Discovering Hidden Structures in Complex Networks

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University of Michigan

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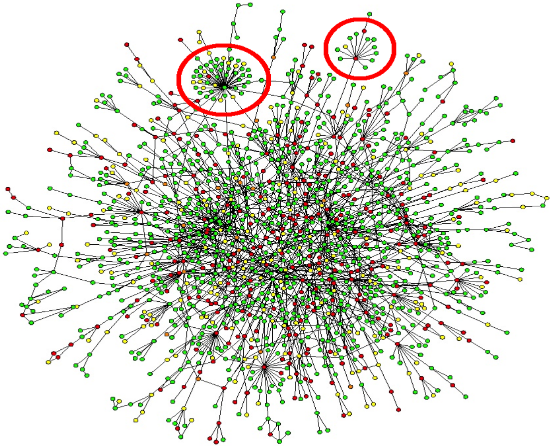
Network Science is highly interdisciplinary.

+ finance + technology + . . .

Many networks have fascinating structure.

Some structures are apparent, local.



Protein interaction network

[A.-L. Barabási & Z. Oltvai, Nature Reviews Genetics 5, 101–113, Feb. 2004]

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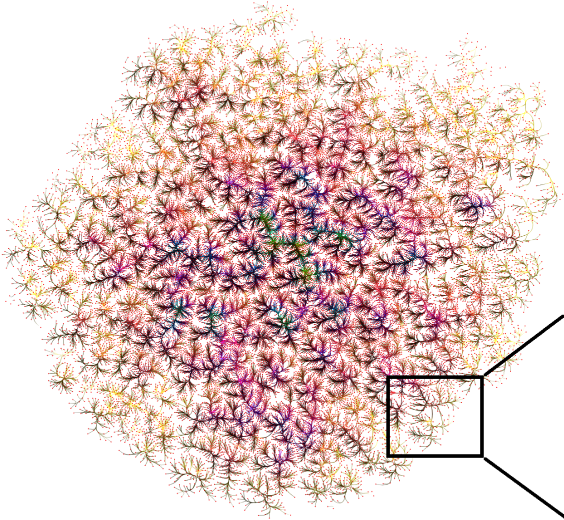

The Internet

(C. Hurter et al., Eurographics Conference on Visualization 2012)

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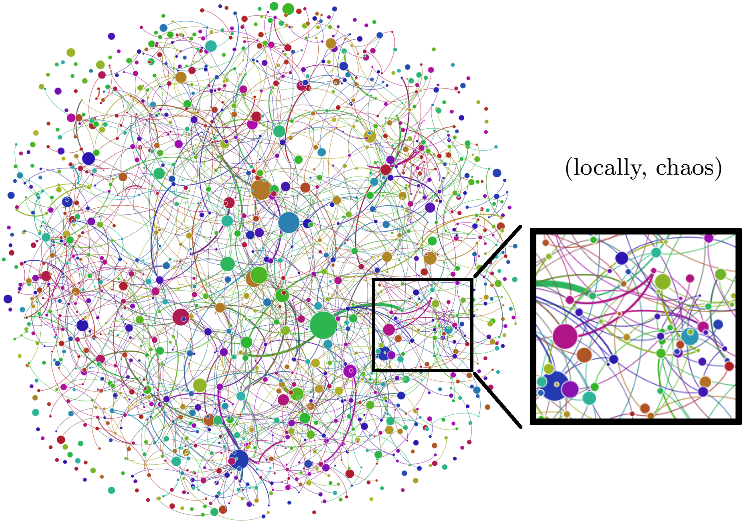
Other structures are latent, global...



(locally, chaos)

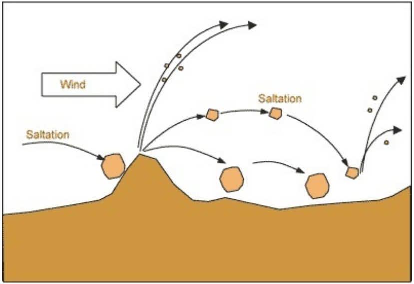
Collaboration network of economists

(AER, JPE, Econometrica, RES, QJE. www.cloudycnet.net)

Many networks have fascinating structure.

... just like in nature:

global structure



local chaos

Basic Questions

- How can we find latent structures in real networks?
- How can we explain and model these structures?

Mathematical perspective

Model large networks as random graphs. (Edges drawn at random.)

A leap of faith.

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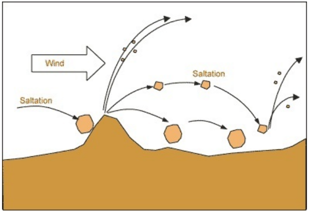
Randomness at the microscopic level averages out at the macroscopic level:



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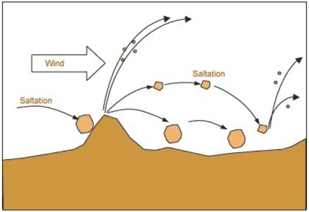

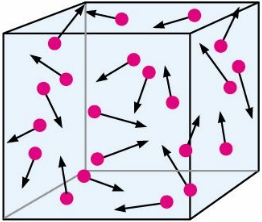

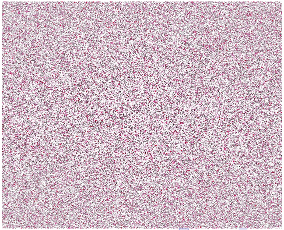

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Edges drawn independently at random, with probability $p \in [0, 1]$.

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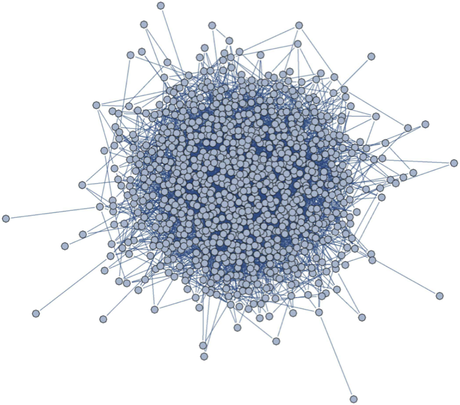
$G(n, p)$ with $n = 1000$, $p = 0.00095$



(A. Novozhilov's course in Mathematics of Networks, NDSU)

Inhomogeneous Erdös-Rényi model $G(n, (p_{ij}))$

Edges are still independent, but can have **different** probabilities p_{ij}.

Allows to model networks with structure = communities (clusters).

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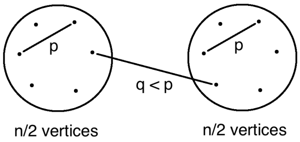
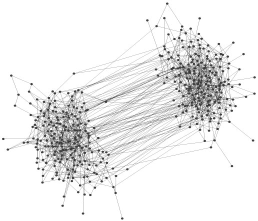
Example. **Stochastic block model** with two communities $G(n, p, q)$:
Edges *within* each community: probability p; *across* communities: probability $q < p$.





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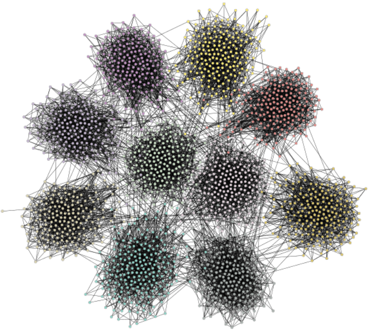
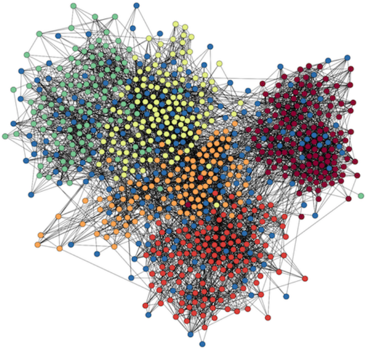
Multiple communities are possible to model, too:

Stochastic block model



Real data (aggression network of students)



(UC Davis Center for Visualization)

Network Model Recovery

Model Recovery Problem. Observe one instance of a network from $G(n, (p_{ij}))$. Recover the model, i.e. the connection probabilities p_{ij}.

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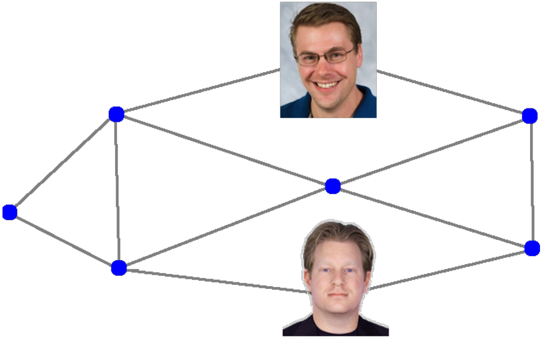

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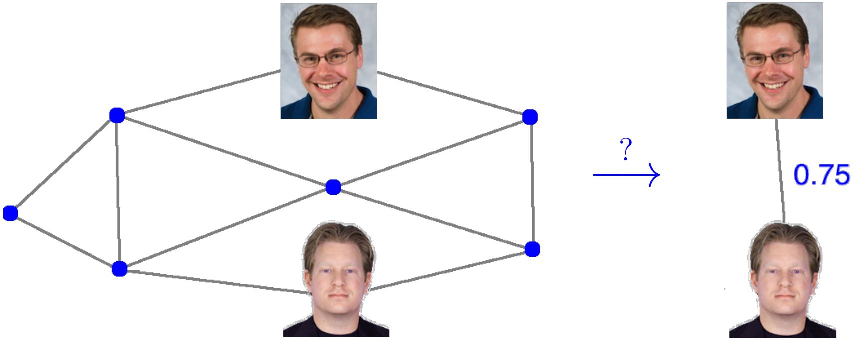


p_{ij} = *"latent bonds"* between vertices.

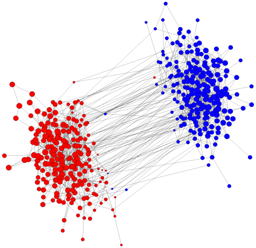
Link prediction.

Network Model Recovery Problem

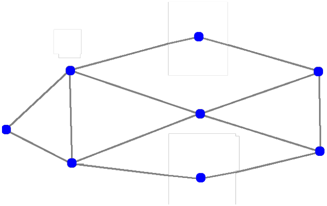
A particular case, for stochastic block models:

Community Detection Problem. Observe a network drawn from the stochastic block model $G(n, p, q)$. Recover the two communities.

$\xrightarrow{?}$



Adjacency matrix A:



$$\longrightarrow \qquad A = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 1 & 0 & 1 & 0 \end{bmatrix}$$

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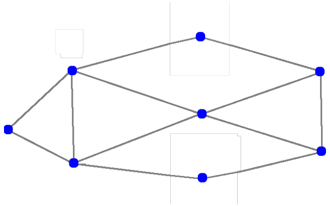

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For inhomogeneous Erdös-Rényi model:

$$A = (\mathrm{Bernoulli}(p_{ij})) \qquad \mathbb{E}\, A = (p_{ij})$$

From graphs to matrices

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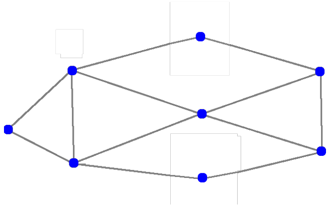

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Model Recovery Problem. Observe A; recover $\mathbb{E}\, A$.

Relation to matrix completion

Evident but not thoroughly explored.

Matrix completion: recover a low-rank matrix from a few randomly chosen entries.

$$\begin{bmatrix} & & & & .1 & & & \\ .7 & & .6 & & & & & .1 \\ & & & .9 & & & & \\ & & .9 & & & .1 & & \\ .1 & & & & & & & .5 \\ & .1 & & & .8 & & & \\ .3 & & & & & & & \\ & & & & & .6 & & \end{bmatrix} \xrightarrow{?} \begin{bmatrix} 1 & .7 & .6 & .7 & .1 & .4 & .3 & .2 \\ .7 & 1 & .6 & .5 & .2 & .1 & .2 & .1 \\ .6 & .6 & 1 & .9 & .4 & .2 & .3 & .3 \\ .7 & .5 & .9 & 1 & .2 & .1 & .3 & .2 \\ .1 & .2 & .4 & .2 & 1 & .8 & .6 & .5 \\ .4 & .1 & .2 & .1 & .8 & 1 & .7 & .6 \\ .3 & .2 & .3 & .3 & .6 & .7 & 1 & .9 \\ .2 & .1 & .3 & .2 & .5 & .6 & .9 & 1 \end{bmatrix}$$

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Network model recovery: recover a (low-rank?) matrix $\mathbb{E}\,A = (p_{ij})$ from random measurements $A = (\text{Bernoulli}(p_{ij}))$.

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Most relevant comparison is to **single-bit matrix completion** [Davenport et al '12].

Existing approaches

Mostly apply to **stochastic block models**.

Insights from Combinatorics, Computer Science, Statistics, Physics:

- combinatorial techniques (min-cut, hierarchical clustering)
- spectral methods – this talk
- statistical inference (likelihood maximization)
- variational methods
- Markov chain Monte Carlo
- belief propagation
- convex optimization
- semidefinite programming – this talk
- ...

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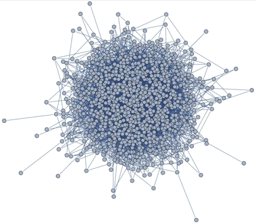
Is this true? In other words:

Question. Do random graphs concentrate near their "expected" graphs?

Dense random graphs concentrate

Consider an inhomogeneous Erdös-Rényi random graph $G(n,(p_{ij}))$ with *expected degrees* $np_{ij} \sim d$.



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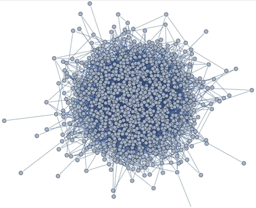

Theorem. *A random graph with expected degrees* $d \gtrsim \log n$ *concentrates:*

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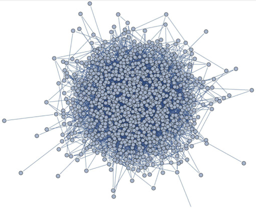

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Proofs:

- [Kahn-Szemeredi 89] → [Feige-Ofek 05, Lei-Rinaldo 13, Chin-Rao-Vu 15]: Simple concentration of $x^\mathsf{T}(A - \mathbb{E}\, A)y$ for *fixed* x, y; then complicated union bound over x, y (tailored the coefficient profiles of x, y).

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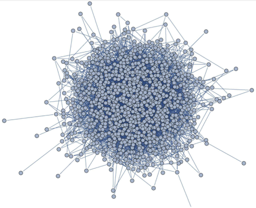

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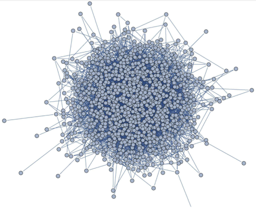

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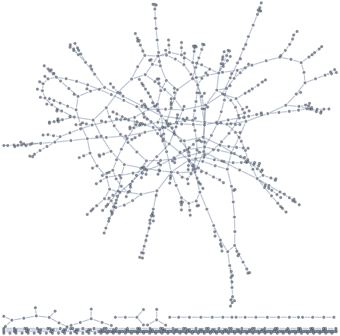
- Other approaches: [Hajek-Wu-Xu 14; Bandeira-van Handel 14; Le-Vershynin 15].
- Weaker results: [Furedi-Komlos 80] with $d \gtrsim \log^4 n$; [Oliveira 10] with $\|A - \mathbb{E}\,A\| \lesssim \sqrt{d \log n}$ by matrix Bernstein inequality.

Sparse random graphs do not concentrate

Observation. *A random graph* $G(n,p)$ *with expected degrees* $d = np \ll \log n$ *does* *not* *concentrate:*

$$\|A - \mathbb{E}\, A\| \gg \|\mathbb{E}\, A\|.$$

See [Krivelevich-Sudakov 03].



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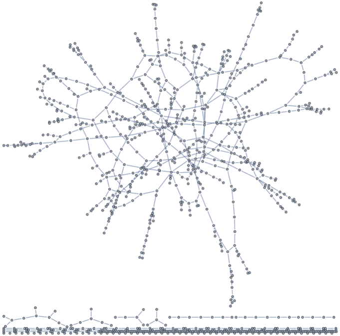
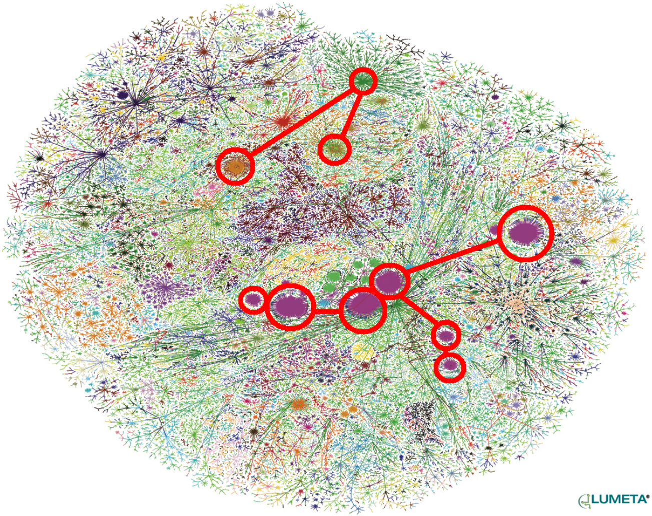


What is wrong with sparse graphs?

The degrees are wild, do not concentrate near d anymore.
High-degree vertices blow up $\|A\|$: some columns of A are too large.

Sparse random graphs do not concentrate

High-degree vertices dominate the picture. Spectral methods reveal only those vertices. *Local information*, no latent structure [Mihail-Papadimitriou 02].



The Internet

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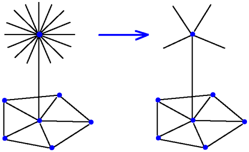

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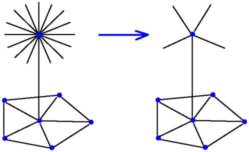

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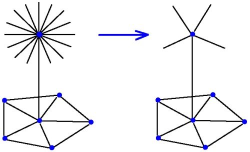

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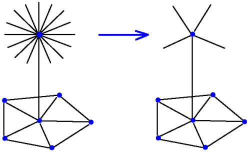

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- Yes, in full generality. Any type of regularization helps, as long as it brings down the degrees to $\sim d$. [Le-Levina-V, Le-V 05].

Regularization and concentration: theory

Inhomogeneous E-R random graph with $d = \max np_{ij}$.

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[Le-Levina-V, Le-V 05]; partial case in [Feige-Ofek] (complete removal of vertices).

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$$\|A' - \mathbb{E}\, A\| \lesssim \sqrt{d} \quad w.h.p.$$

[Le-Levina-V, Le-V 05]; partial case in [Feige-Ofek] (complete removal of vertices).

The graph can be very sparse, $d = O(1)$.

Regularization and concentration: theory

Inhomogeneous E-R random graph with $d = \max np_{ij}$.

Regularize vertices with degrees $> 2d$:
make all degrees $\leq 2d$ by reducing the weights of edges arbitrarily.

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The graph can be very sparse, $d = O(1)$.

Proof:

1. simple concentration of A in *cut norm*;
2. upgrade to operator norm on a subgraph by *Grothendieck-Pietsch factorization*;
3. *iteration* to extend the control over all graph. □

By-product: a new graph decomposition.

Eigenvectors reveal the latent structure?

Regularization and concentration: applications

Eigenvectors reveal the latent structure?

Concentration (possibly after regularization) $\Rightarrow$

$$A \approx \mathbb{E}\, A.$$

Davis-Kahan theorem $\Rightarrow$ eigenvectors satisfy

$$v_i(A) \approx v_i(\mathbb{E}\, A).$$

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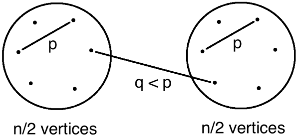
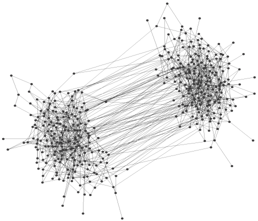
Eigenvectors $v_i(\mathbb{E}\, A)$ carry information about **network structure**.

Eigenvectors reveal the network structure.

Example. **Community detection** in stochastic block model $G(n, p, q)$.





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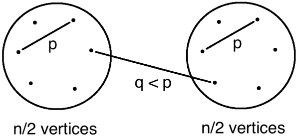

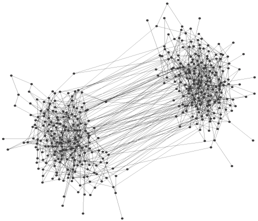

$$\mathbb{E}\,A = \left[\begin{array}{cc|cc} p & p & q & q \\ p & p & q & q \\ \hline q & q & p & p \\ q & q & p & p \end{array}\right] \text{ has rank 2;} \qquad v_1(\mathbb{E}\,A) = \left[\begin{array}{c} 1 \\ 1 \\ \hline 1 \\ 1 \end{array}\right], \quad v_2(\mathbb{E}\,A) = \left[\begin{array}{c} 1 \\ 1 \\ \hline -1 \\ -1 \end{array}\right].$$

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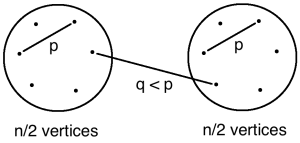

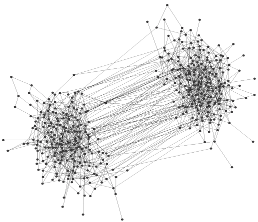

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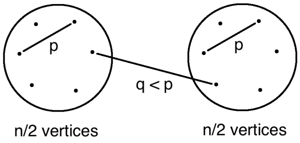

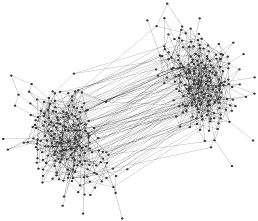

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Spectral Clustering Algorithm: given a graph with adjacency matrix A,

- Compute the second leading *eigenvector* of A;
- Recover communities based on the *signs of its coefficients*.

Using eigenvectors: theory.

Corollary **(Community Detection).** Consider the stochastic block model $G(n, p, q)$ with $p = a/n$ and $q = b/n$. Suppose

$$(a-b)^2 \geq C_\varepsilon (a+b).$$

Then the *regularized* spectral clustering algorithm recovers communities up to εn misclassified vertices, and with high probability.

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Detection threshold. The condition on is *optimal* up to C_ε, which must $\to \infty$. No algorithm can succeed if

$$(a-b)^2 \leq 2(a+b).$$

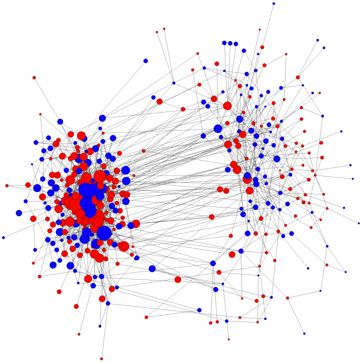
There are algorithms that do *better than random guess* if

$$(a-b)^2 > 2(a+b).$$

See [Mossel-Neeman-Sly 13-14; Massoulié 13; Bordenave-Lelarge-Massoulié 15].

Performance of regularized spectral clustering

Without regularization



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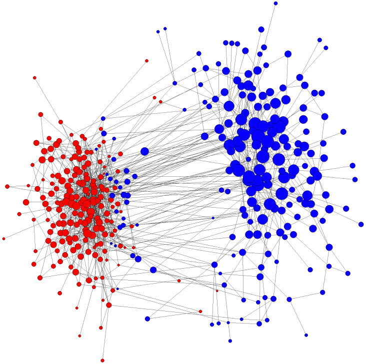

$n = 400$ vertices, expected degree 5. Connection probabilities $p = 5/n$ and $b = 0.5/n$.

Application: network visualization by PCA

Further application of

$$\text{eigenstructure}(A) \approx \text{eigenstructure}(\mathbb{E}\, A).$$

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Assume $\mathbb{E}\, A$ has low rank, exactly or approximately.
Then PCA on A should **reveal the latent structure** of the network.

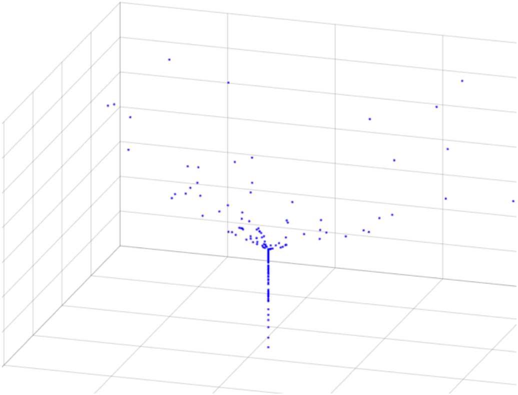
How? project the columns of A onto the space of the 3 leading eigenvectors.

Application: network visualization by PCA

Power grid of U.S.A.

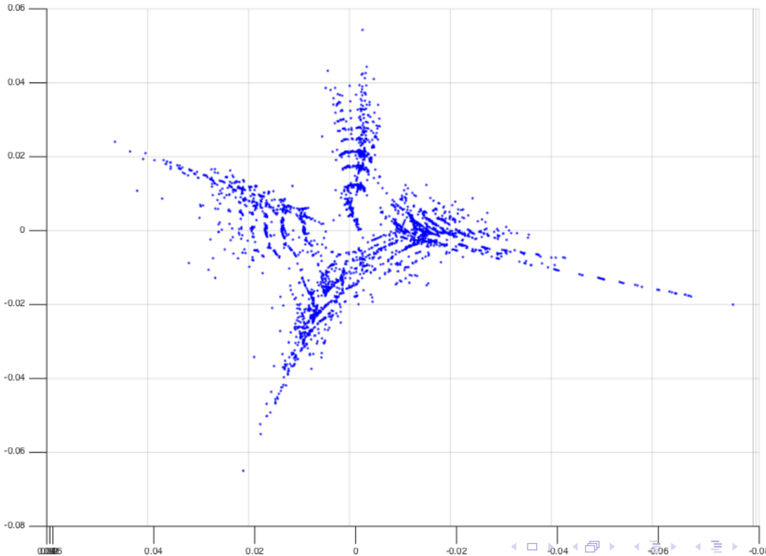
Application: network visualization by PCA

Without regularization:



Not very useful...

With regularization:



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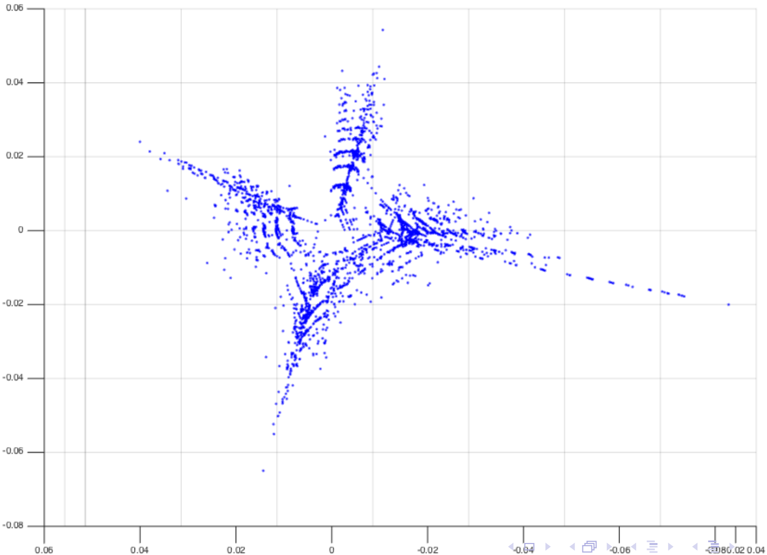

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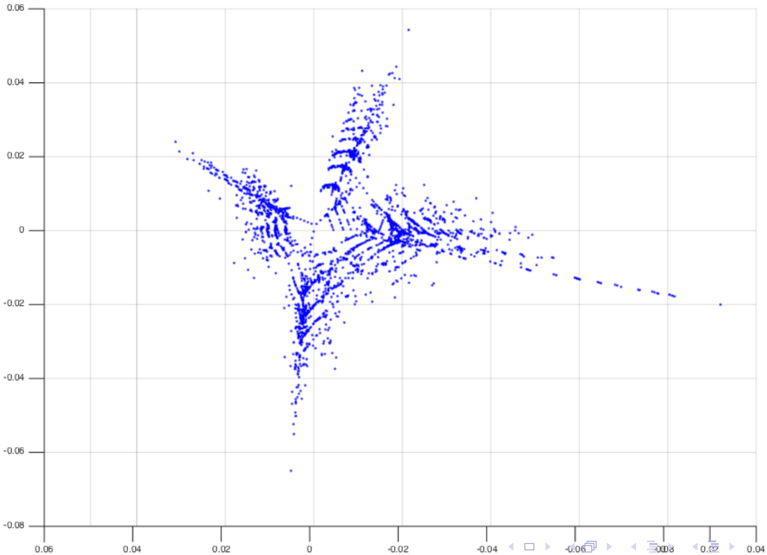

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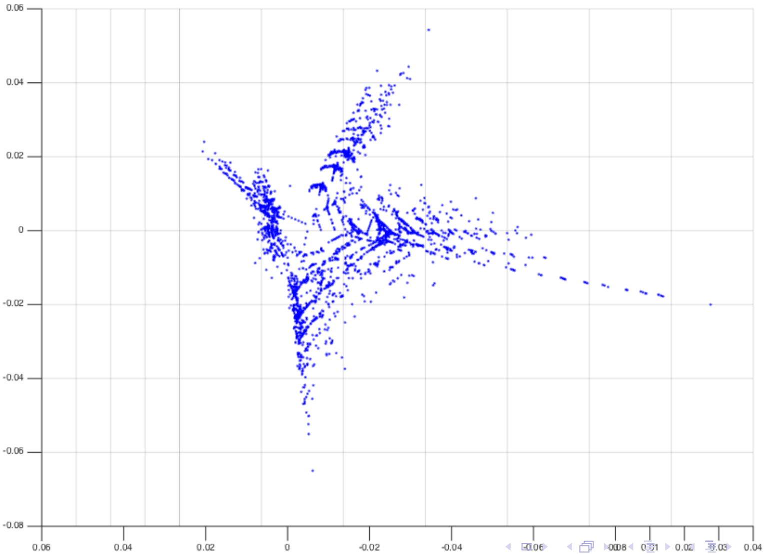

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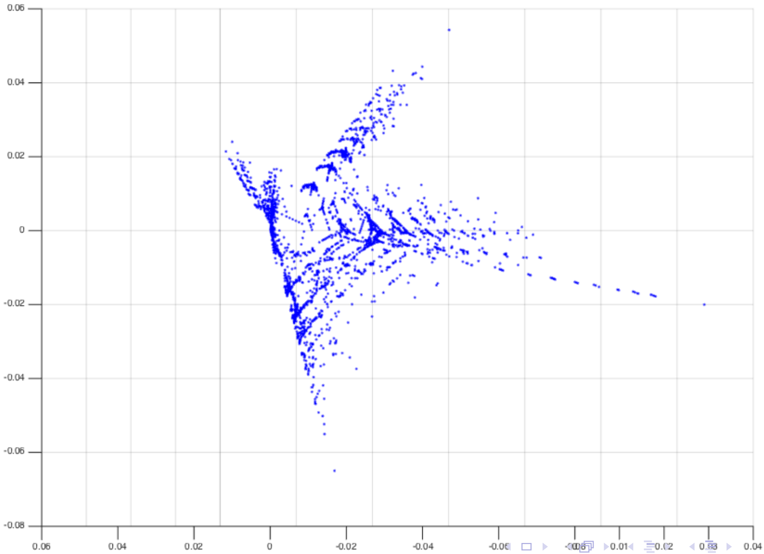

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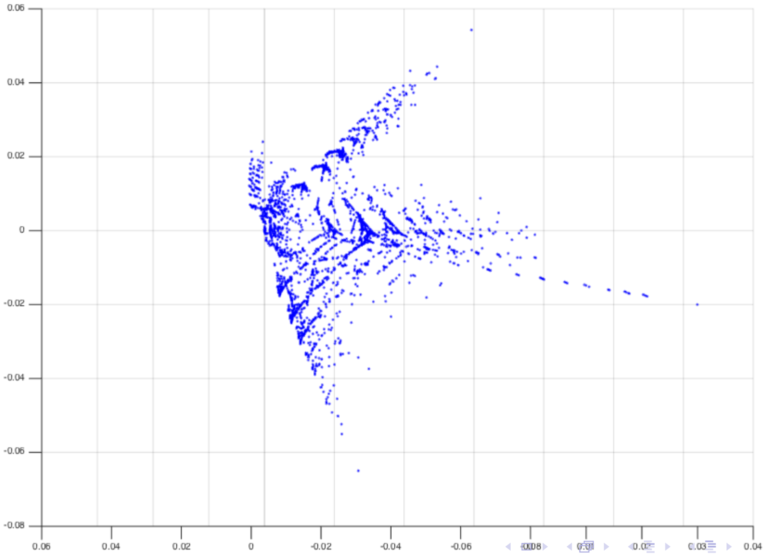

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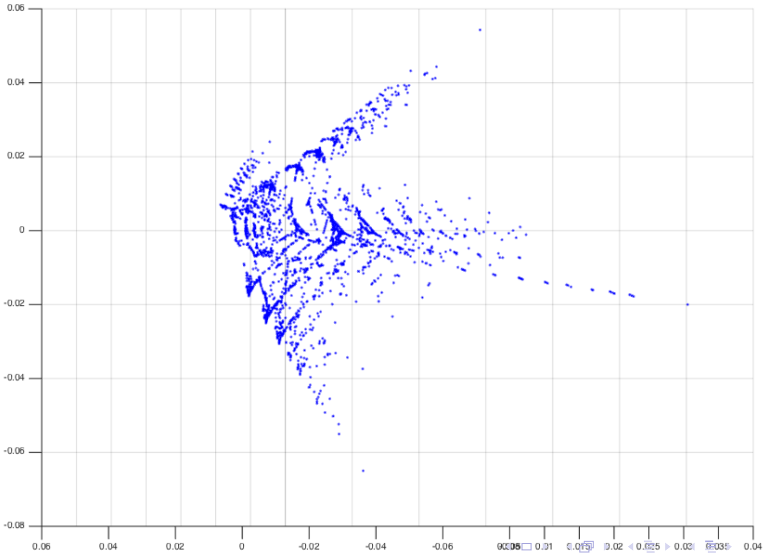

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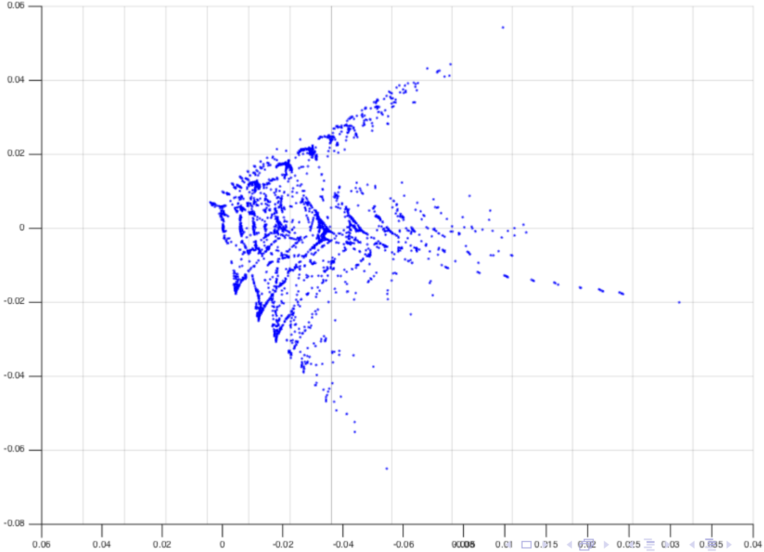

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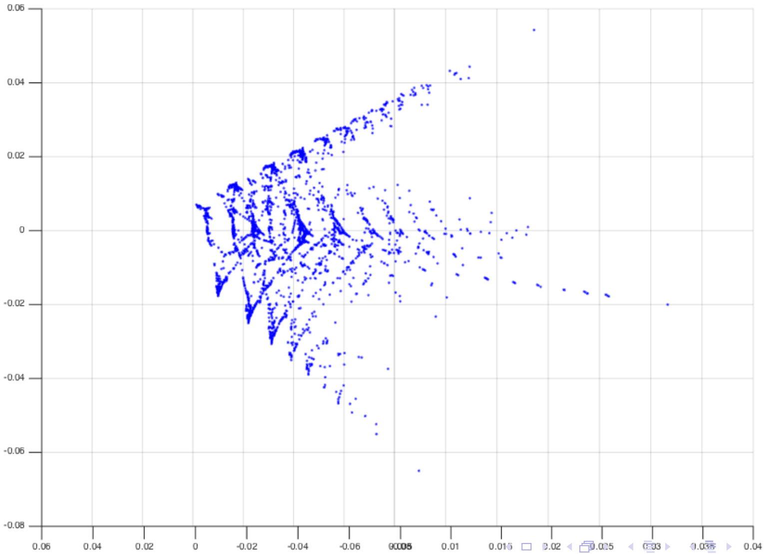

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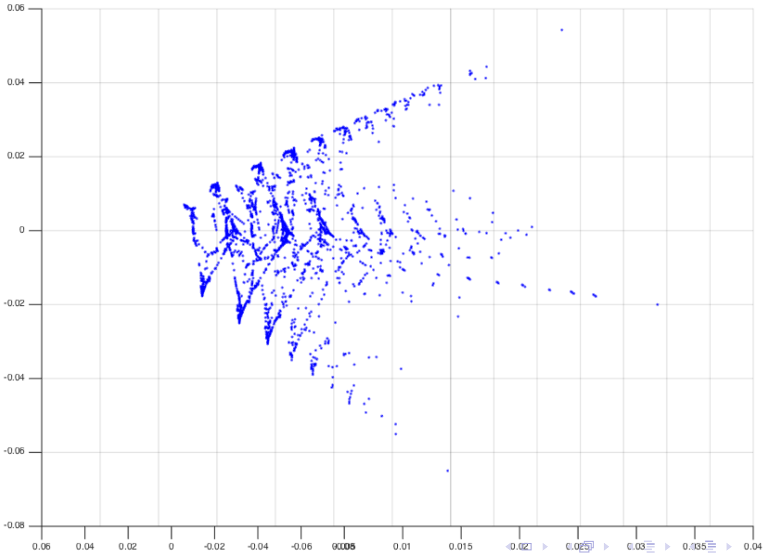

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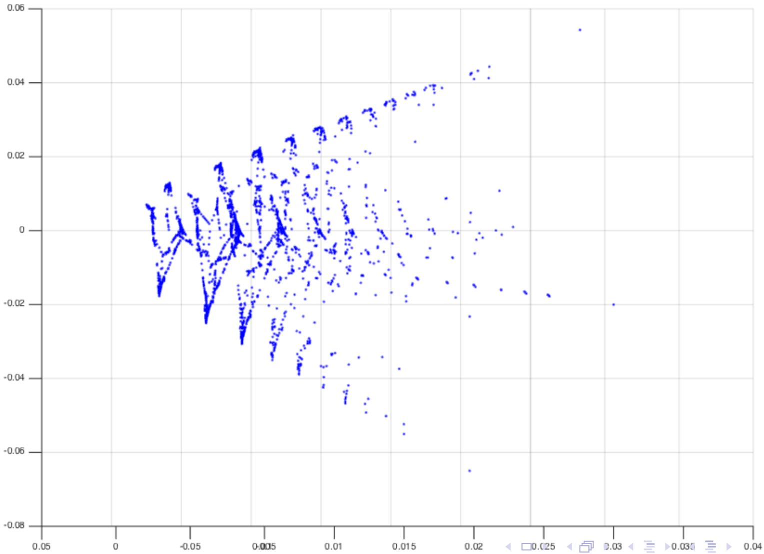

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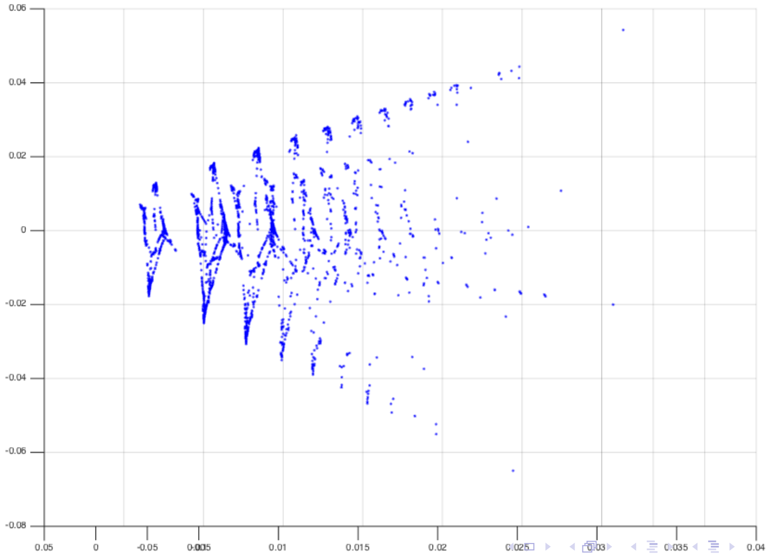

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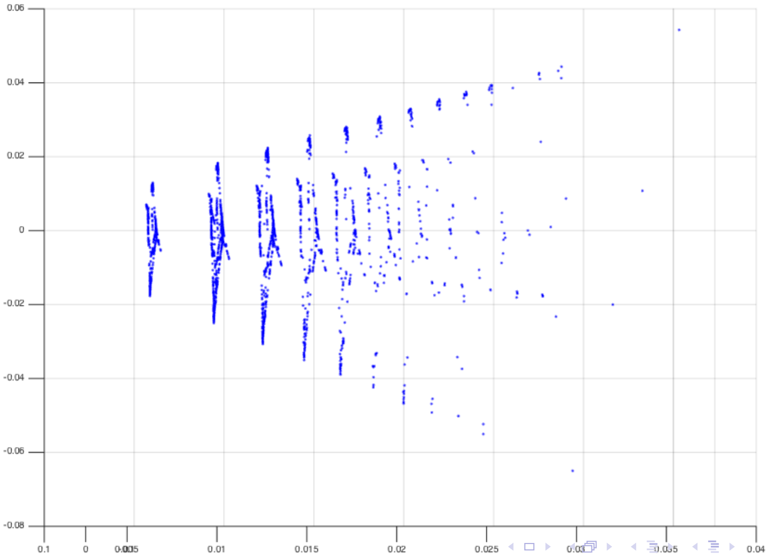

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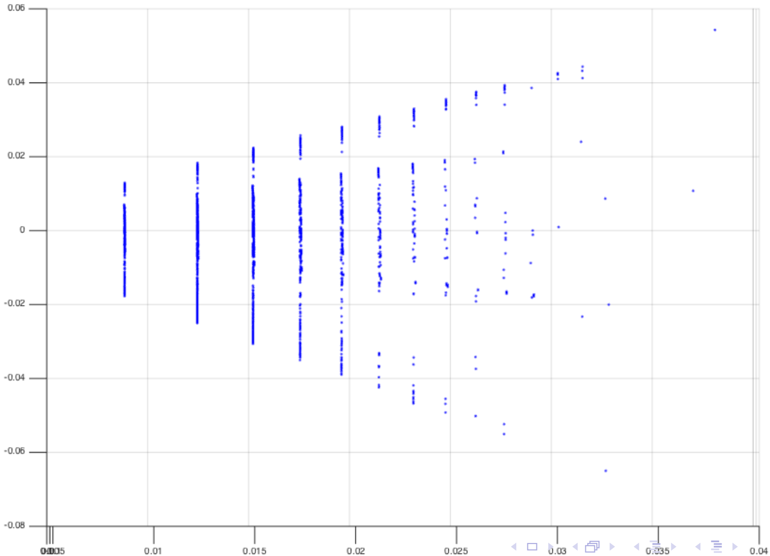

Graph Laplacian

Diffusion approach: heat the graph.

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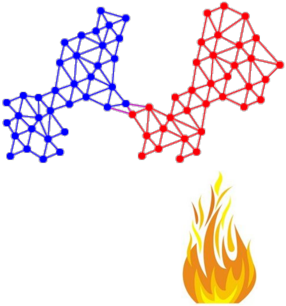
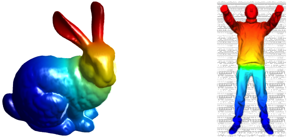
The heat gets trapped in a community $\Rightarrow$ can recover it.



Graph Laplacian

In $\mathbb{R}^2$, the **heat diffusion** is described by the Laplacian $\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$.



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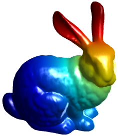 

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On a graph, the discrete Laplacian is the $n \times n$ matrix

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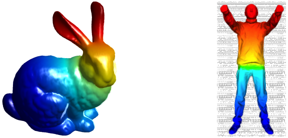

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Adjacency and Laplacian are two most fundamental matrices associated to graphs.

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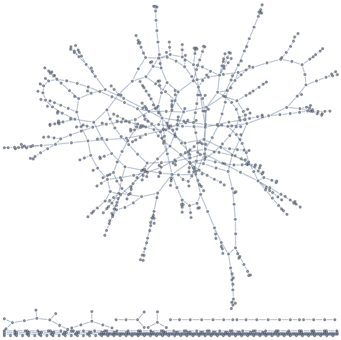
What's wrong? Low-degree vertices: isolated vertices, trees. (They get overheated.)



Concentration of Laplacian

Would regularization help?

Concentration of Laplacian

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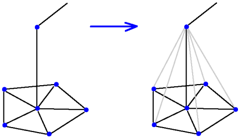
Connect low-degree vertices to the rest of the graph by *light weighted edges*; bring up all degrees to $\sim d$.



$$\Longleftrightarrow \qquad A_{ij} \mapsto A_{ij} + d/n$$

Proposed by network scientists [Chaudhuri+ 12, Amini+ 13].

Concentration of regularized Laplacian: theory

Theorem. *The Laplacian* Δ' *of the regularized graph concentrates:*

$$\|\Delta' - \mathbb{E}\,\Delta'\| \lesssim \frac{1}{\sqrt{d}} \quad \textit{while} \quad \|\Delta'\| \sim 1.$$

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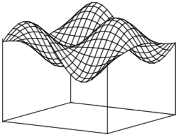
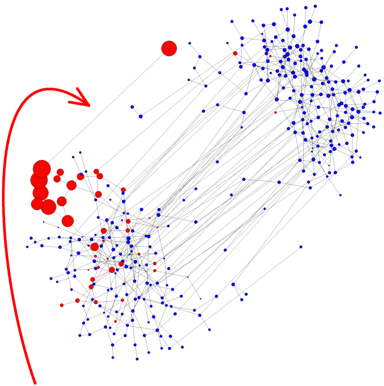
Physical interpretation: Make the graph vibrate; the wave with lowest frequency recovers the communities.



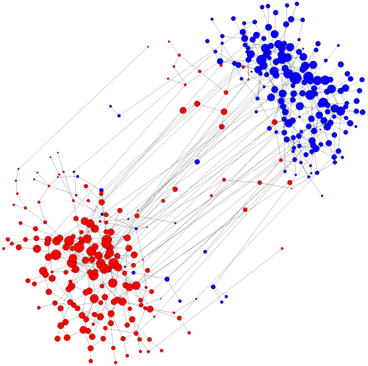
Performance of regularized spectral clustering

Artificial data: sparse stochastic block model

Without regularization



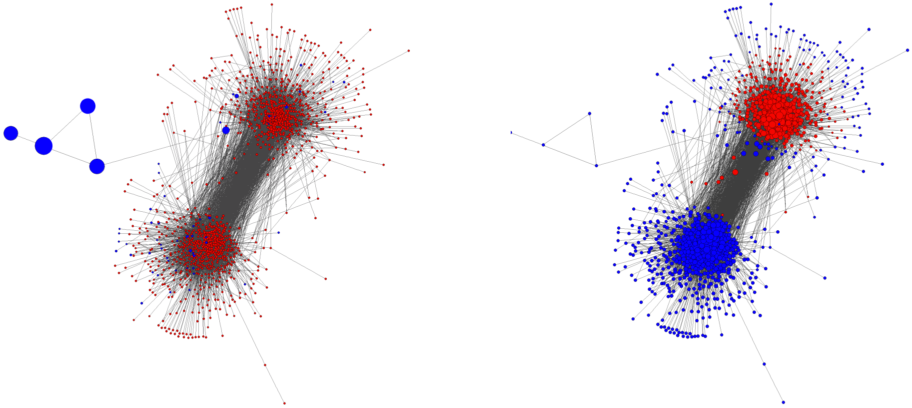
With regularization



This tree gets overheated

Real data: political blogs after 2004 U.S. presidential election [Adamic-Glance 04].

Without regularization — With regularization



1,222 vertices (liberal/conservative); edges = hyperlinks; average degree = 27.

Optimization Methods

Goal: fit the desired type of structure to a given network.

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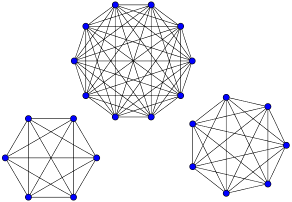
Optimization: $\max \langle A, Z \rangle$ where $A =$ adjacency matrix of the network, $Z =$ adjacency matrix of a union of cliques with k edges.



$$Z = \begin{bmatrix} 1 & 1 & 1 & 1 & & & & & \\ 1 & 1 & 1 & 1 & & & & & \\ 1 & 1 & 1 & 1 & & & & & \\ 1 & 1 & 1 & 1 & & & & & \\ & & & & 1 & 1 & 1 & & \\ & & & & 1 & 1 & 1 & & \\ & & & & 1 & 1 & 1 & & \\ & & & & & & & 1 & 1 \\ & & & & & & & 1 & 1 \end{bmatrix}$$

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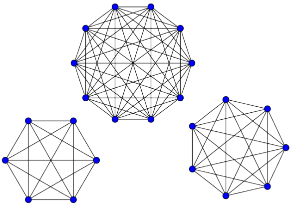

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Optimization. $\max \langle A, Z \rangle$: $Z \in \{0,1\}^{n \times n}$ is block-diagonal, $\sum Z_{ij} = k$.

Integer optimization problem. NP-hard.

Semidefinite relaxation

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Fact. A matrix $Z \in \{0,1\}^{n\times n}$ is block diagonal $\Leftrightarrow$ Z is positive semidefinite.

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A semidefinite relaxation:

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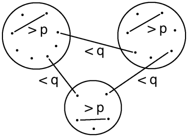
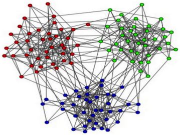
General stochastic block model: $\forall$ many communities, $\forall$ connection probabilities p_{ij}, *within* communities $> p$; *across* communities $< q$. (Not necessarily low rank!)





Semidefinite relaxation: theory

SDP. $\max \langle A, Z \rangle$: $Z \in [0,1]^{n \times n}$ is positive semidefinite, $\sum Z_{ij} = k$.

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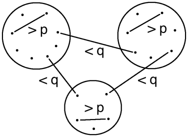

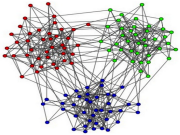

Theorem (Community Detection by SDP). Consider a general stochastic block model with $p = a/n$ and $q = b/n$. Suppose

$$(a-b)^2 \geq C_\varepsilon (a+b).$$

Then the SDP (with k=number of edges) recovers communities up to εn misclassified vertices, and with high probability.

[Guedon-V. 14].

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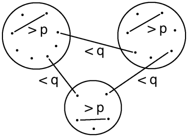

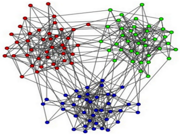

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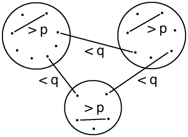

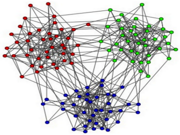

Theorem **(Community Detection by SDP).** Consider a general stochastic block model with $p = a/n$ and $q = b/n$. Suppose

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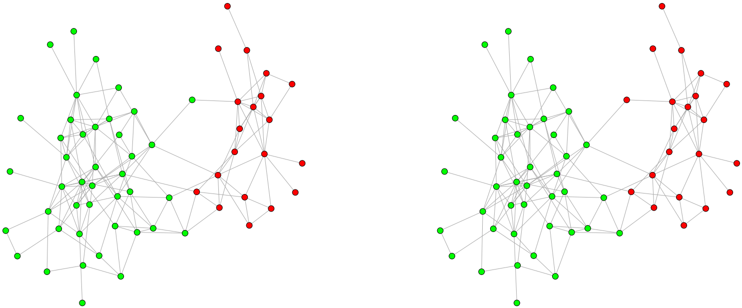
[Guedon-V. 14]. Proof: Grothendieck inequality + concentration in cut norm. □

Exact recovery for *dense* networks ($a, b \geq \log n$); thresholds known [Abbe et al. 14].

Semidefinite relaxation in action

Example. Dolphins in Doubtful Sound, New Zealand [Lusseau et al. 03].



True communities

Communities found by SDP

Semidefinite relaxation in action

Take a closer look at

SDP. $\max \langle A, Z \rangle$: $Z \in [0,1]^{n \times n}$ is positive semidefinite, $\sum Z_{ij} = k$.

Semidefinite relaxation in action

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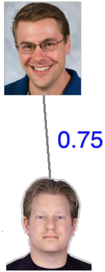

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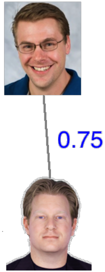
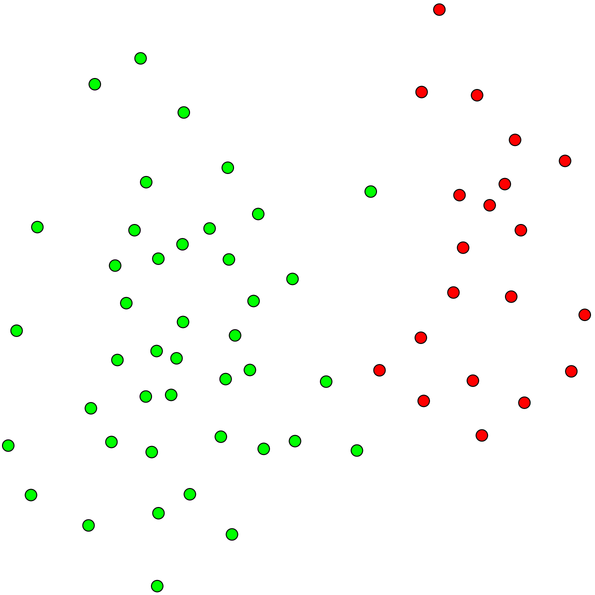
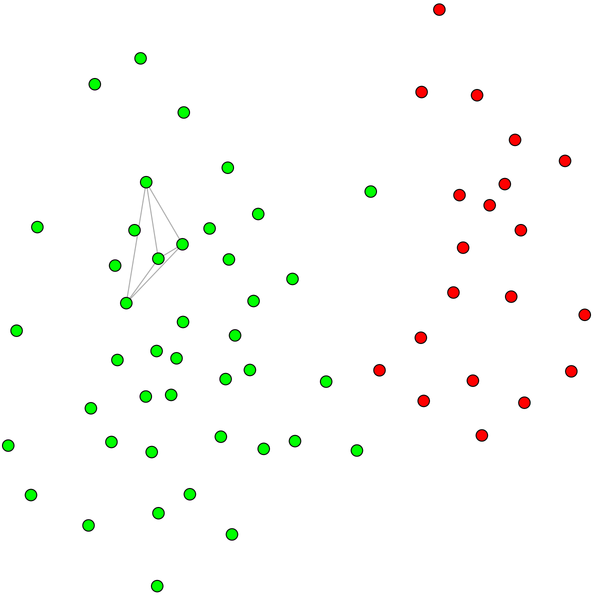
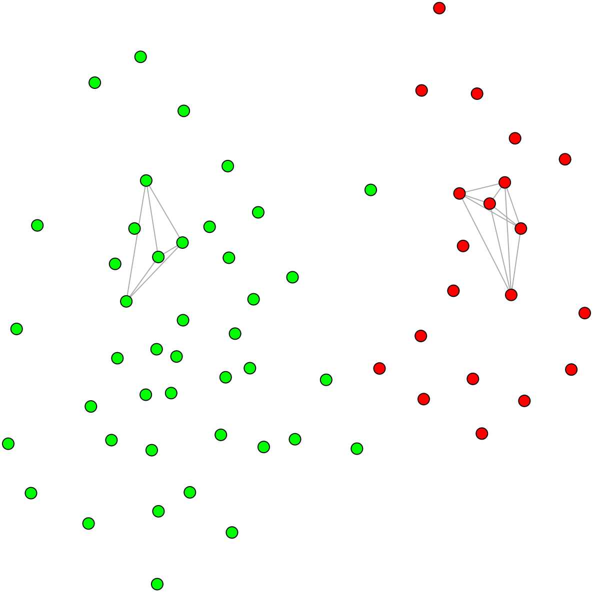
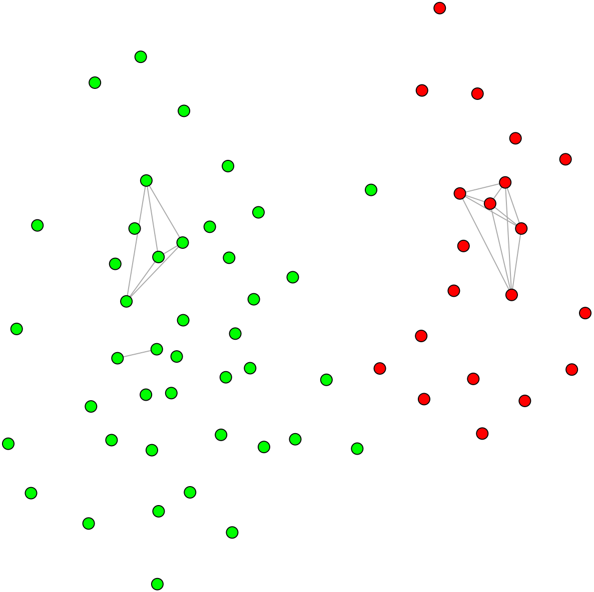


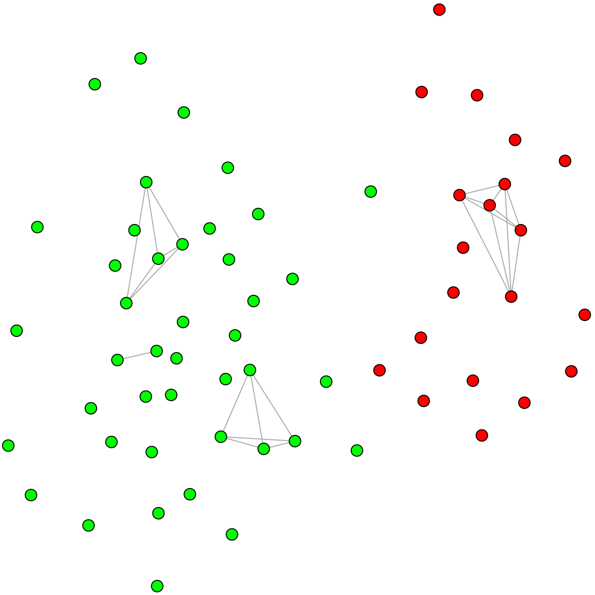
Next slide: increase k gradually $\Rightarrow$ dynamic picture.

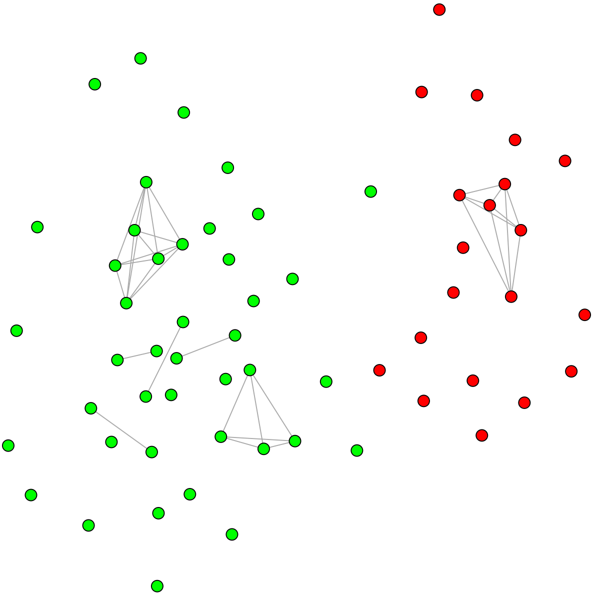


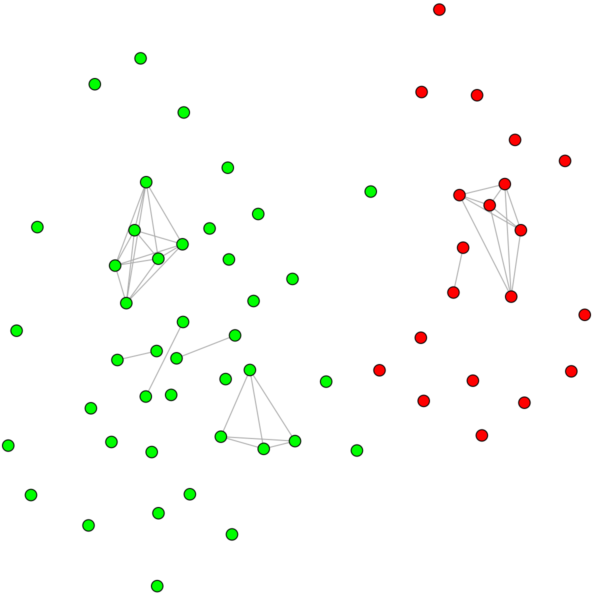


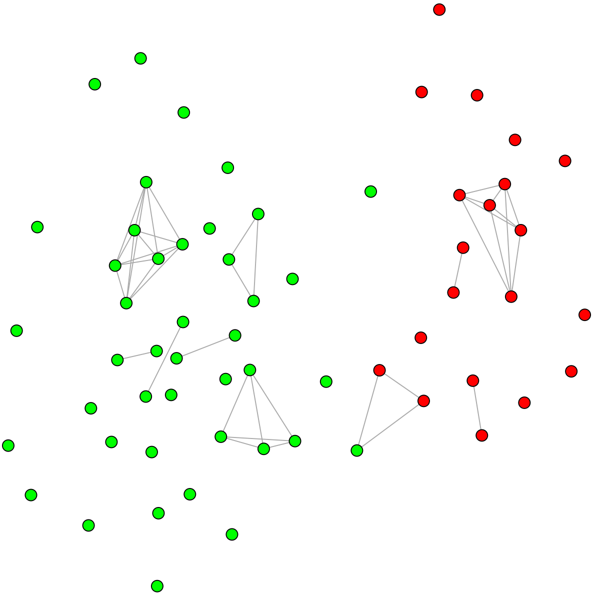


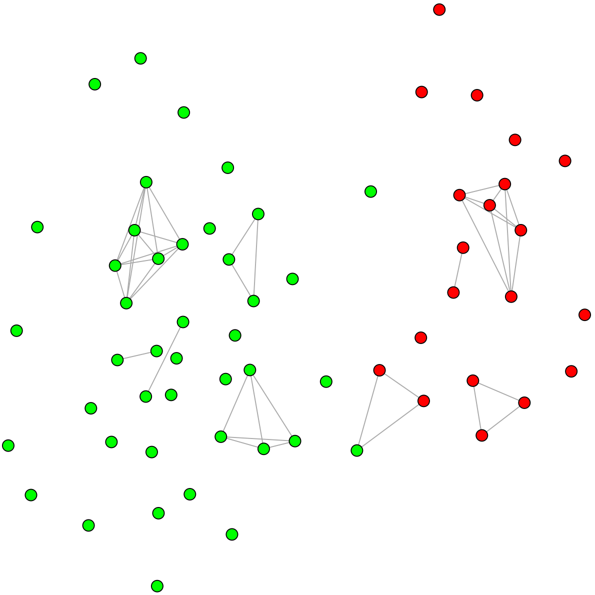


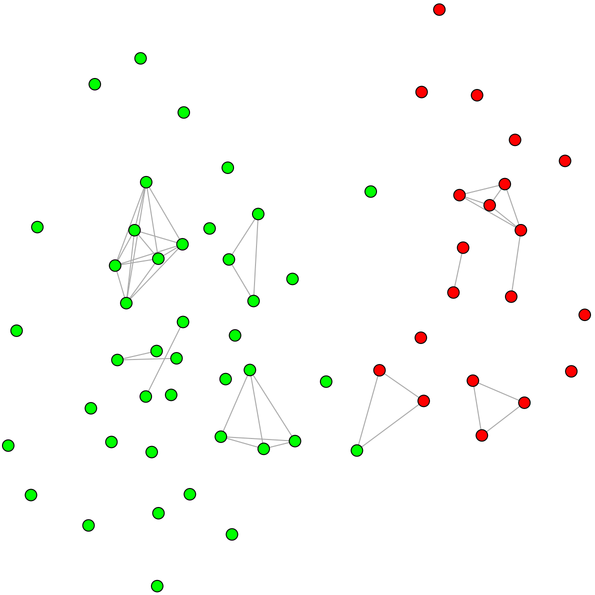


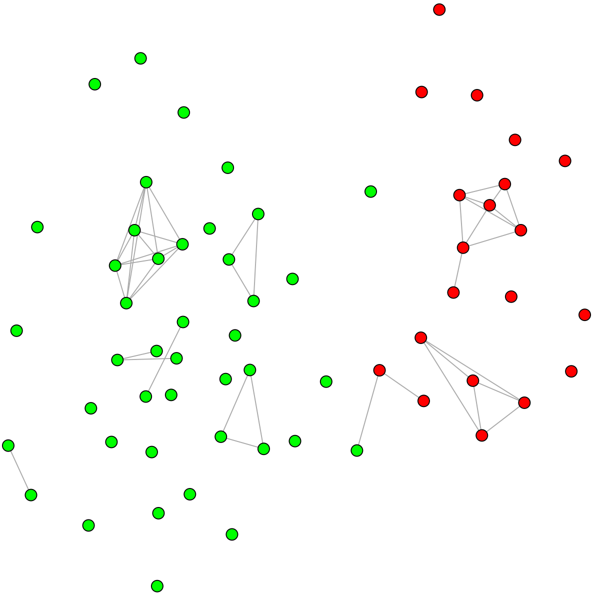


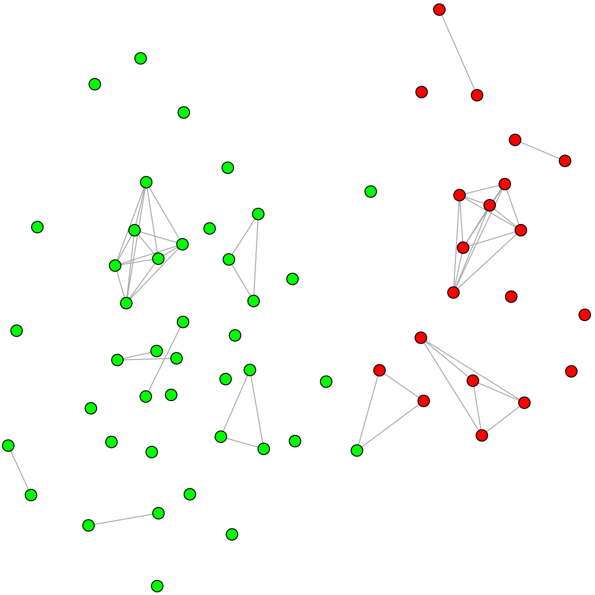


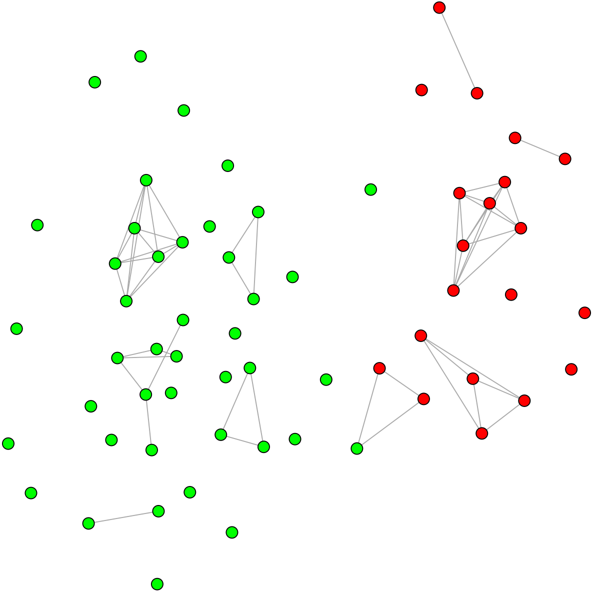


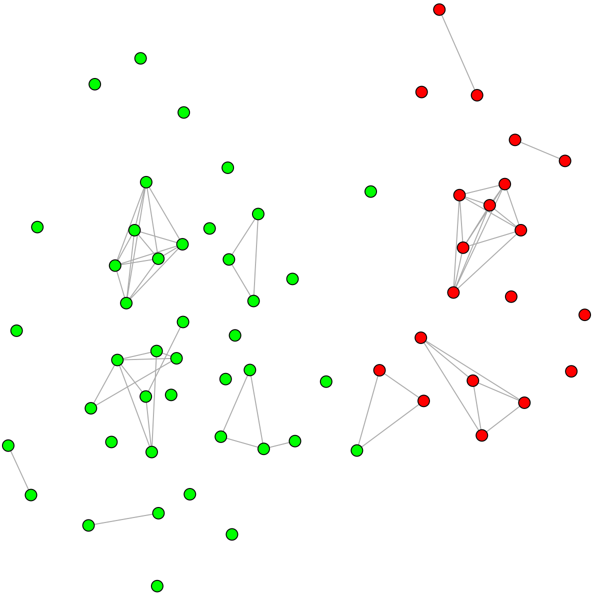


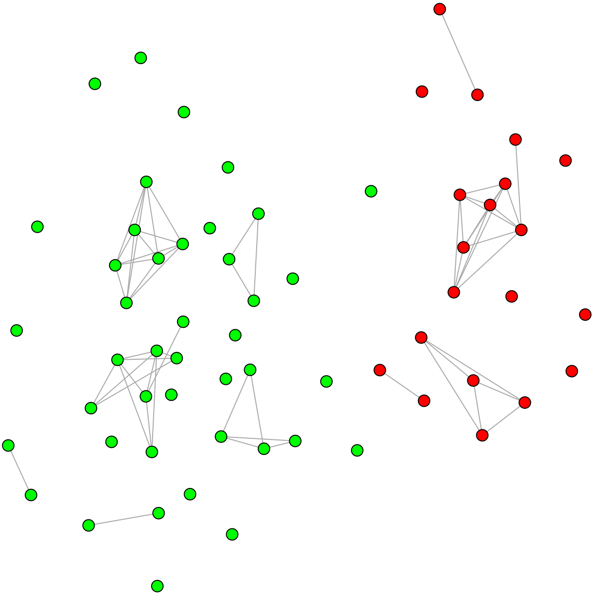


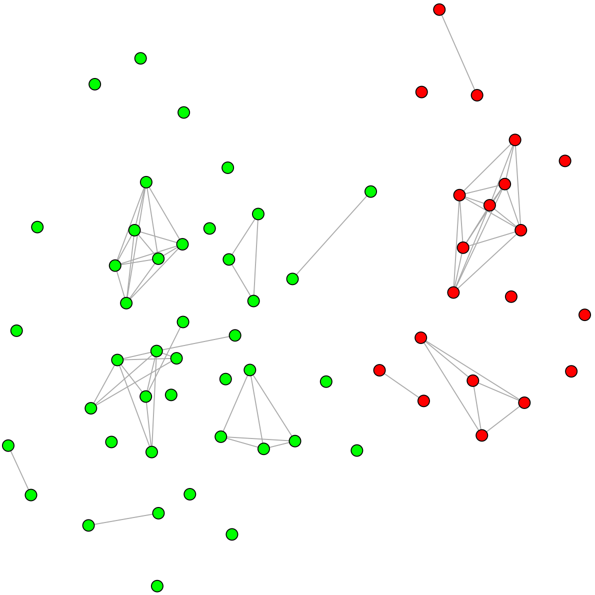


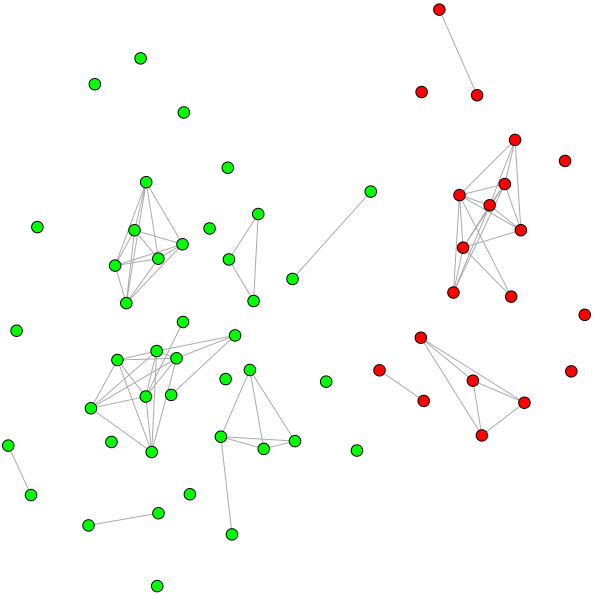


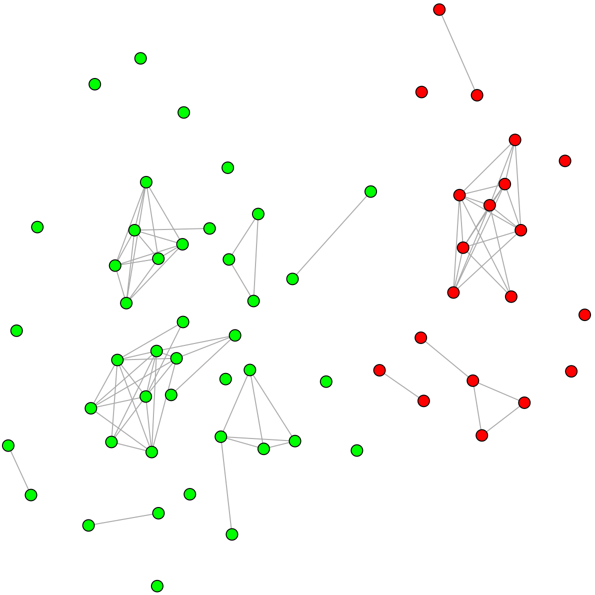


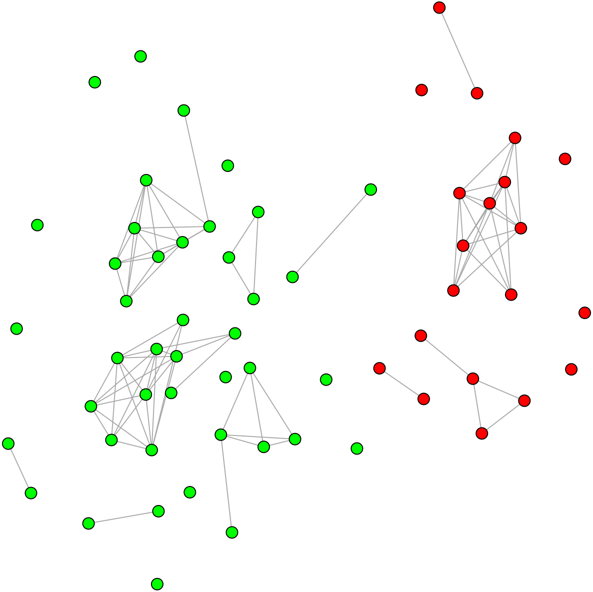


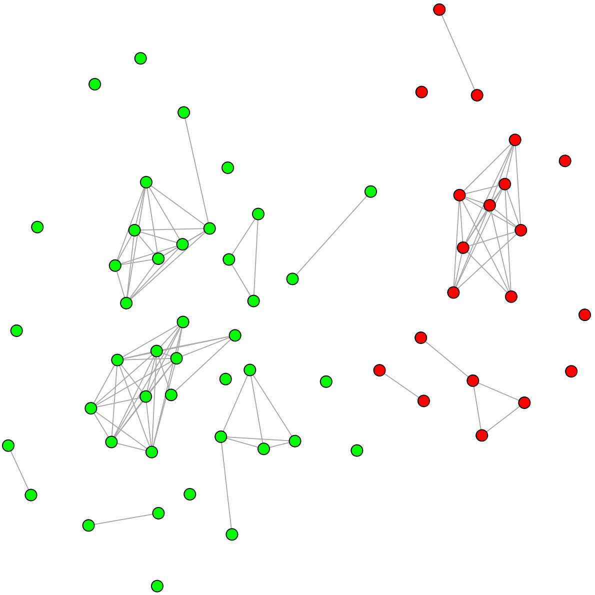


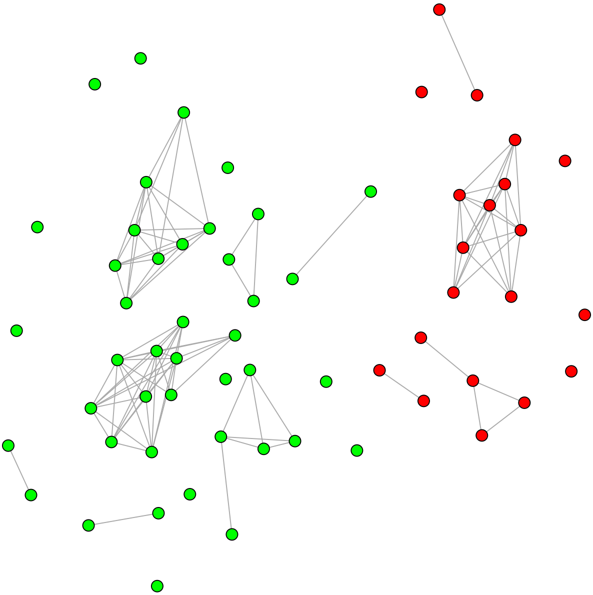


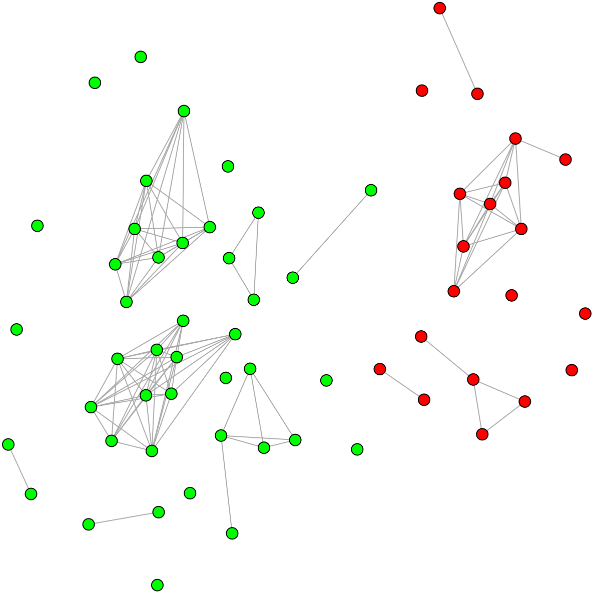


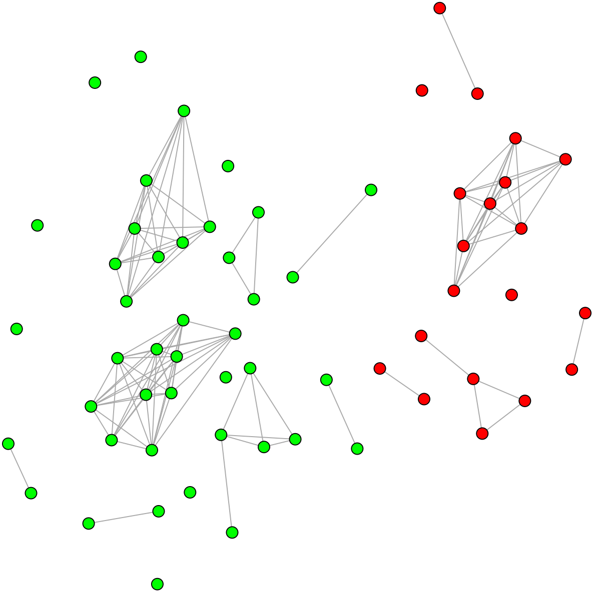


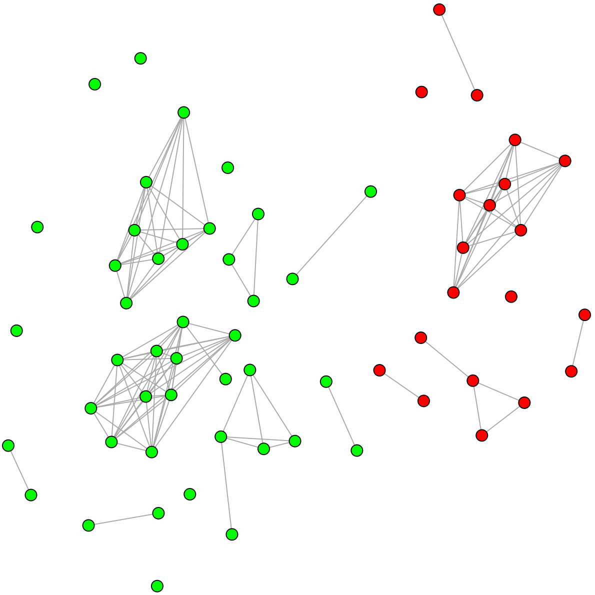


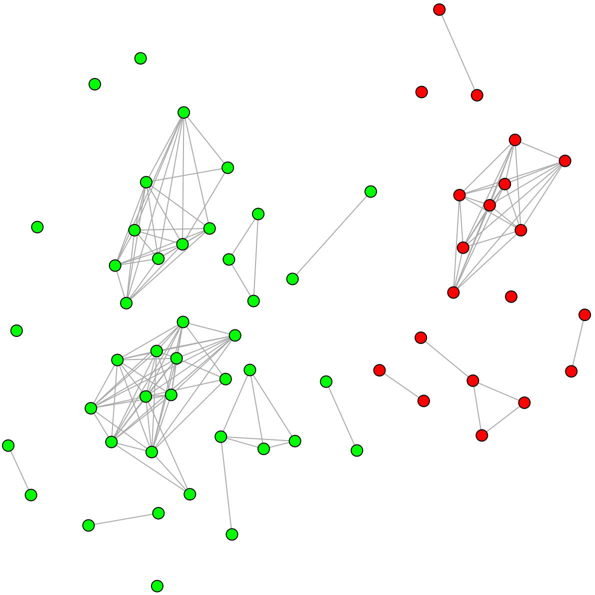


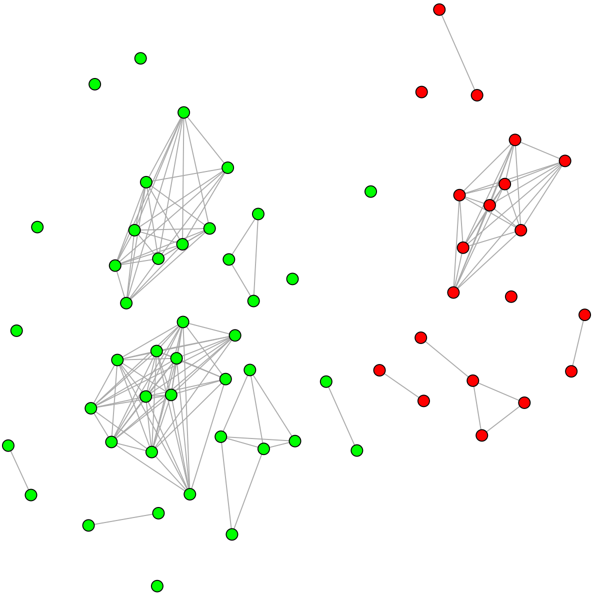


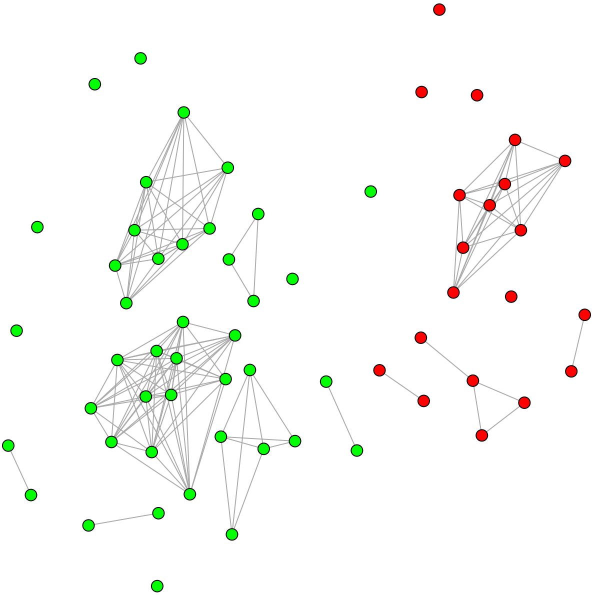


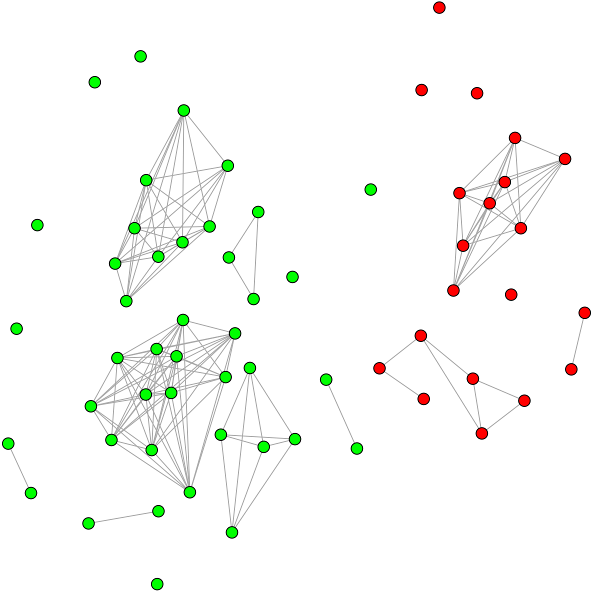


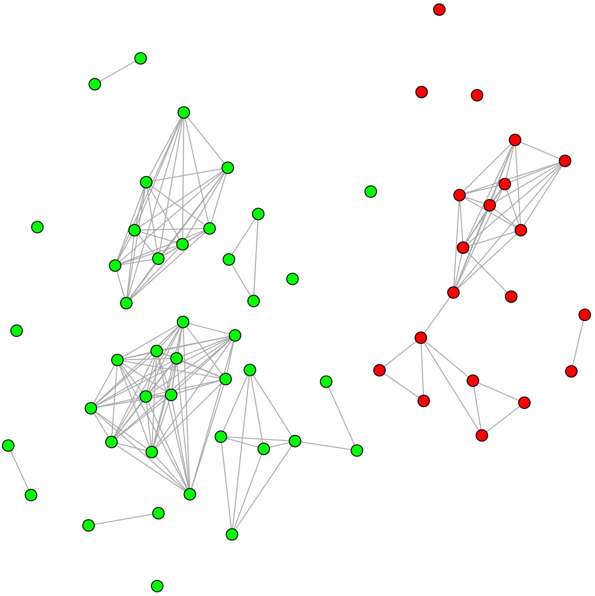


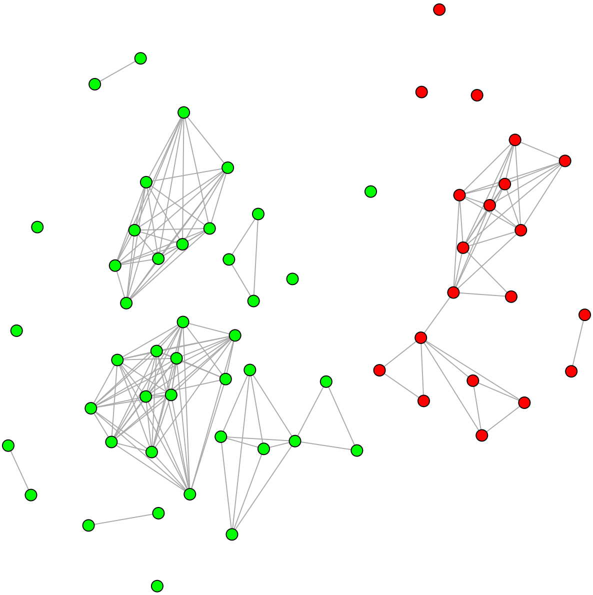


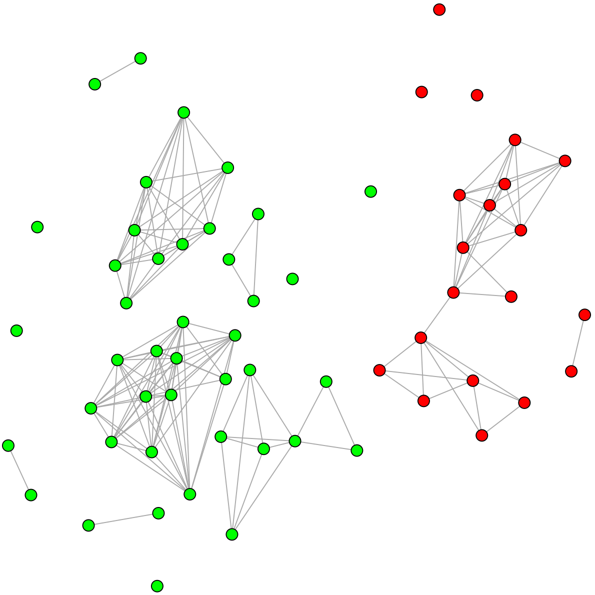


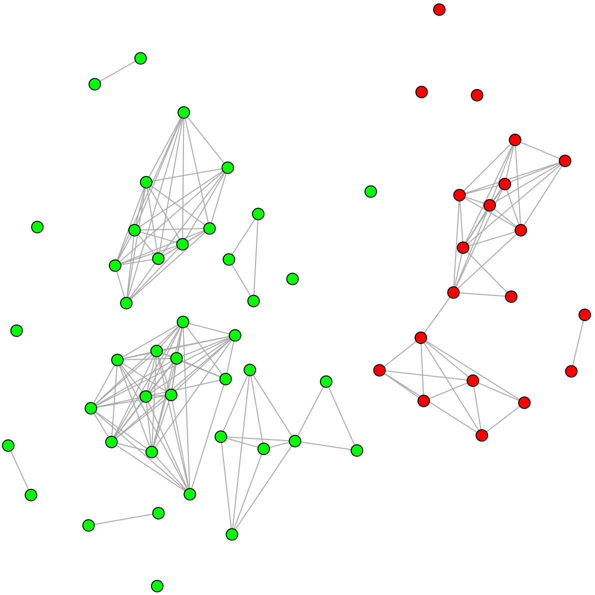


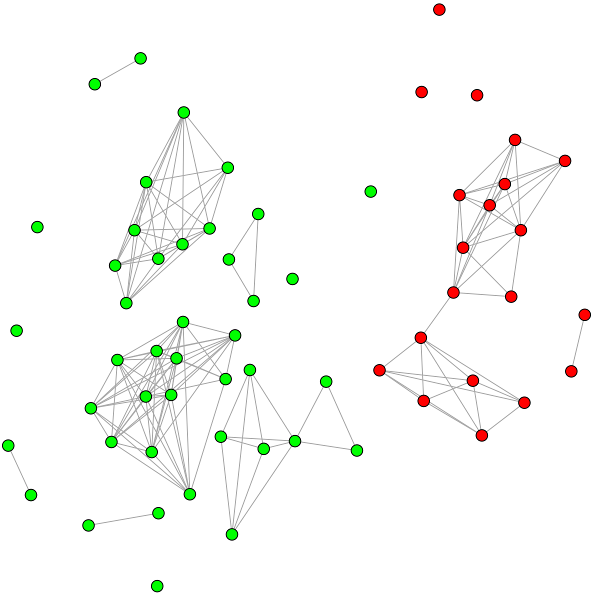


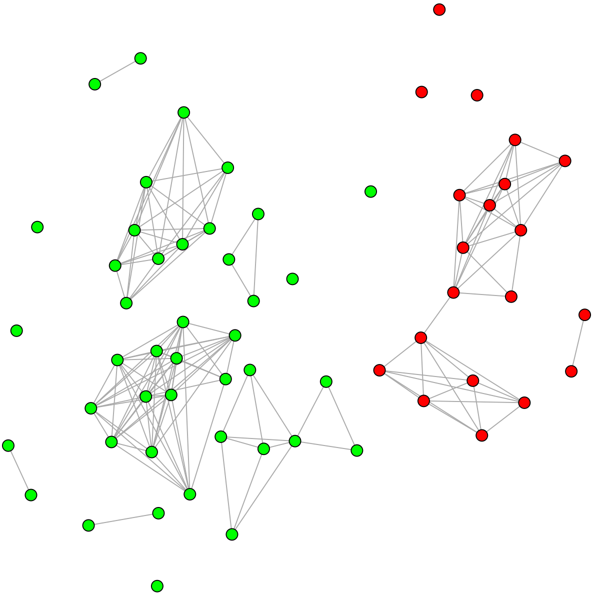


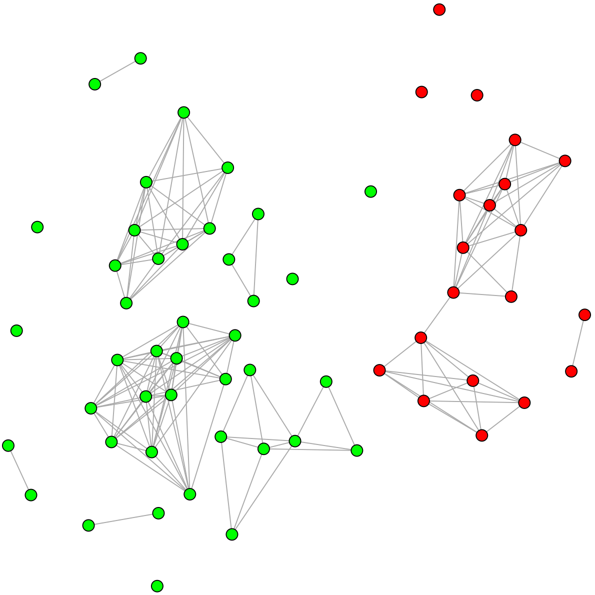


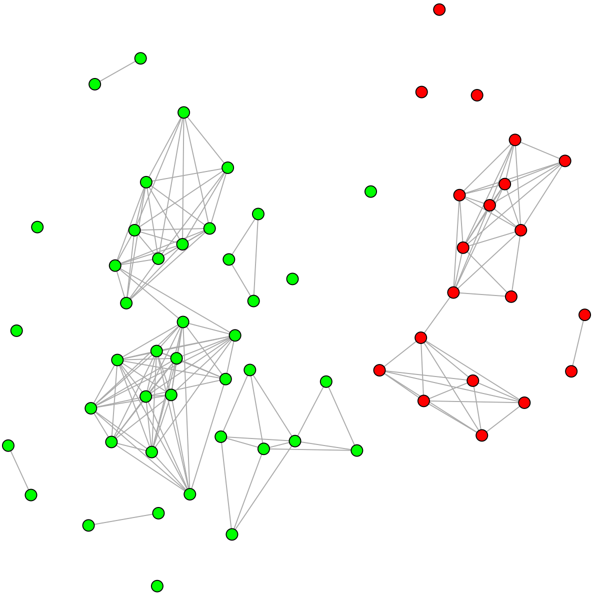


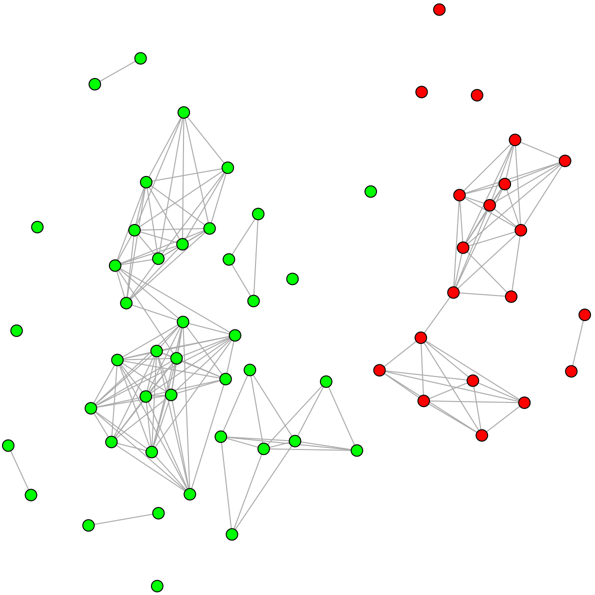


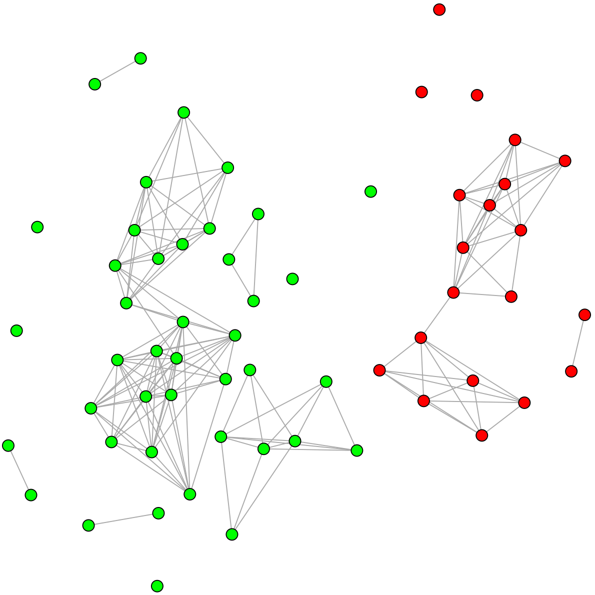


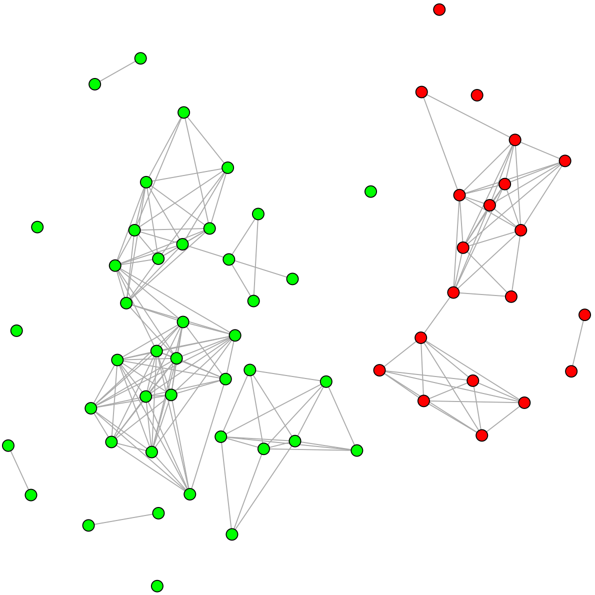


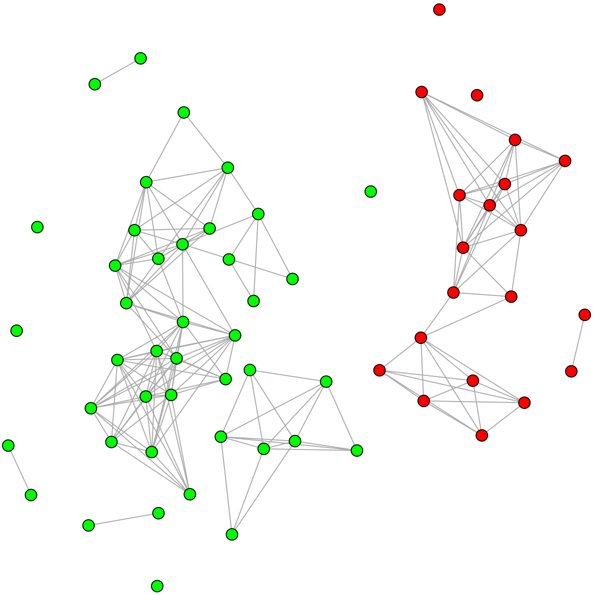


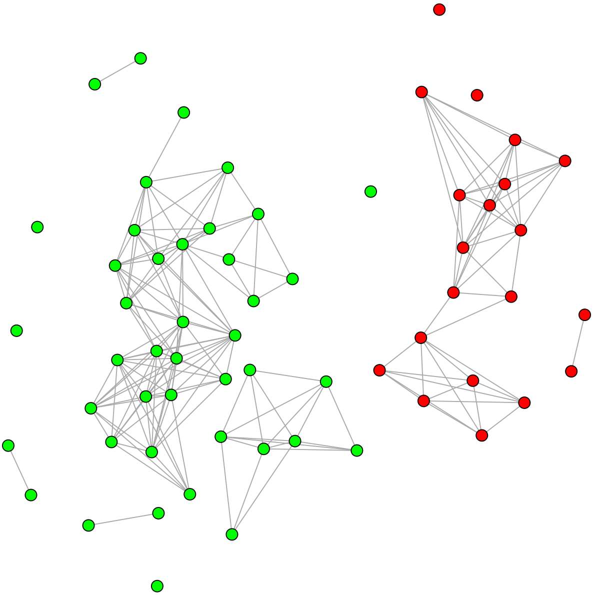


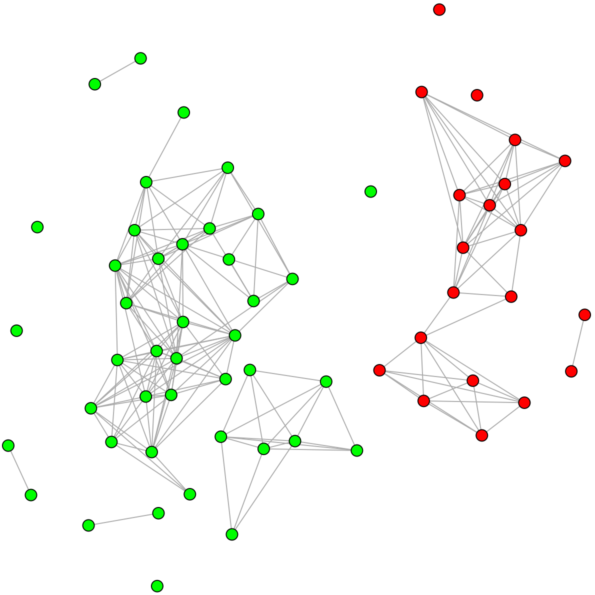


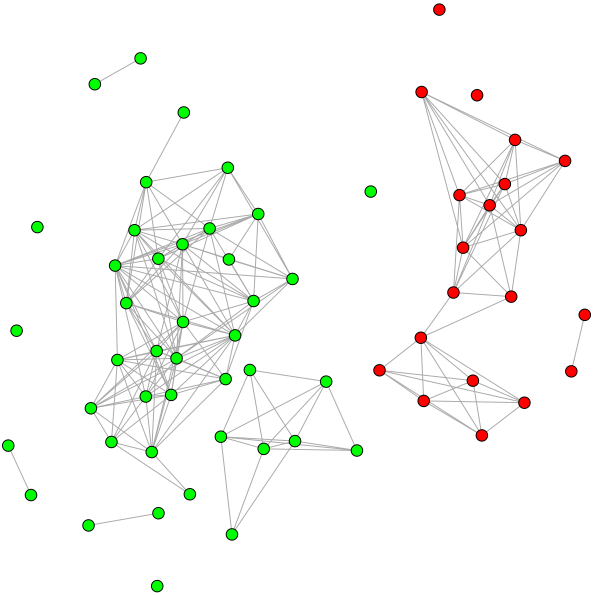


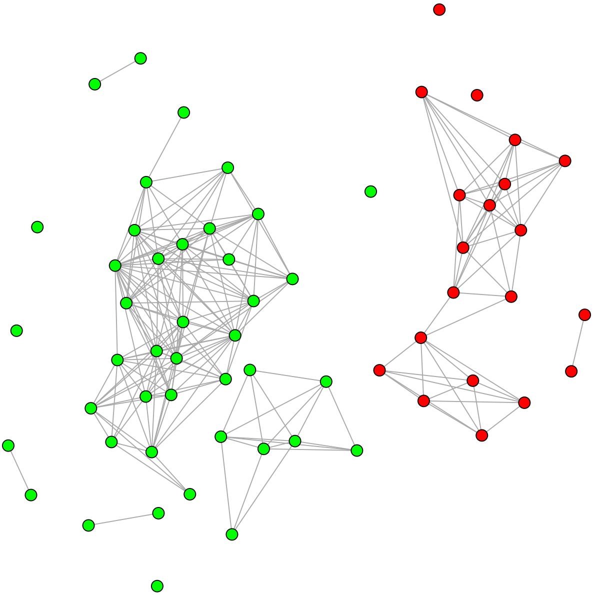


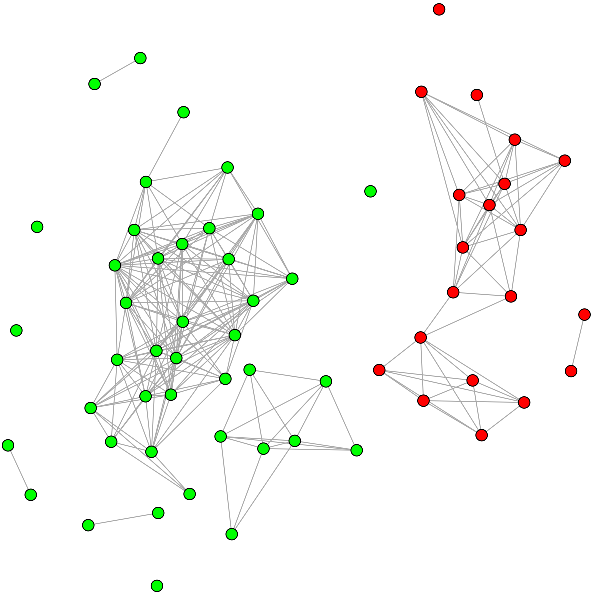


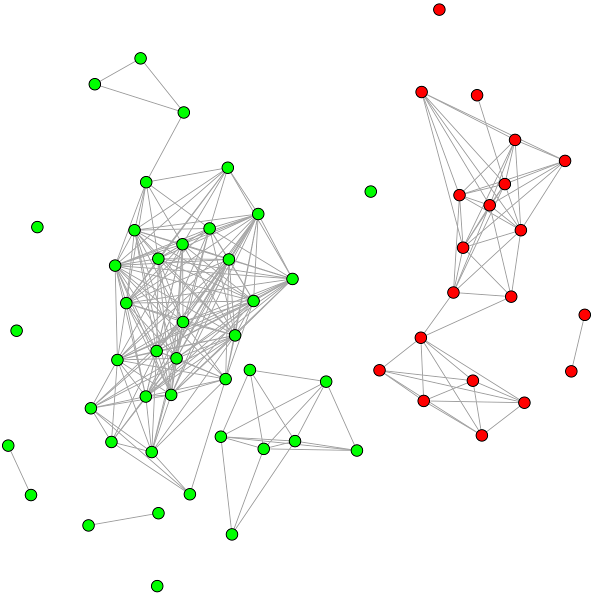


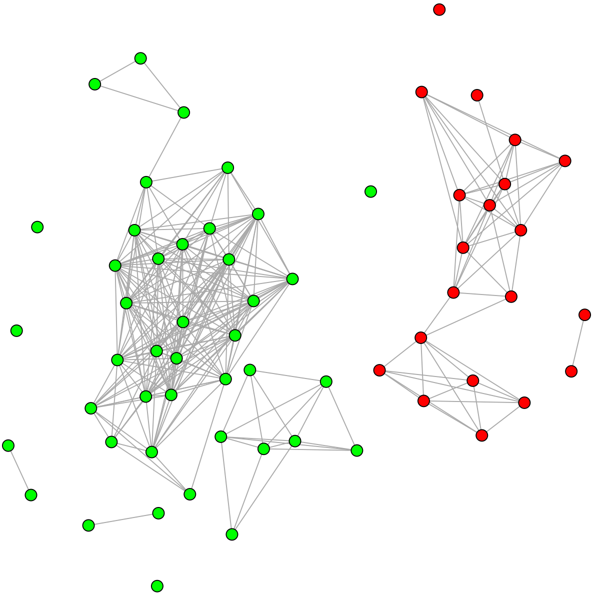


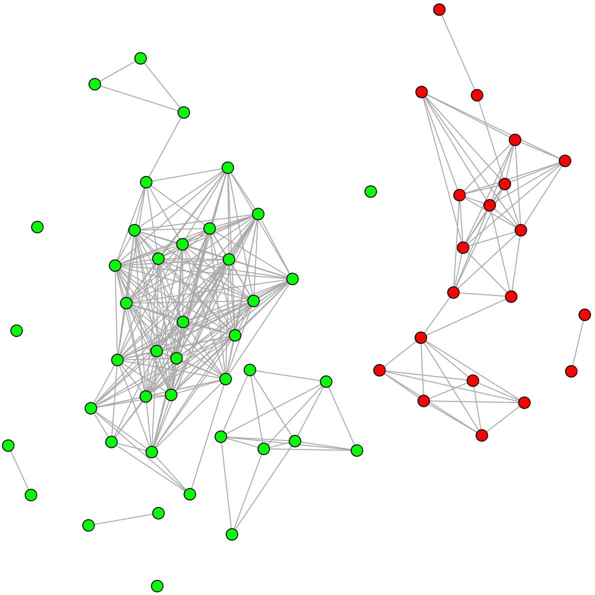


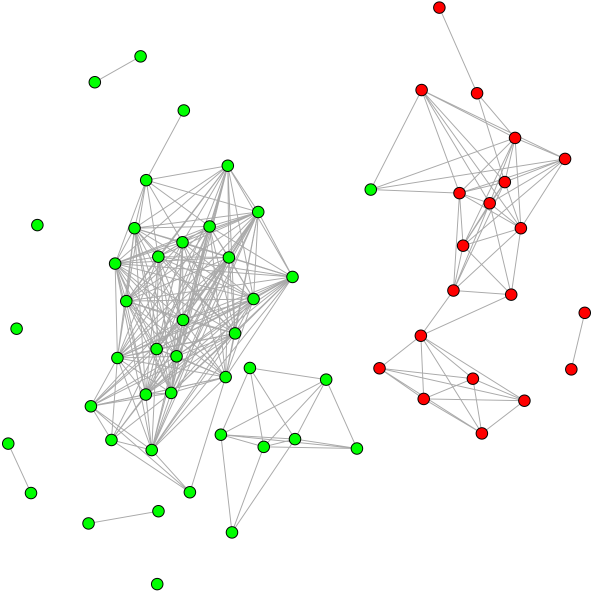


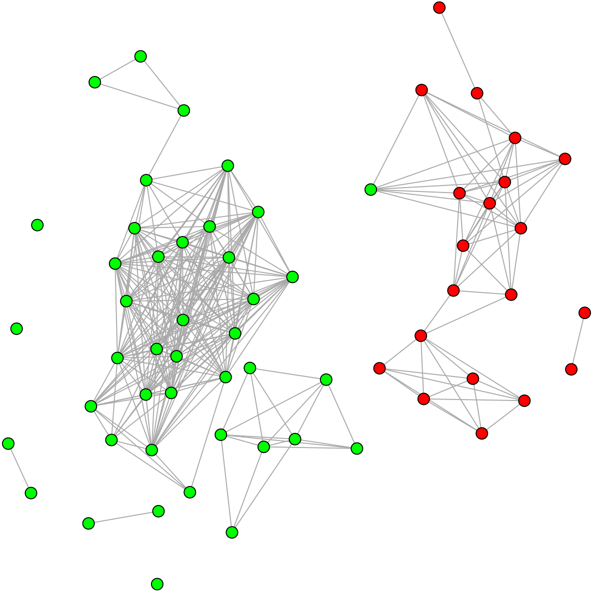


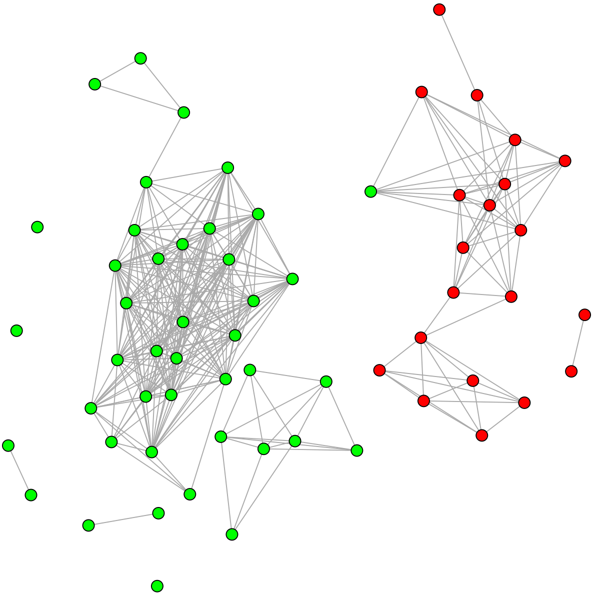


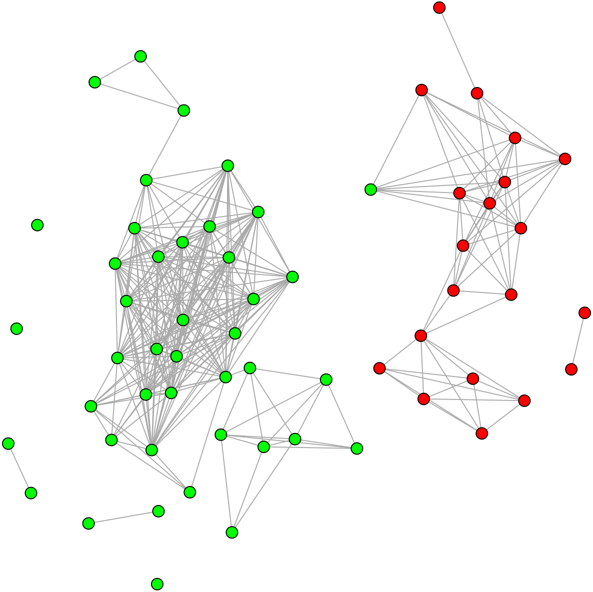


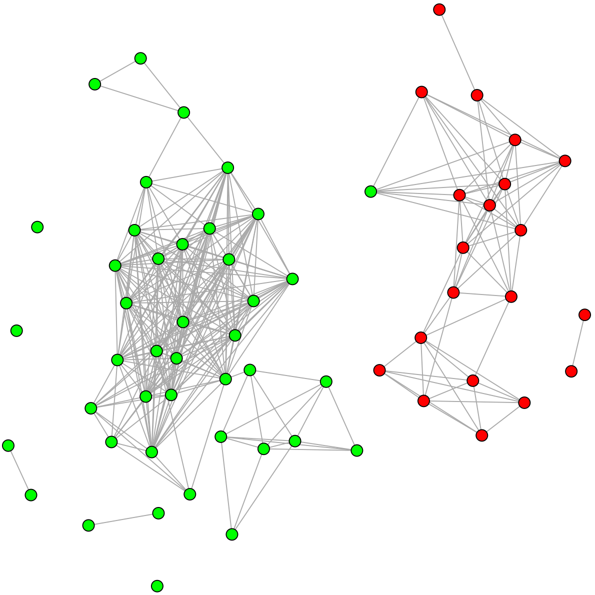


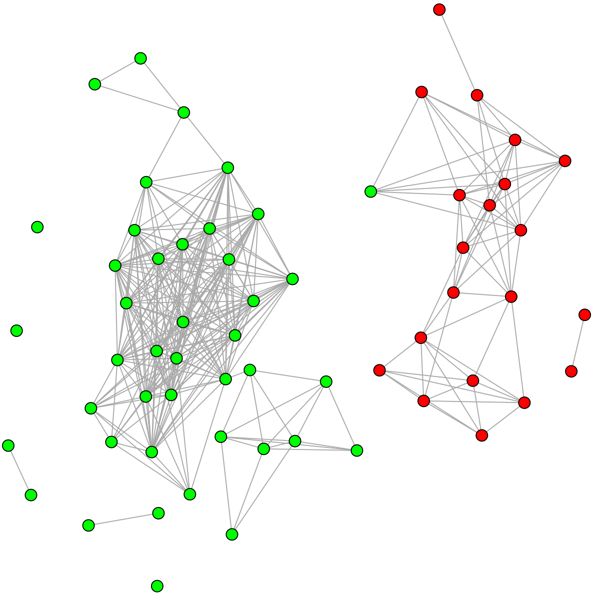


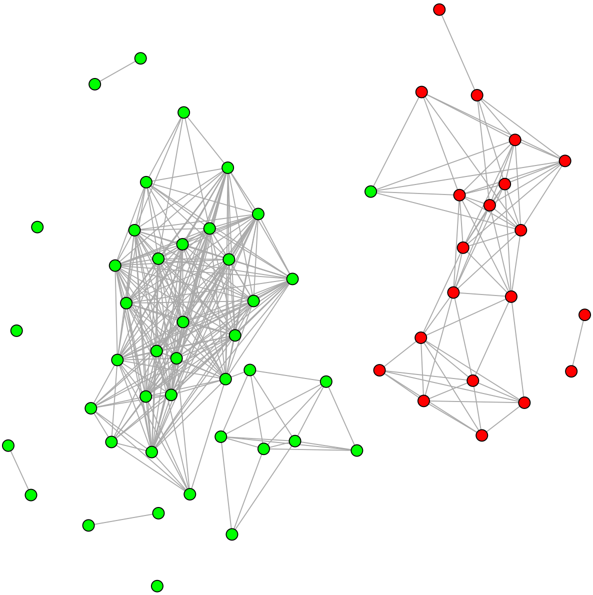


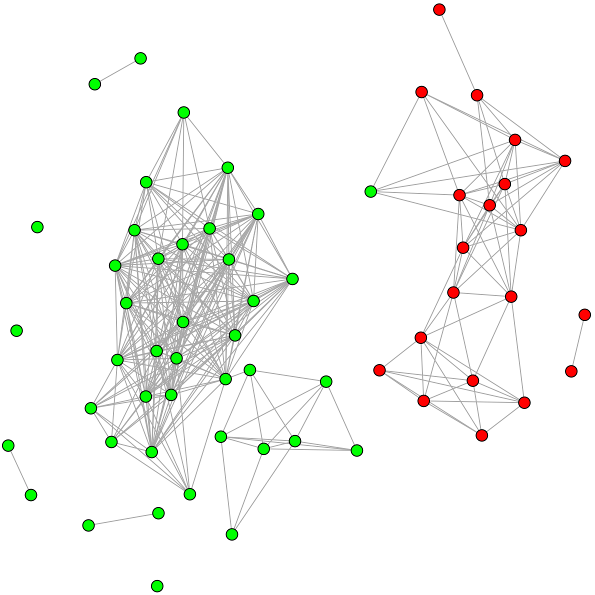


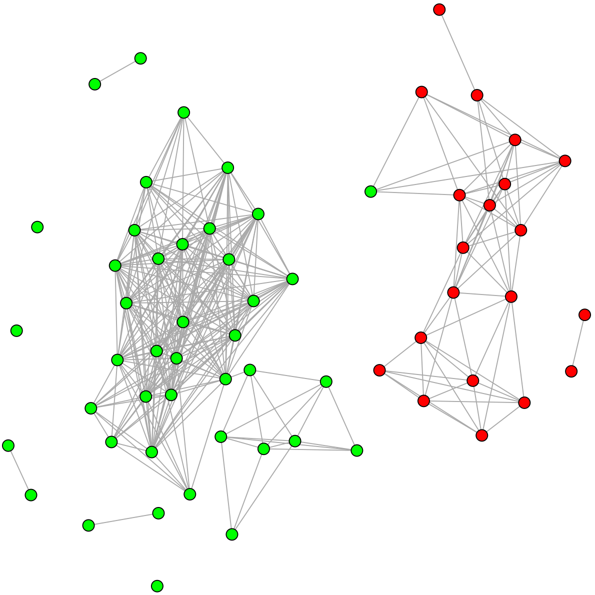


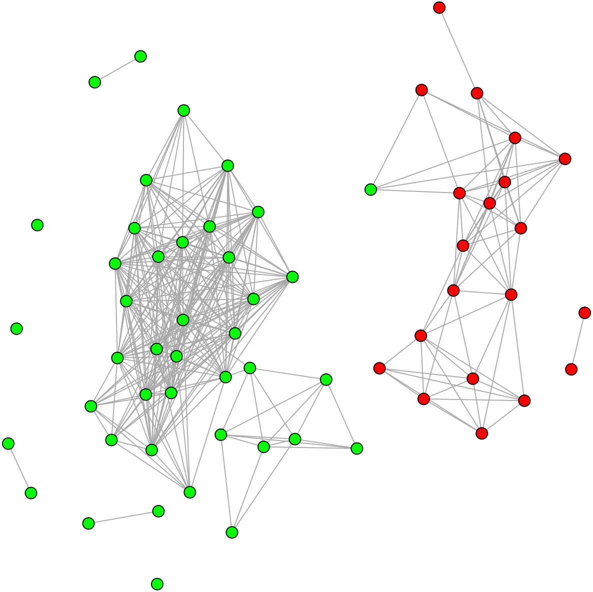


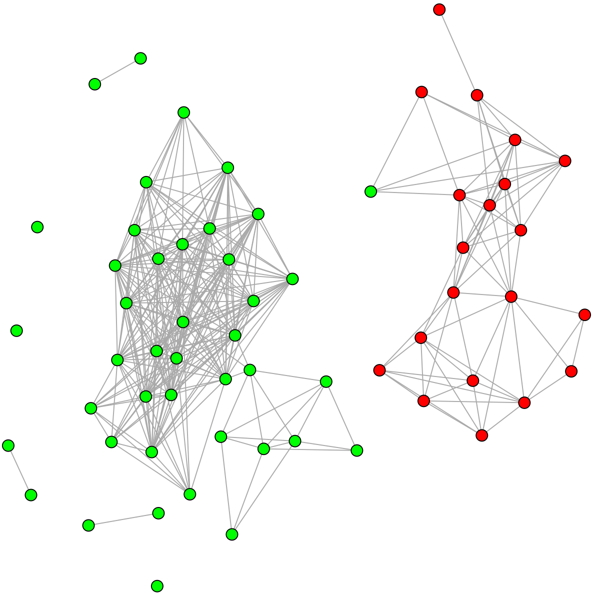


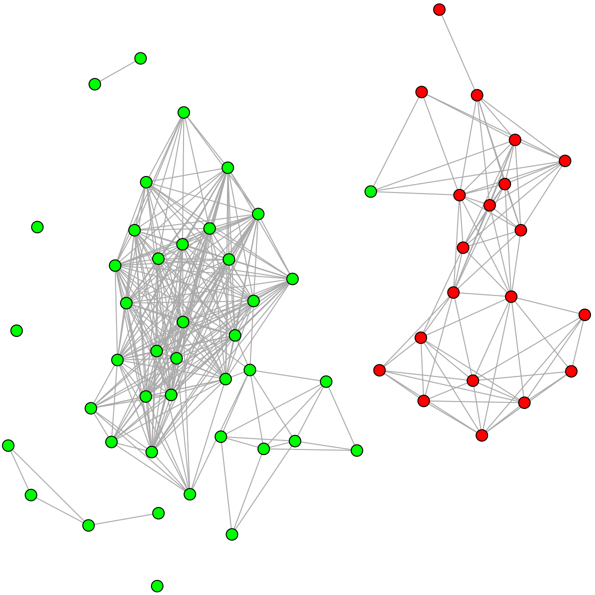


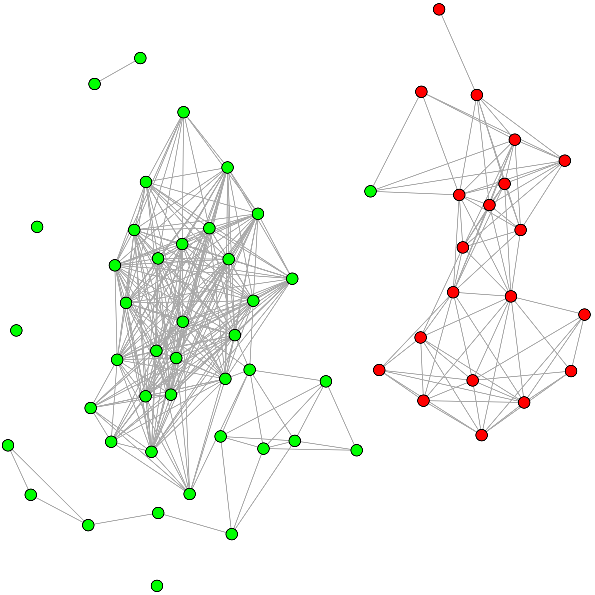


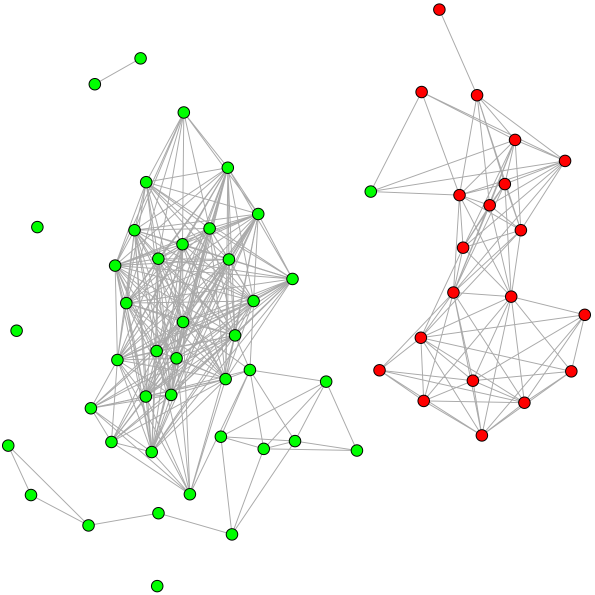


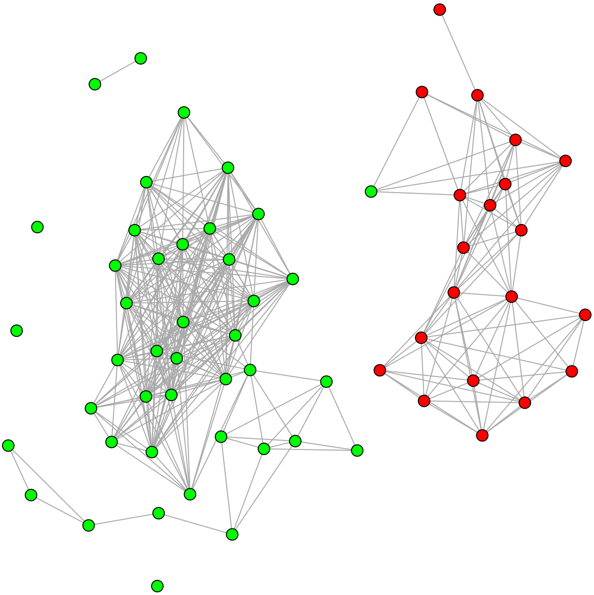


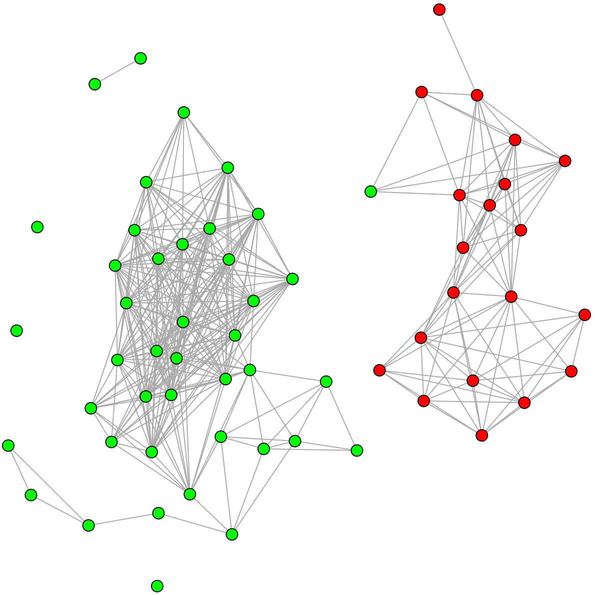


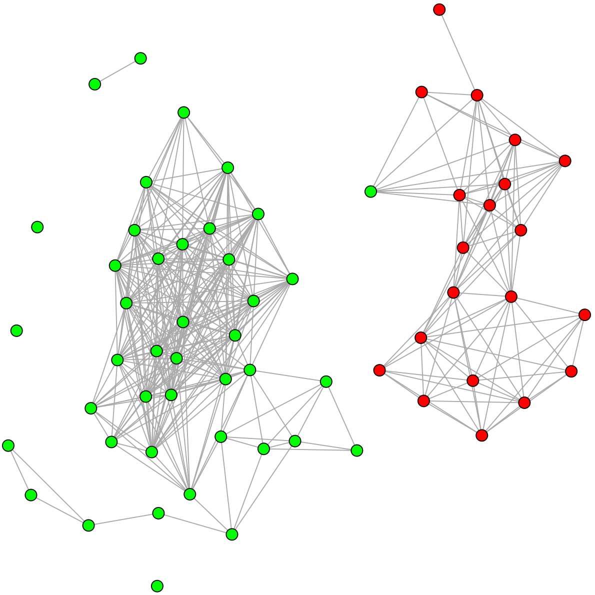


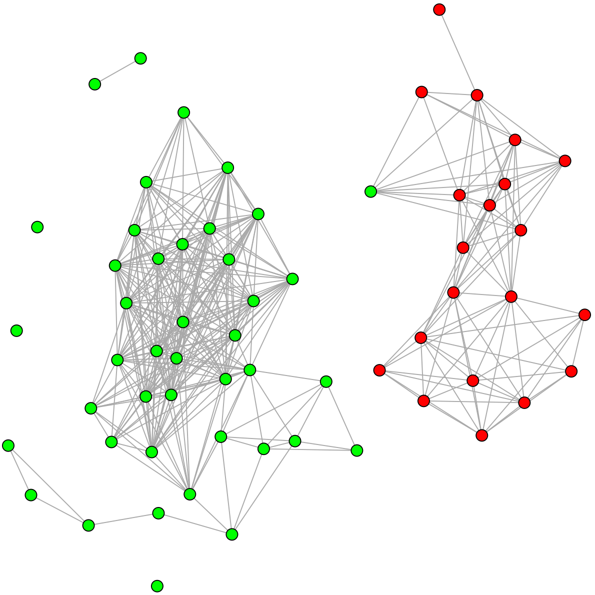


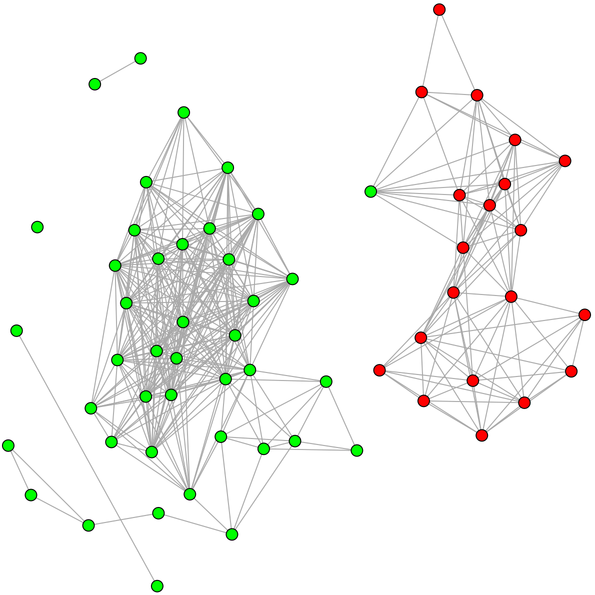


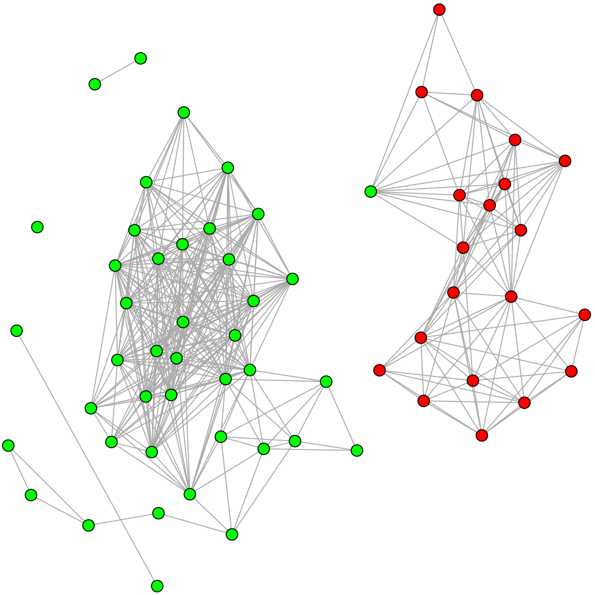


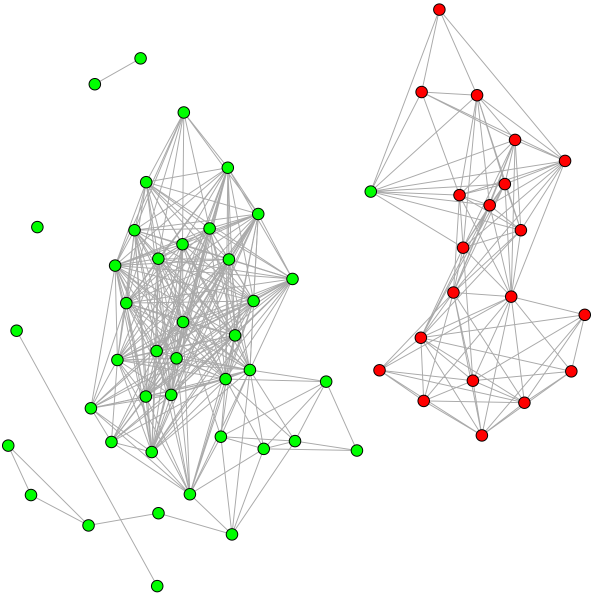


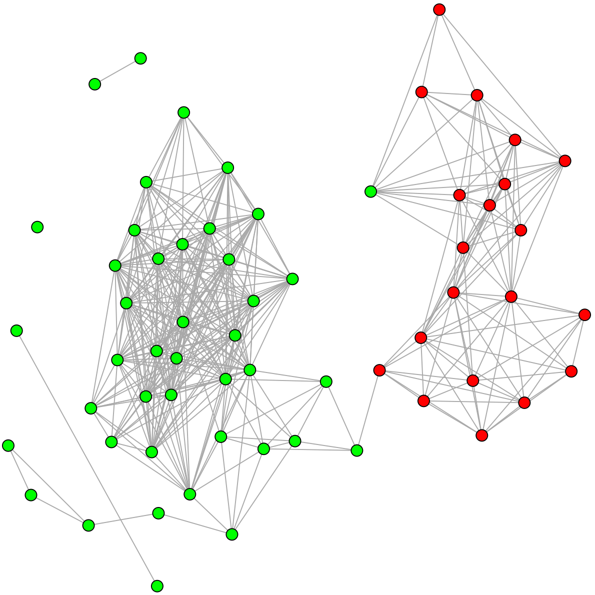


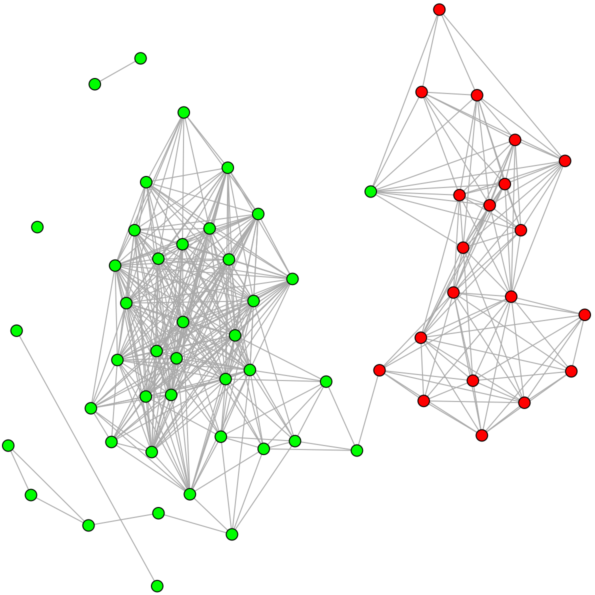


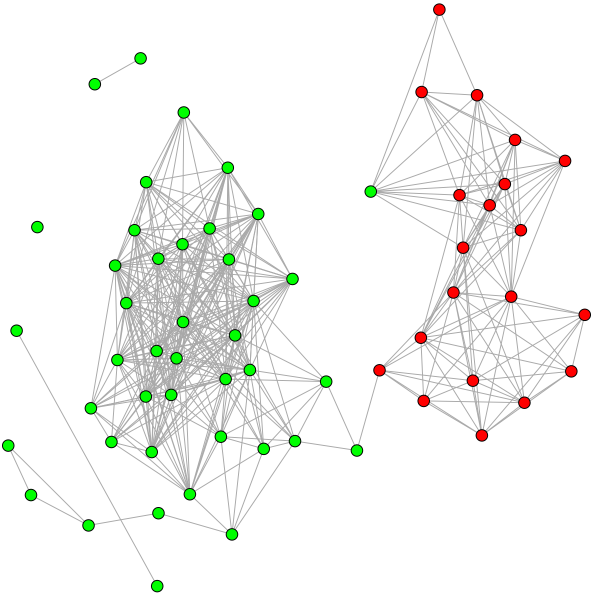


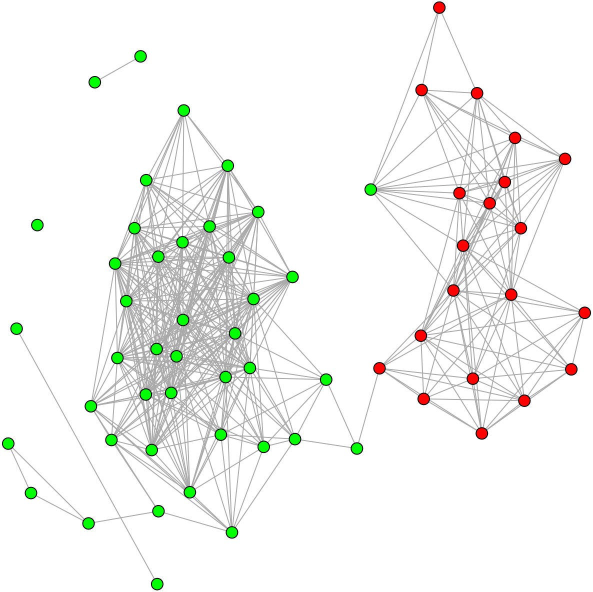


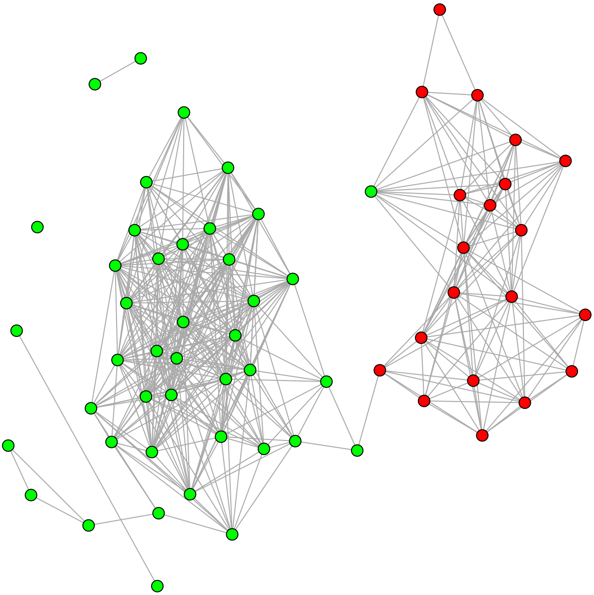


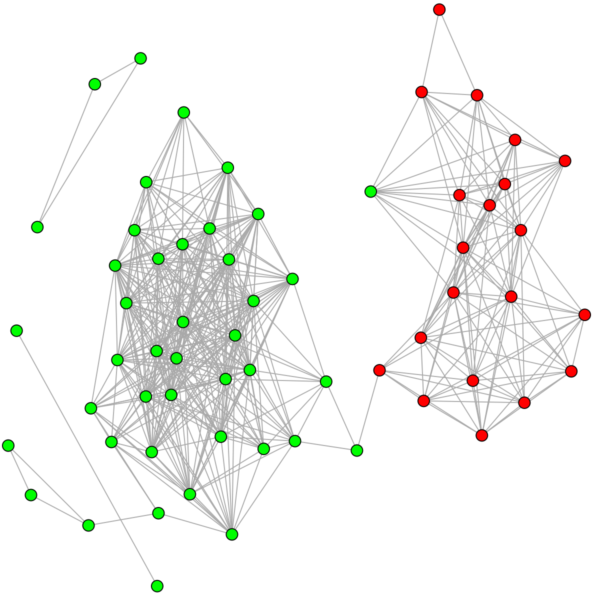


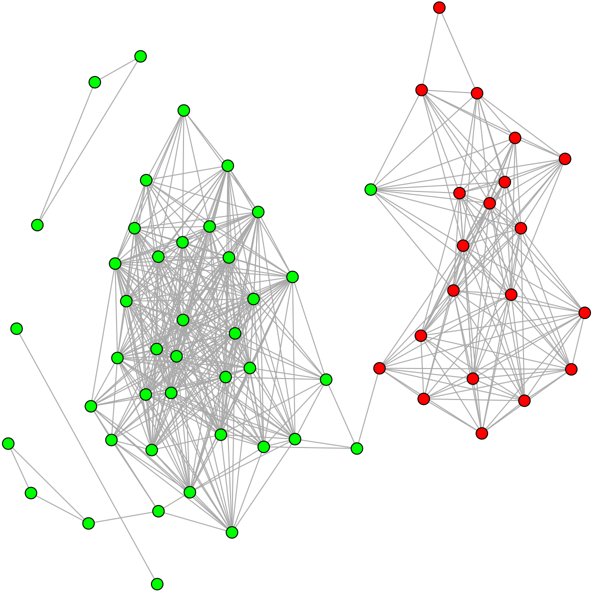


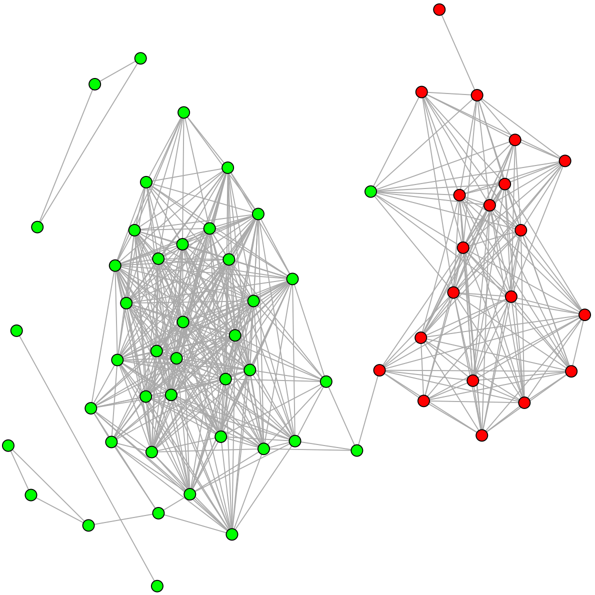


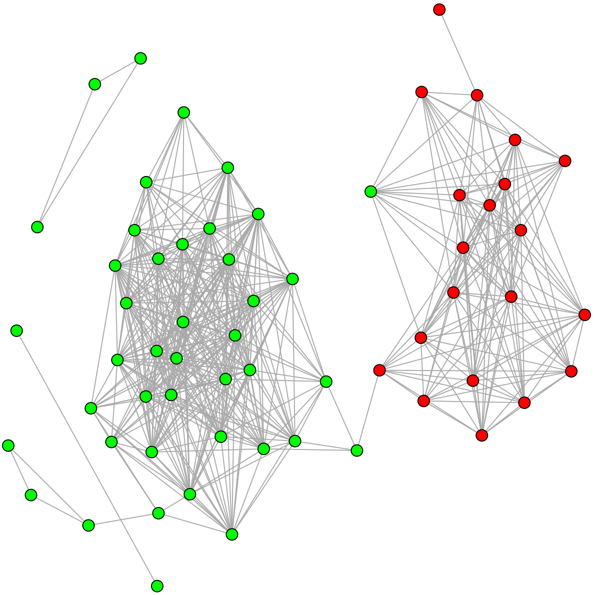


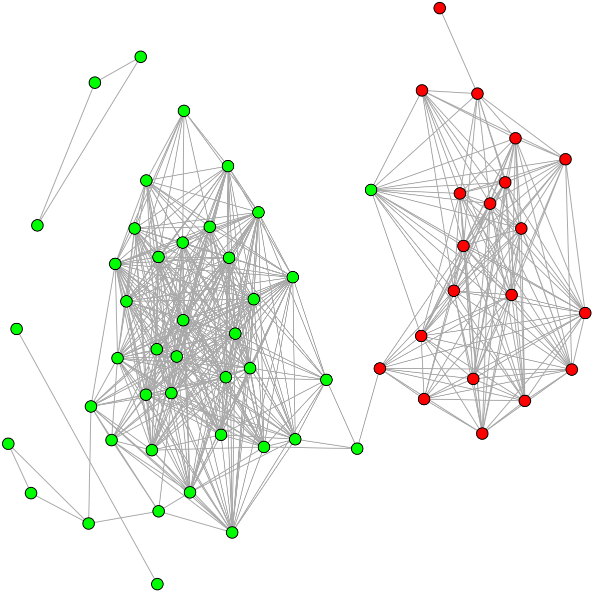


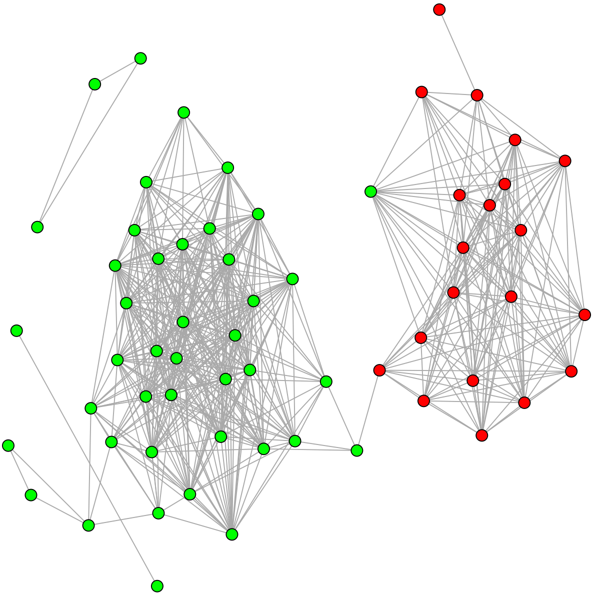


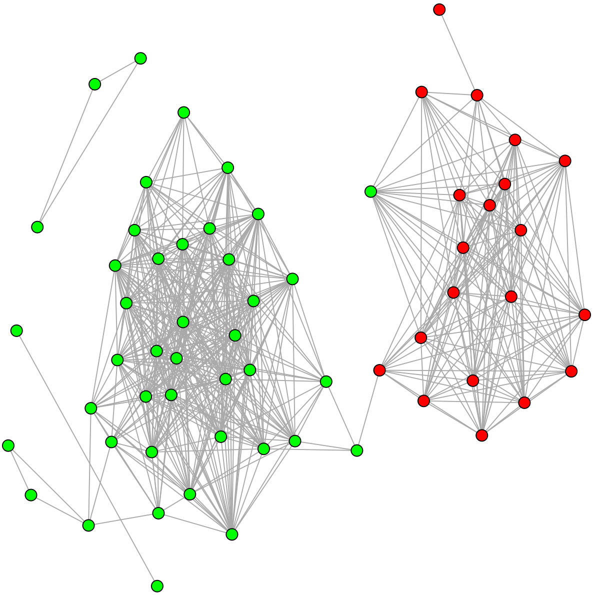


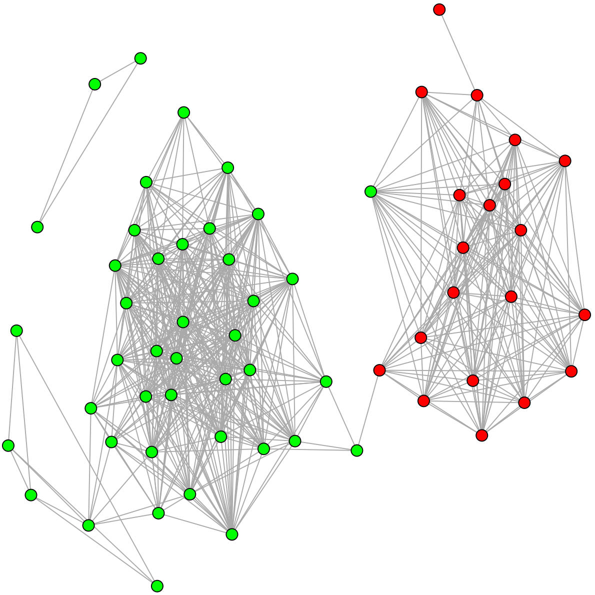


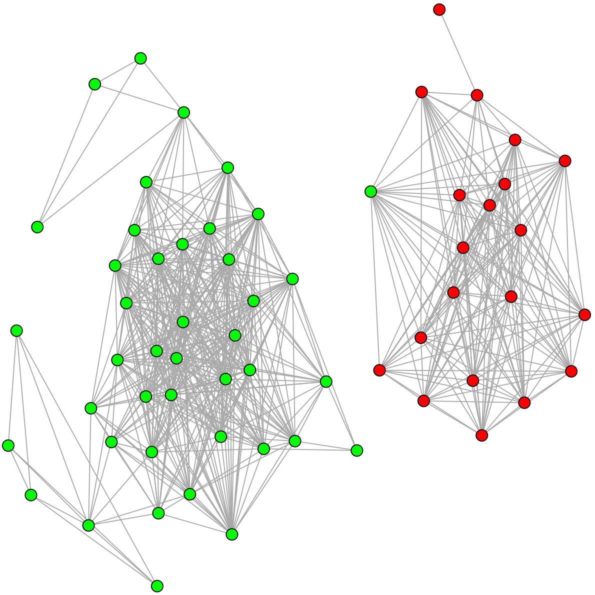


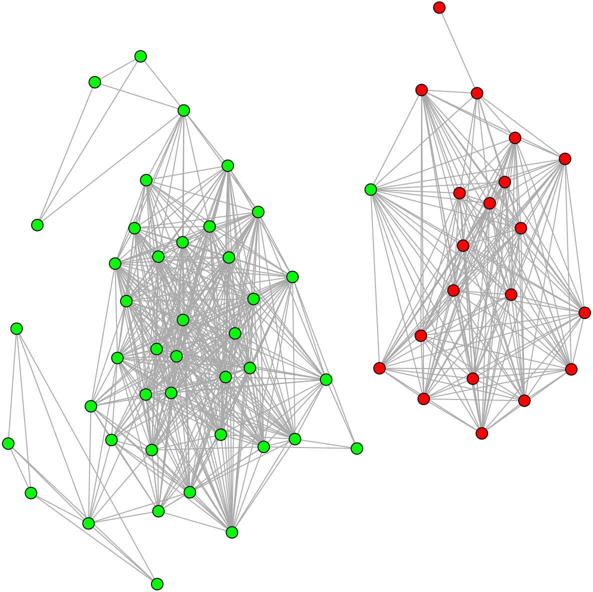


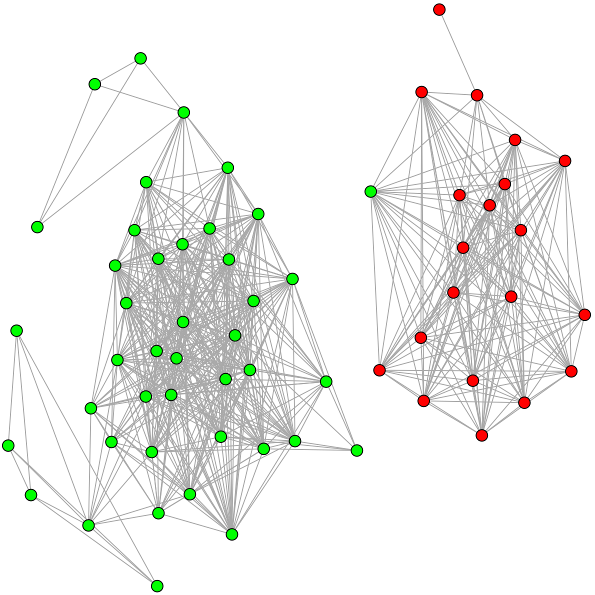


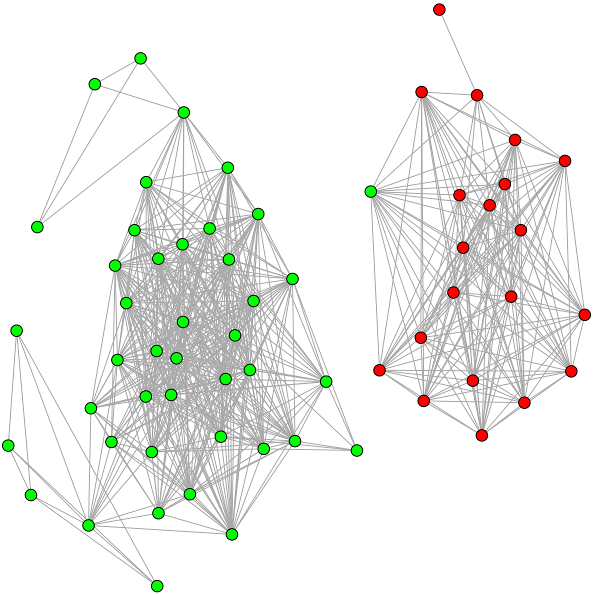


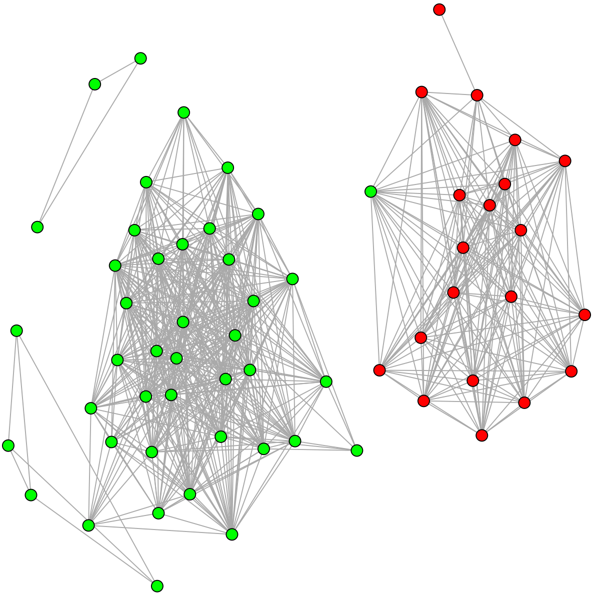


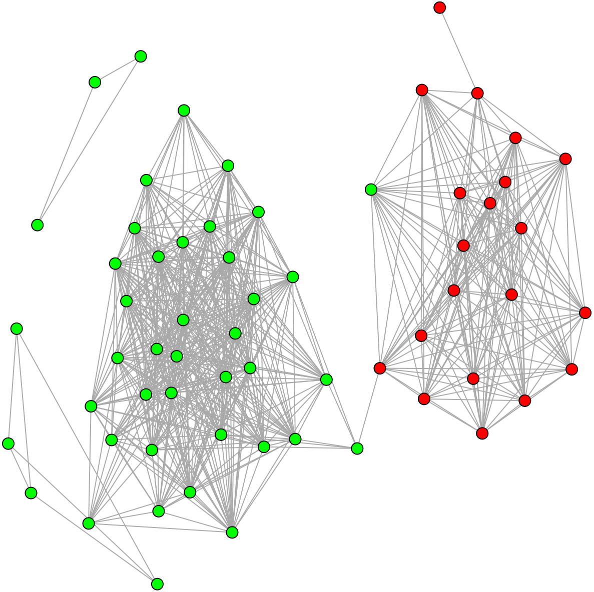


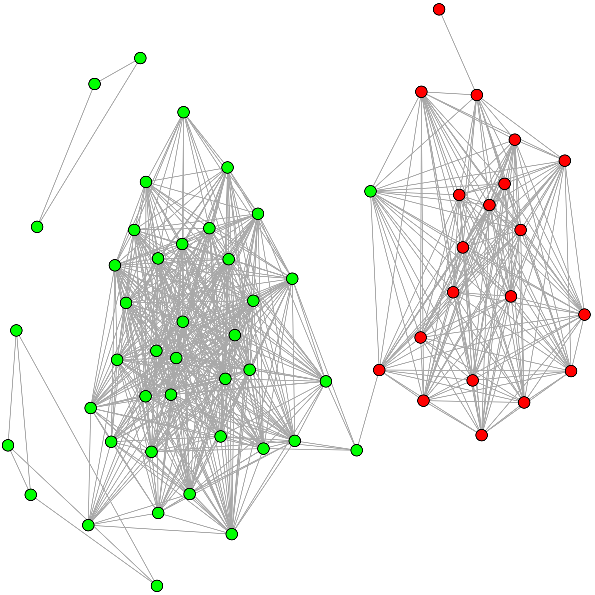


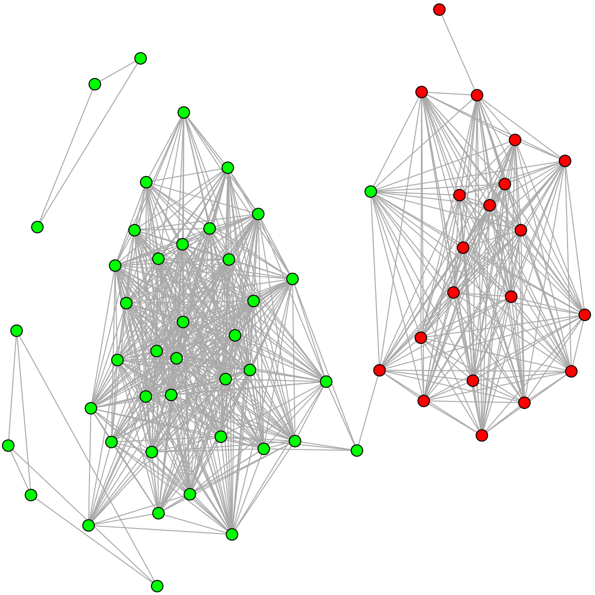


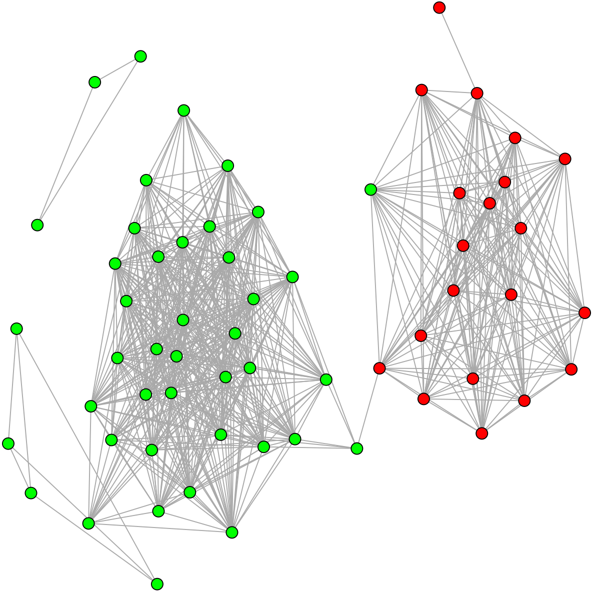


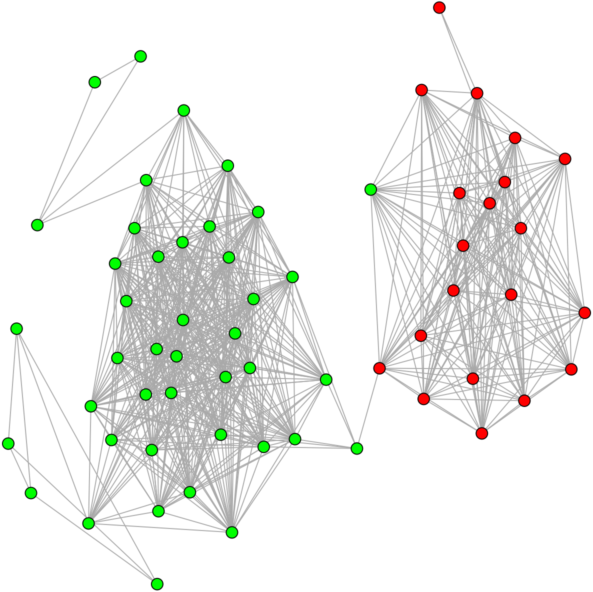


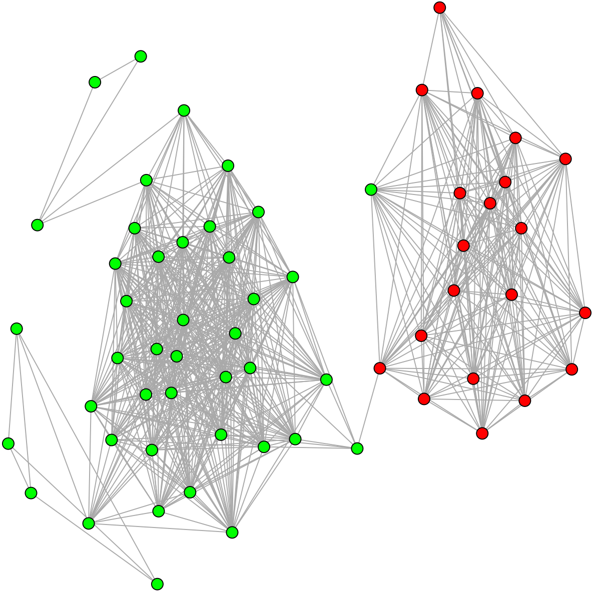


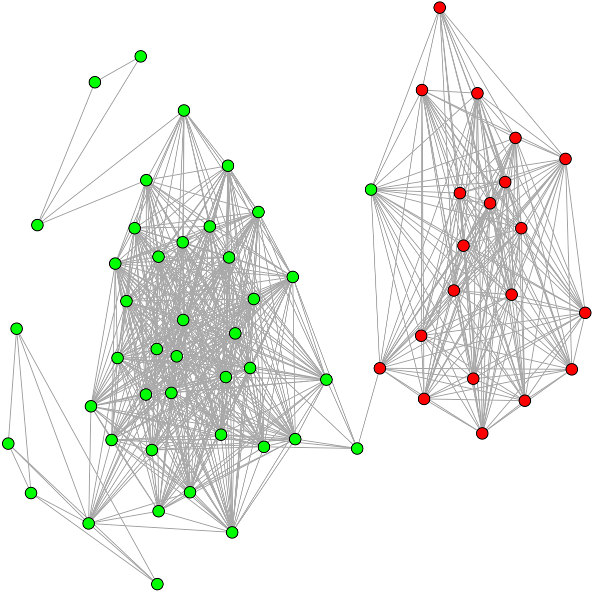


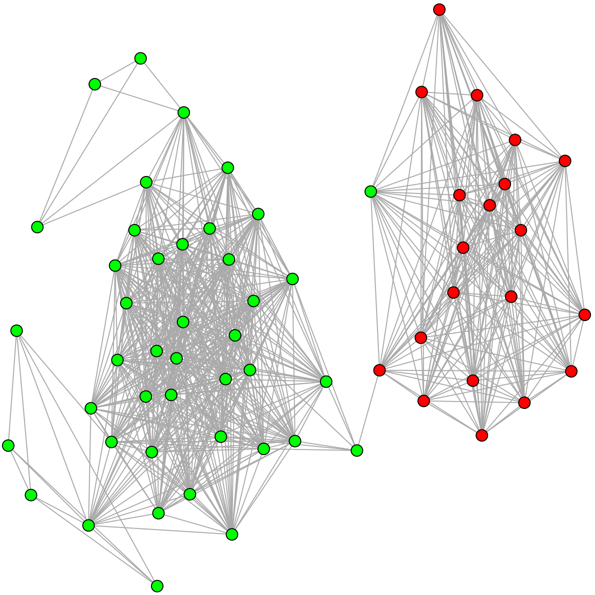


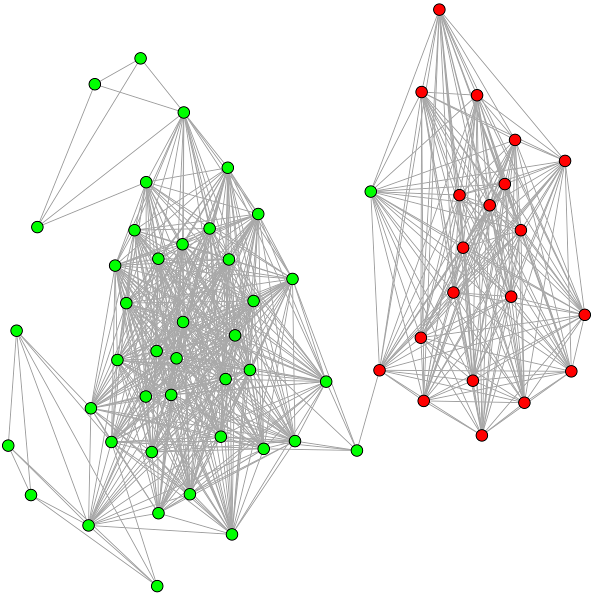


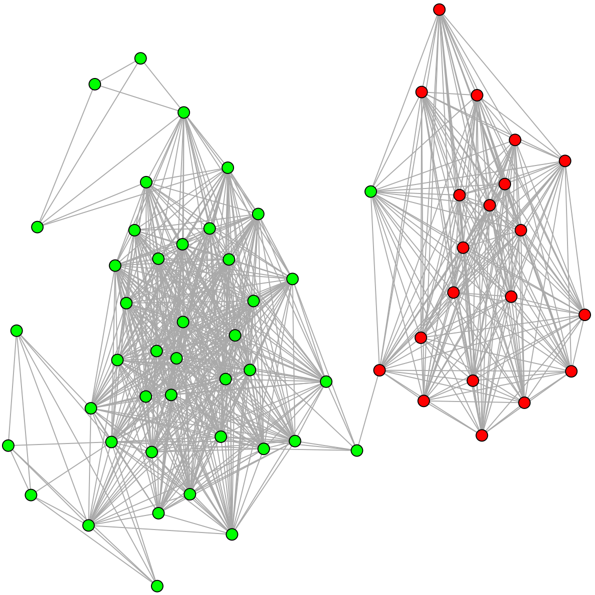


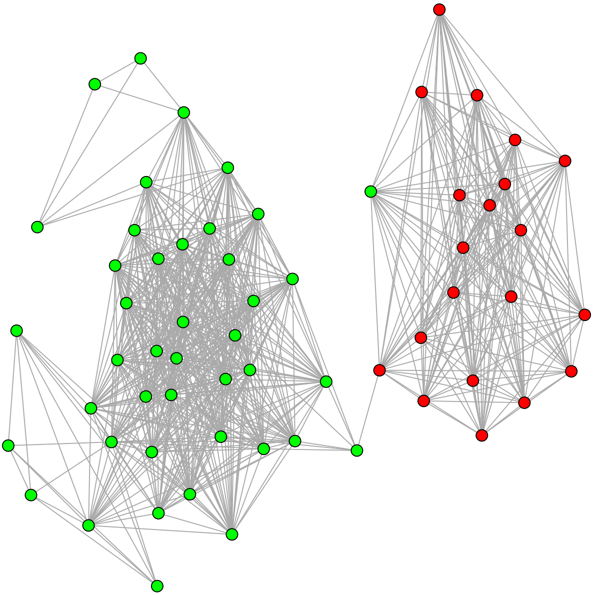


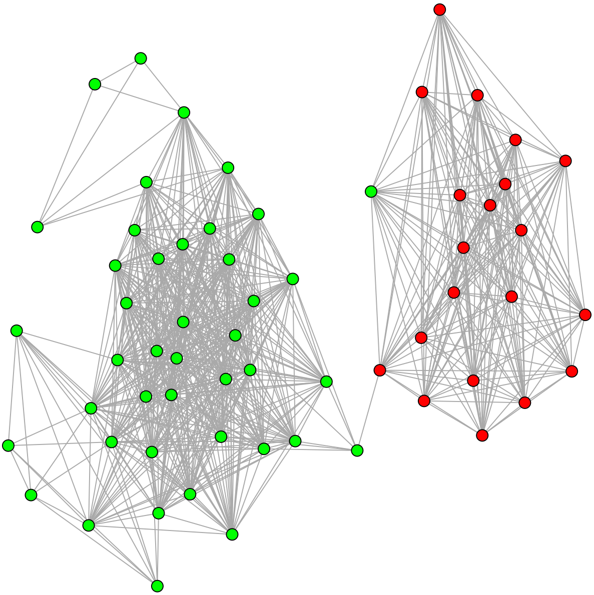


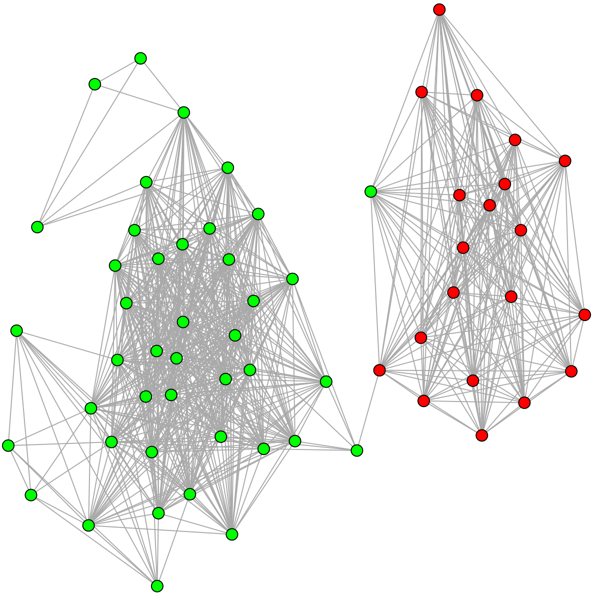






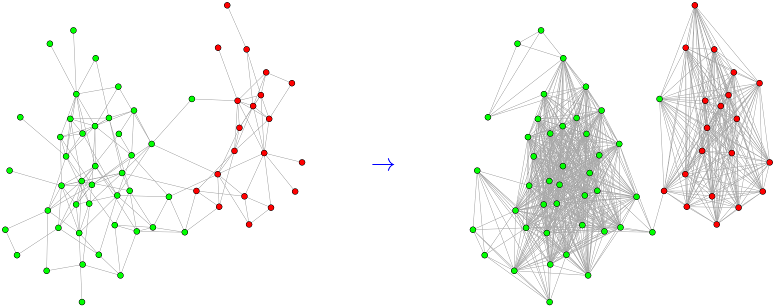






Performance of semidefinite relaxation

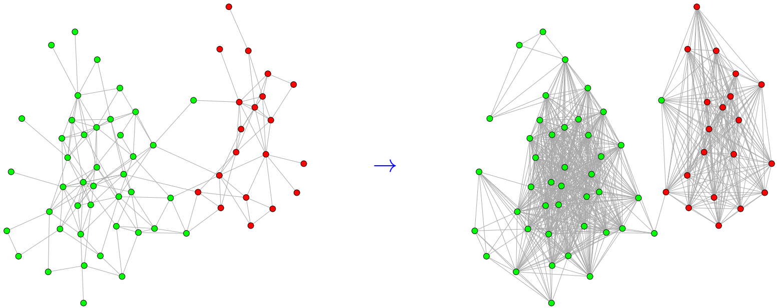
SDP enhances the latent structure of the network:



SDP *densifies* communities, *sparsifies* cuts across communities.

Performance of semidefinite relaxation

SDP enhances the latent structure of the network:



SDP *densifies* communities, *sparsifies* cuts across communities.

SDP did not know the number of communities in advance.
It decided that 2 communities should fit best.

Compressed sensing vs. networks

Compressed sensing

Signal: vector, matrix
Structure: sparsity, low rank
Measurements: random linear, few
Outliers: permitted in robust PCA
Exact recovery; exact thresholds
Recent blowup (2004+)

Structure recovery in networks

Signal: network model (p_{ij})
Structure: low rank, ??? (open)
Measurements: 0/1 random, few
Outliers: permitted (high/low degree vertices)
Exact recovery; exact thresholds
Recent blowup (2012+)