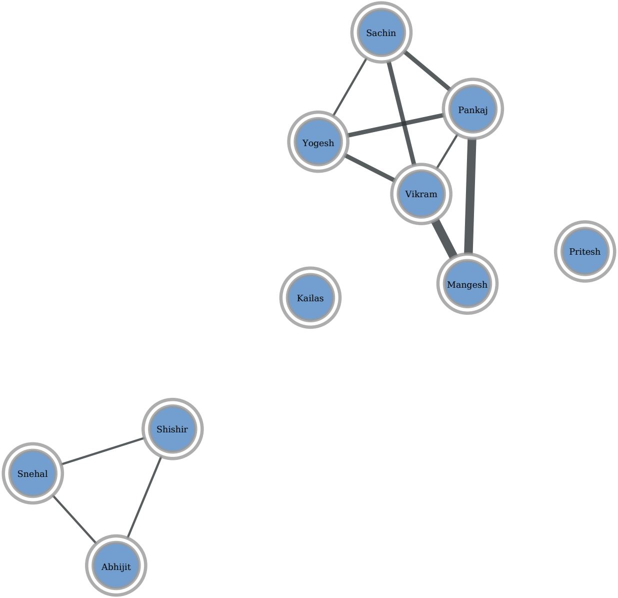
Girvan-Newman algorithm



Girvan-Newman algorithm



Girvan-Newman algorithm



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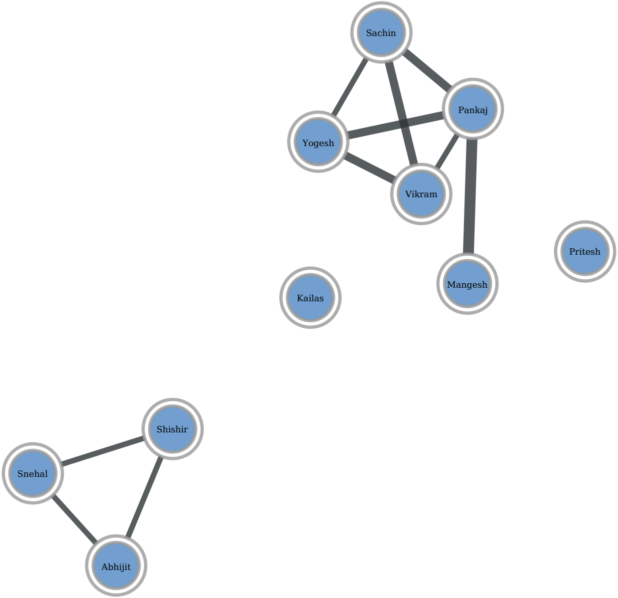

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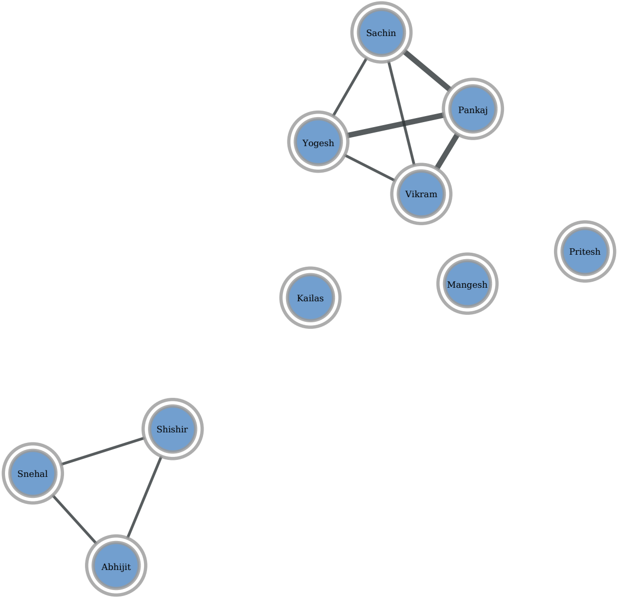
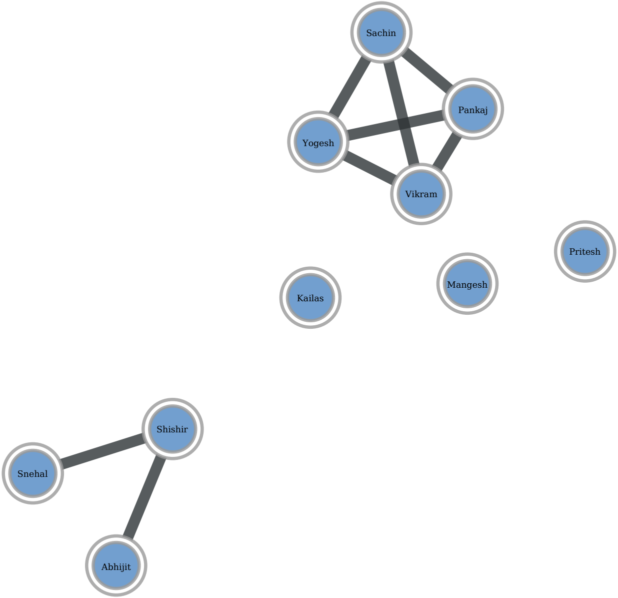


Girvan-Newman algorithm



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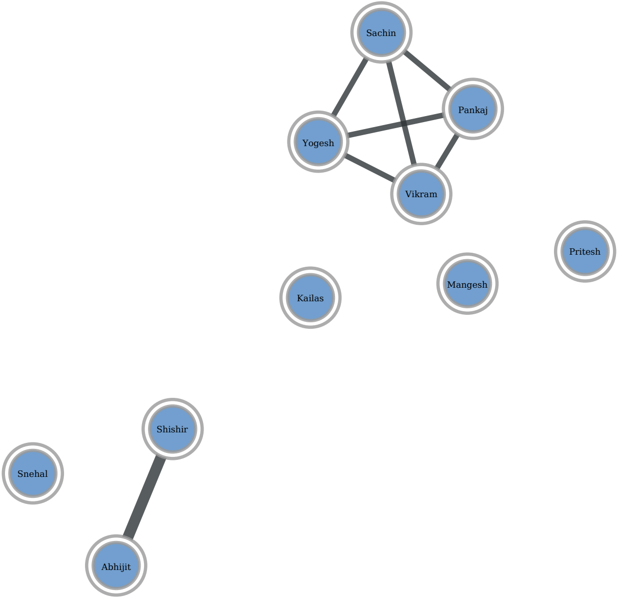

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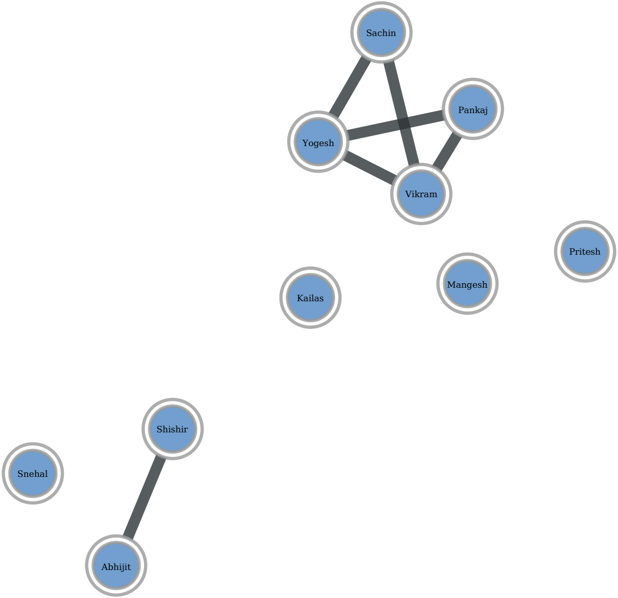
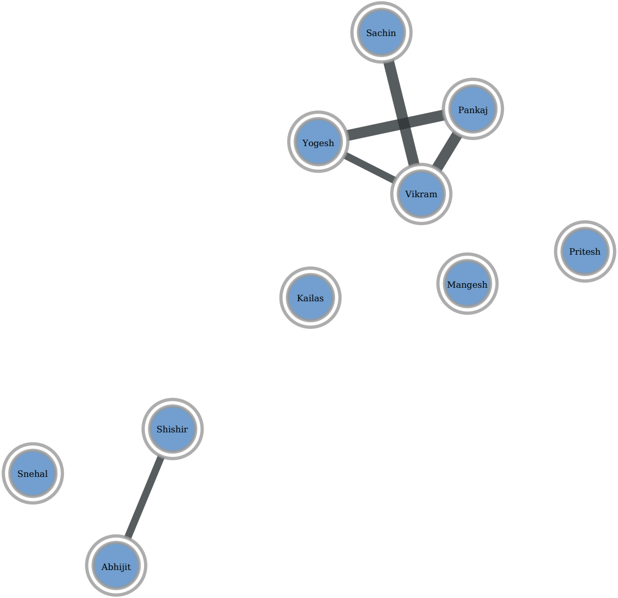
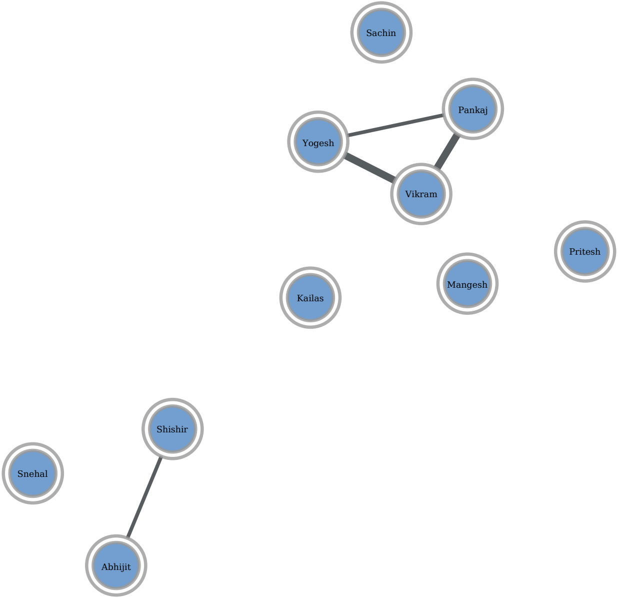


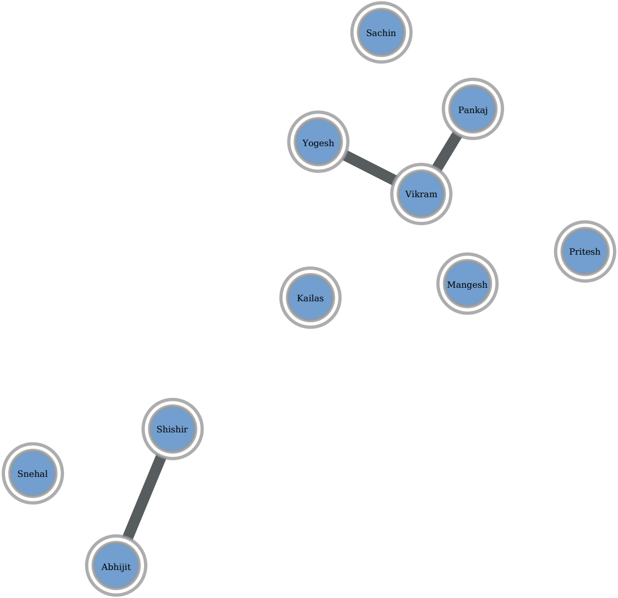
Girvan-Newman algorithm



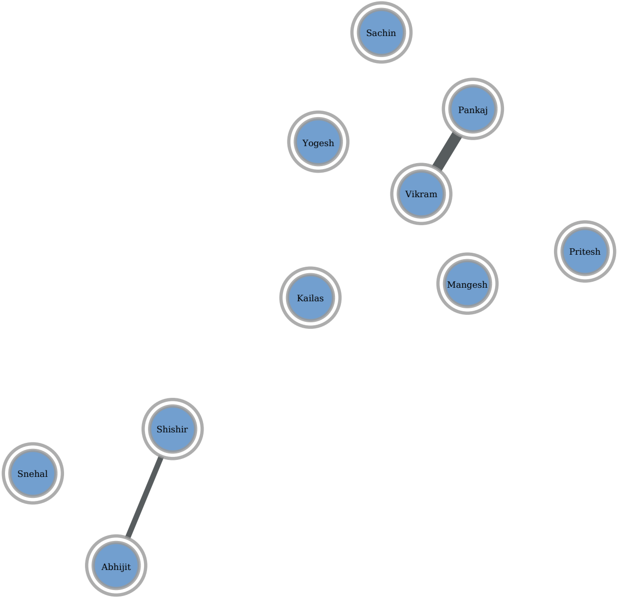
Girvan-Newman algorithm



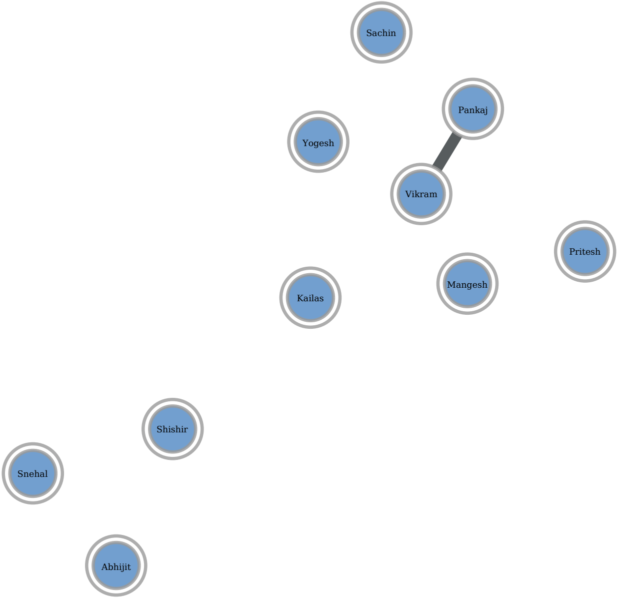
Girvan-Newman algorithm



Girvan-Newman algorithm



Girvan-Newman algorithm



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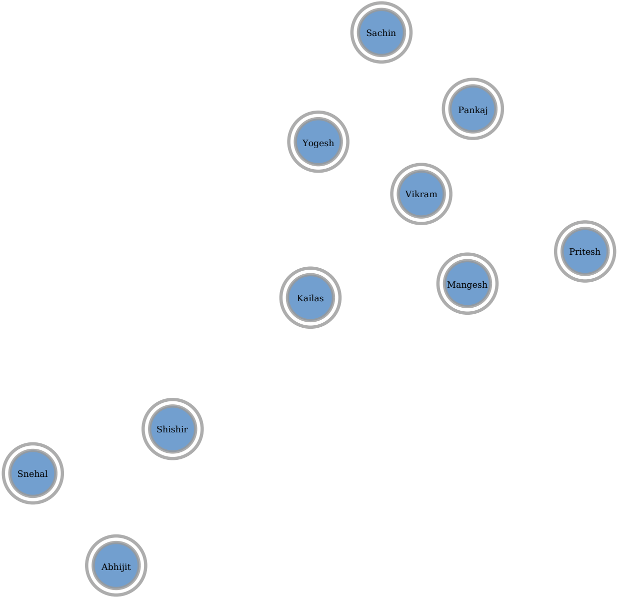
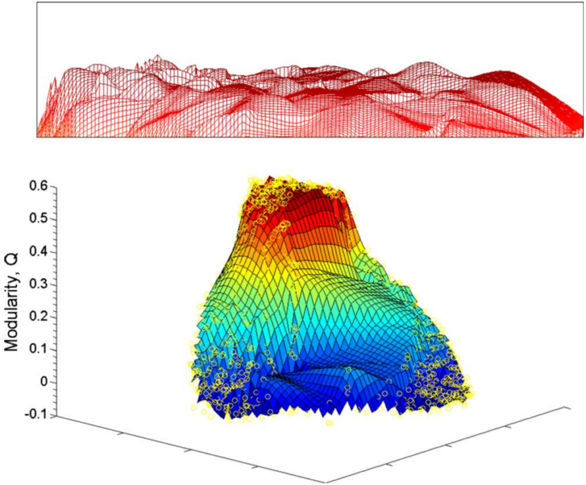


Problems with traditional community detection algorithms

- Degeneracy
- Resolution limit
- Structure vs Noise

Degeneracy



[4]

[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,

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

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]

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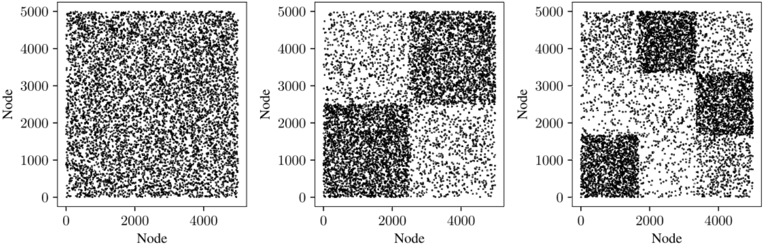
[5] Fortunato, Barthelemy, Resolution limit in community detection, PNAS, (2006)

Structure vs Noise



6

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[6] Tiago Peixoto, Bayesian stochastic blockmodeling

Conclusions

- Community structure is a fundamental property of networks
- Community detection is an ill-defined problem
- (Too) many algorithms exist
- Community detection is still an open problem!

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