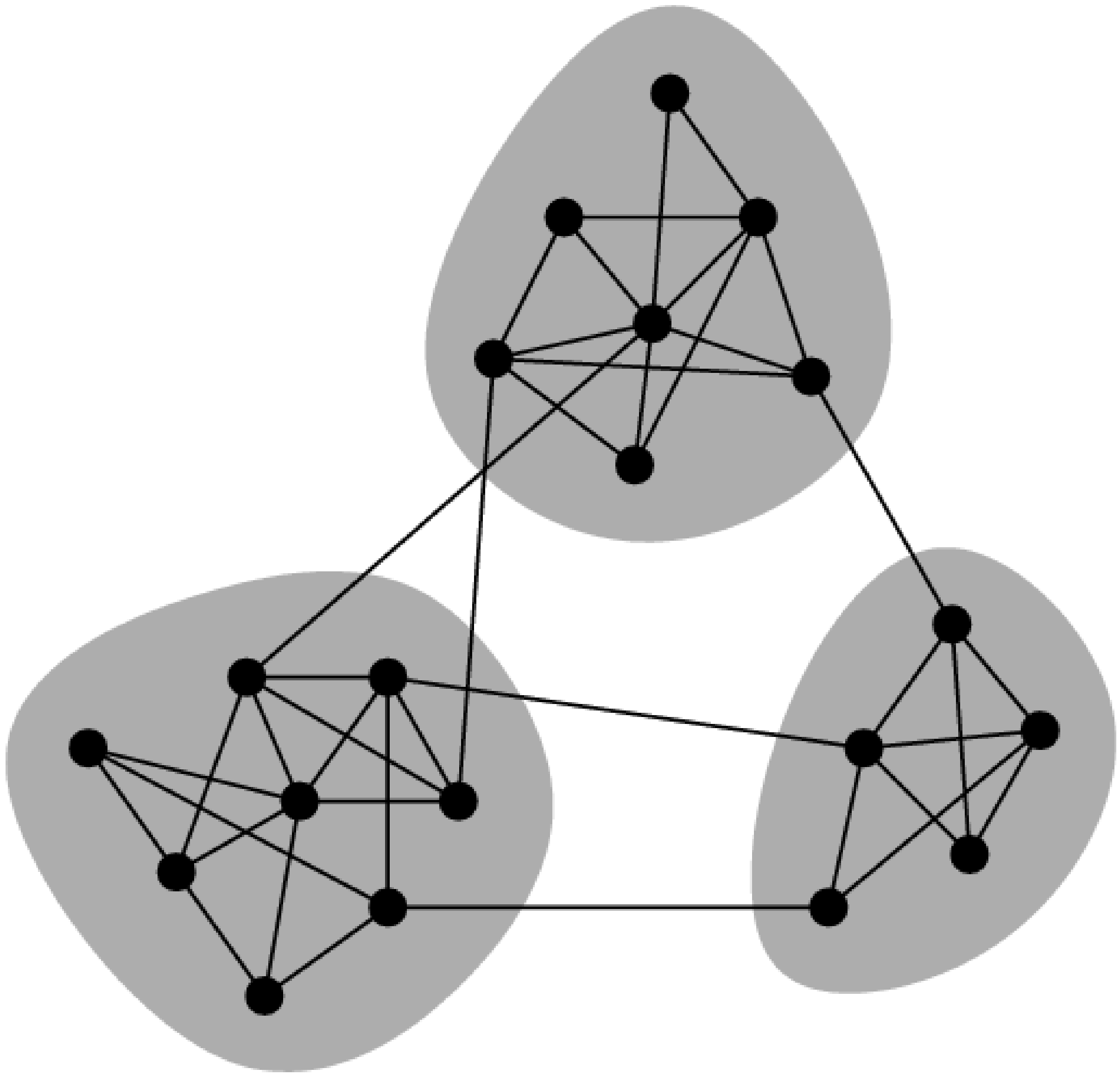
Detecting and Understanding the Large-Scale Structure of Networks

Mark Newman
University of Michigan

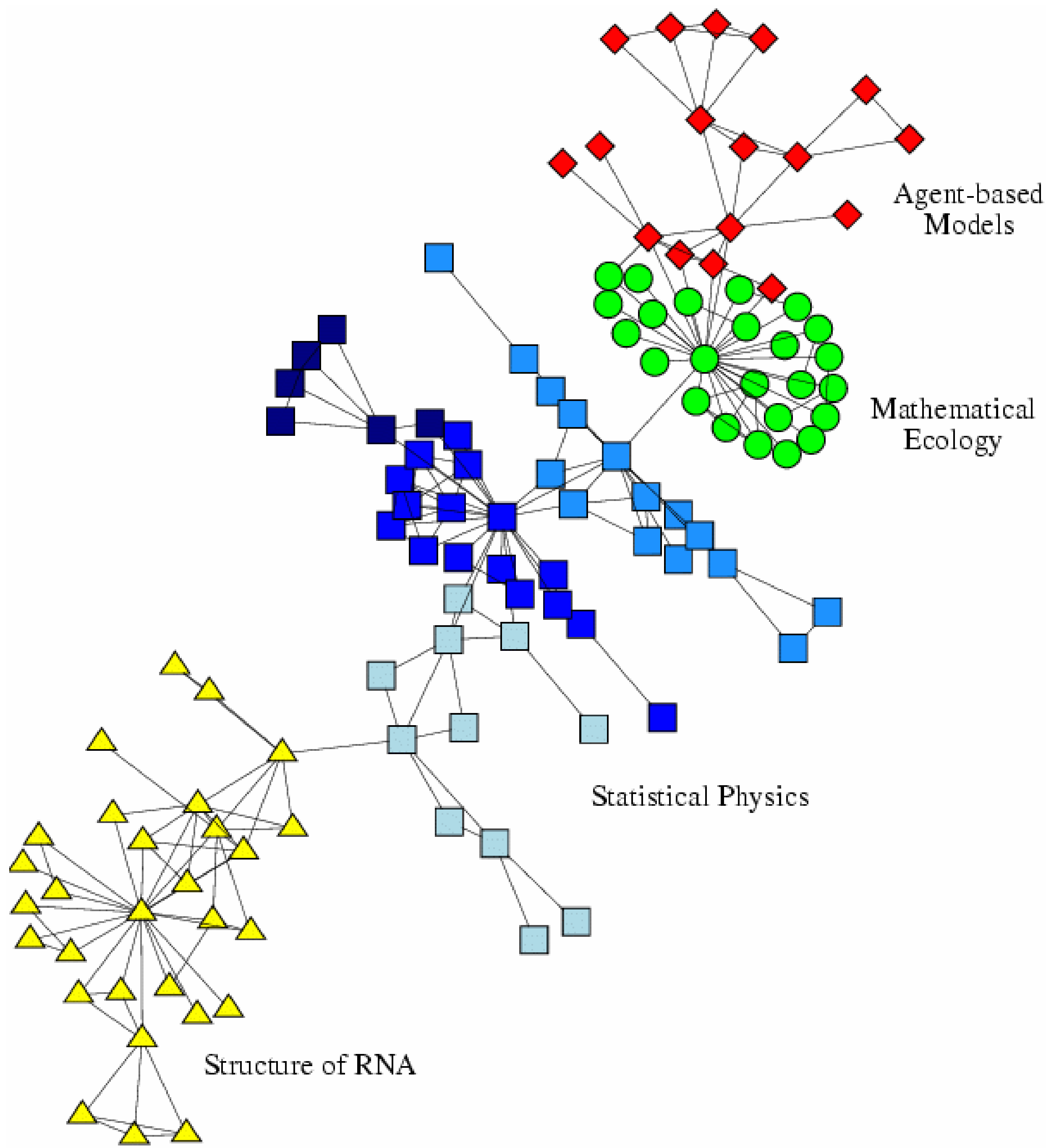
Michelle Girvan (Maryland)
Elizabeth Leicht (Michigan)

Modules, groups, or communities

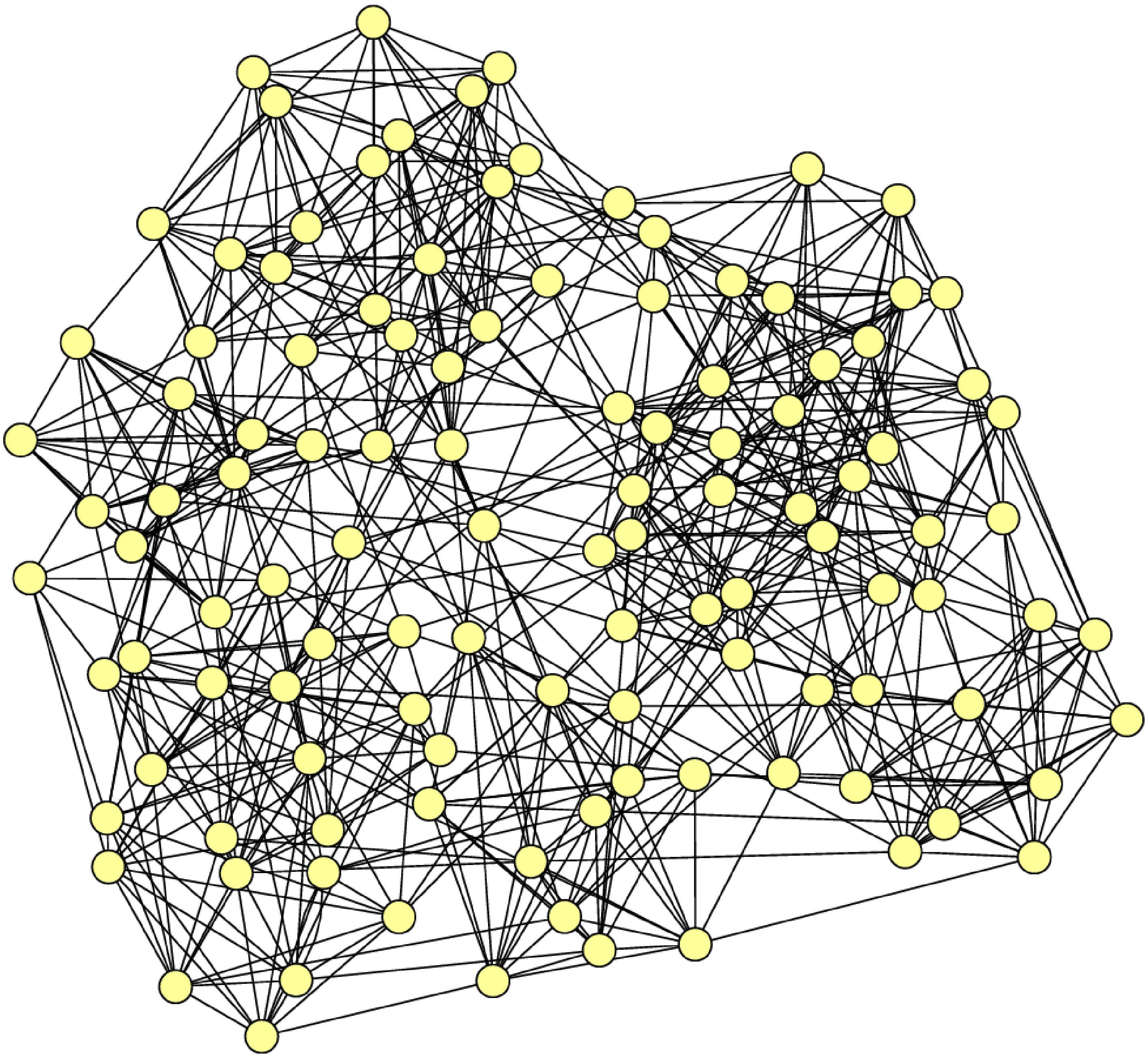


Modular structure

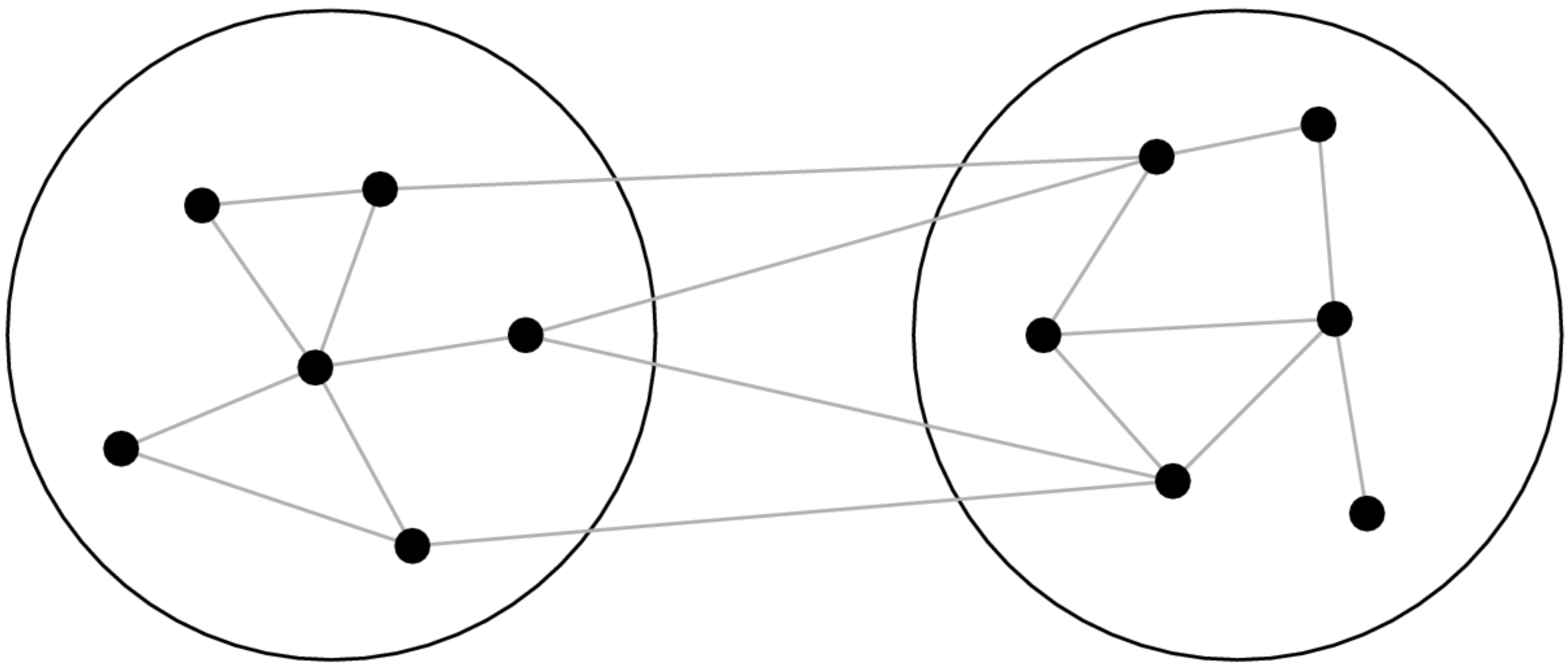
- Modules are of interest in many cases:
  - World Wide Web
  - Citation networks
  - Social networks
  - Metabolic networks
- Properties of modules may be quite different from average properties of a network



Agent-based Models
Mathematical Ecology
Statistical Physics
Structure of RNA



Graph partitioning



- Find the division into groups of given sizes that minimizes the *cut size*, i.e., the number of edges running between groups

Detecting modules

- Maximizing the number of edges within groups (or minimizing the number between groups) is not enough
- A good division into modules not just one with a large number of edges within groups, but one with a *larger than expected* number
- This leads us to the idea of *modularity*

Modularity

(Newman and Girvan 2004, Newman 2006)

Define modularity to be

$$Q = \text{(number of edges within groups)} - \text{(expected number within groups)}.$$

- Modularity is measured relative to a *null model*
  - Defined by P_{ij} = probability of an edge between vertices i and j
  - Examples:
    - ➔ $P_{ij} = p$ (Erdös-Rényi random graph)
    - ➔ $P_{ij} = k_i k_j / 2m$ ("configuration model")

Matrix formulation

Actual number of edges between *i* and *j* is

$$A_{ij} = \begin{cases} 1 & \text{if there is an edge } (i, j), \\ 0 & \text{otherwise.} \end{cases}$$

Expected number of edges is P_{ij}.

Modularity is sum of $A_{ij} - P_{ij}$ over all pairs of vertices (*i*,*j*) falling in the same group

Define:

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

$$
\begin{aligned}
Q &= \frac{1}{2m}\sum_{ij}[A_{ij} - P_{ij}]\,\delta(g_i, g_j) \\
&= \frac{1}{4m}\sum_{ij}[A_{ij} - P_{ij}](s_i s_j + 1) \\
&= \frac{1}{4m}\sum_{ij}[A_{ij} - P_{ij}]s_i s_j \\
&= \frac{1}{4m}\,\mathbf{s}^T\mathbf{B}\mathbf{s}
\end{aligned}
$$

where $B_{ij} = A_{ij} - P_{ij}$

We call **B** the modularity matrix

- Now we write **s** as a linear combination of the eigenvectors $\mathbf{u}_i$ of the modularity matrix:

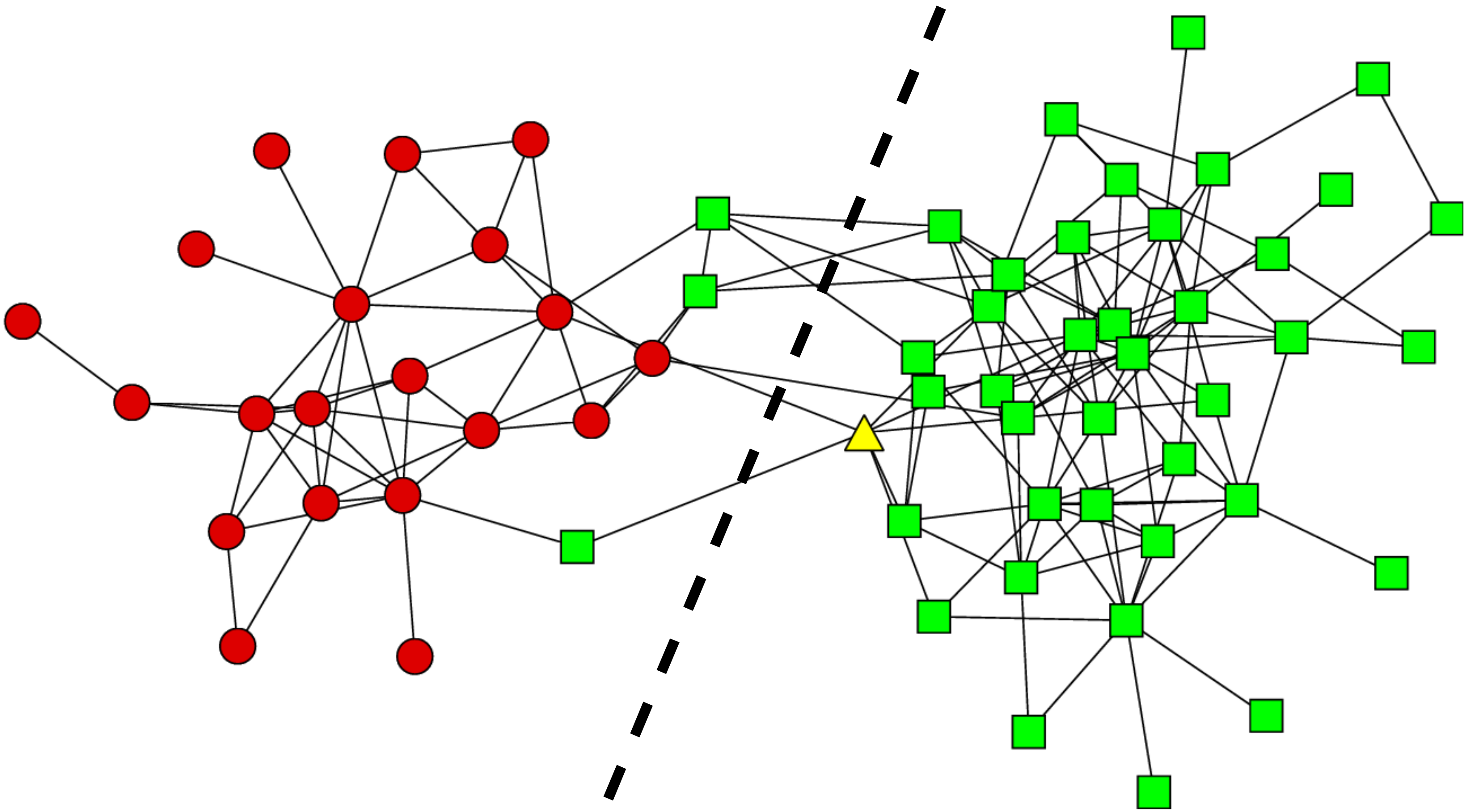
$$\mathbf{s} = \sum_{i=1}^{n} a_i \mathbf{u}_i, \qquad \text{with} \quad a_i = \mathbf{u}_i^T \mathbf{s}$$

$$Q = \frac{1}{4m} \mathbf{s}^T \mathbf{B} \mathbf{s} = \frac{1}{4m} \sum_i a_i^2 \beta_i$$

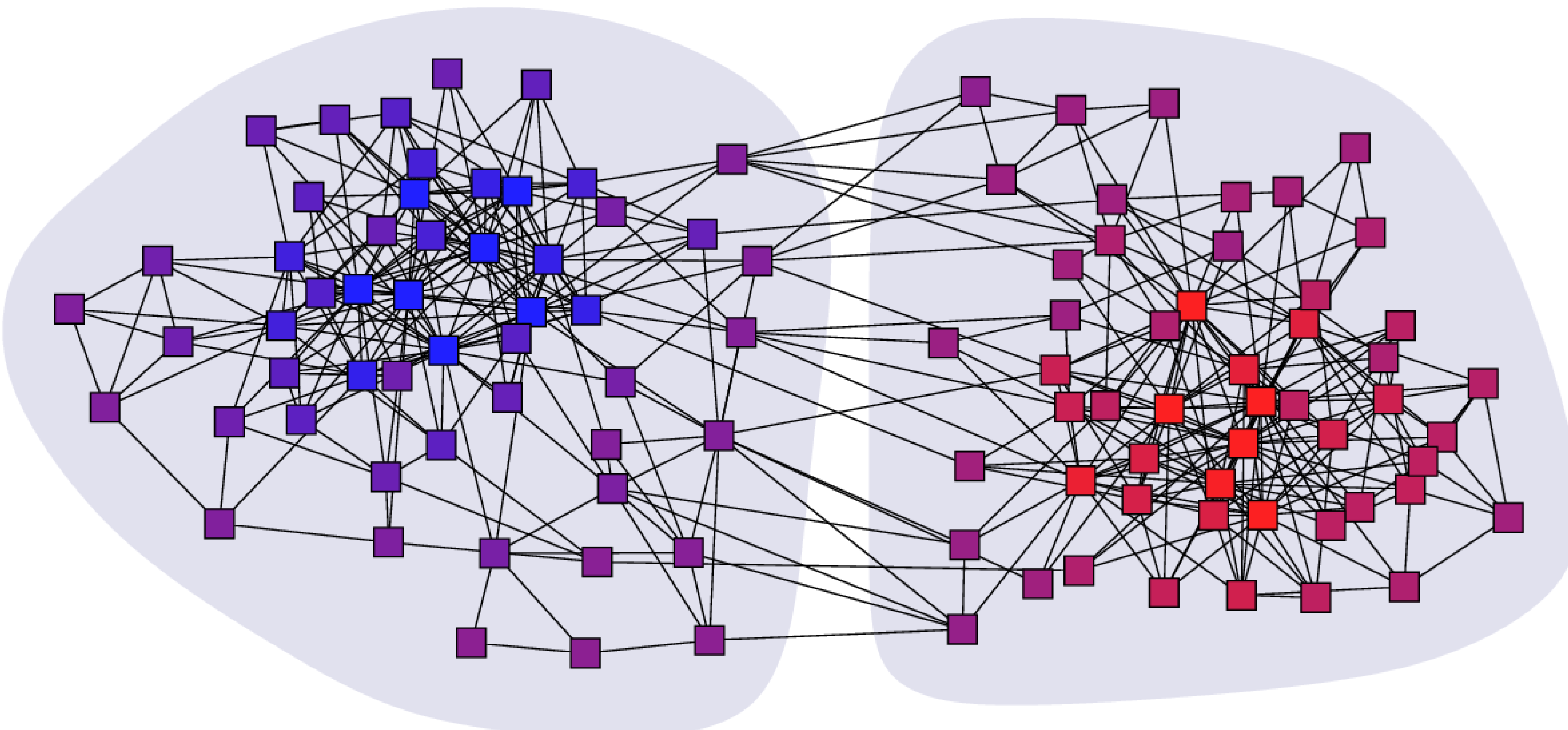
- Maximize by choosing **s** parallel to the leading eigenvector, or failing that, as near parallel as we can

$$s_i = \begin{cases} +1 & \text{if } u_i^{(1)} \geq 0, \\ -1 & \text{if } u_i^{(1)} < 0. \end{cases}$$

Example: animal network



Books about politics



Spectral properties of modularity matrix

- Vector (1, 1, 1, . . .) is always an eigenvector of **B** with eigenvalue zero, corresponding to all vertices in the same group
- Eigenvalues can be either positive or negative
  - So long as there is *any* positive eigenvalue we will never put all vertices in the same group
- But there may be no positive eigenvalues
  - All vertices in same group gives highest modularity
  - We call such networks *indivisible*

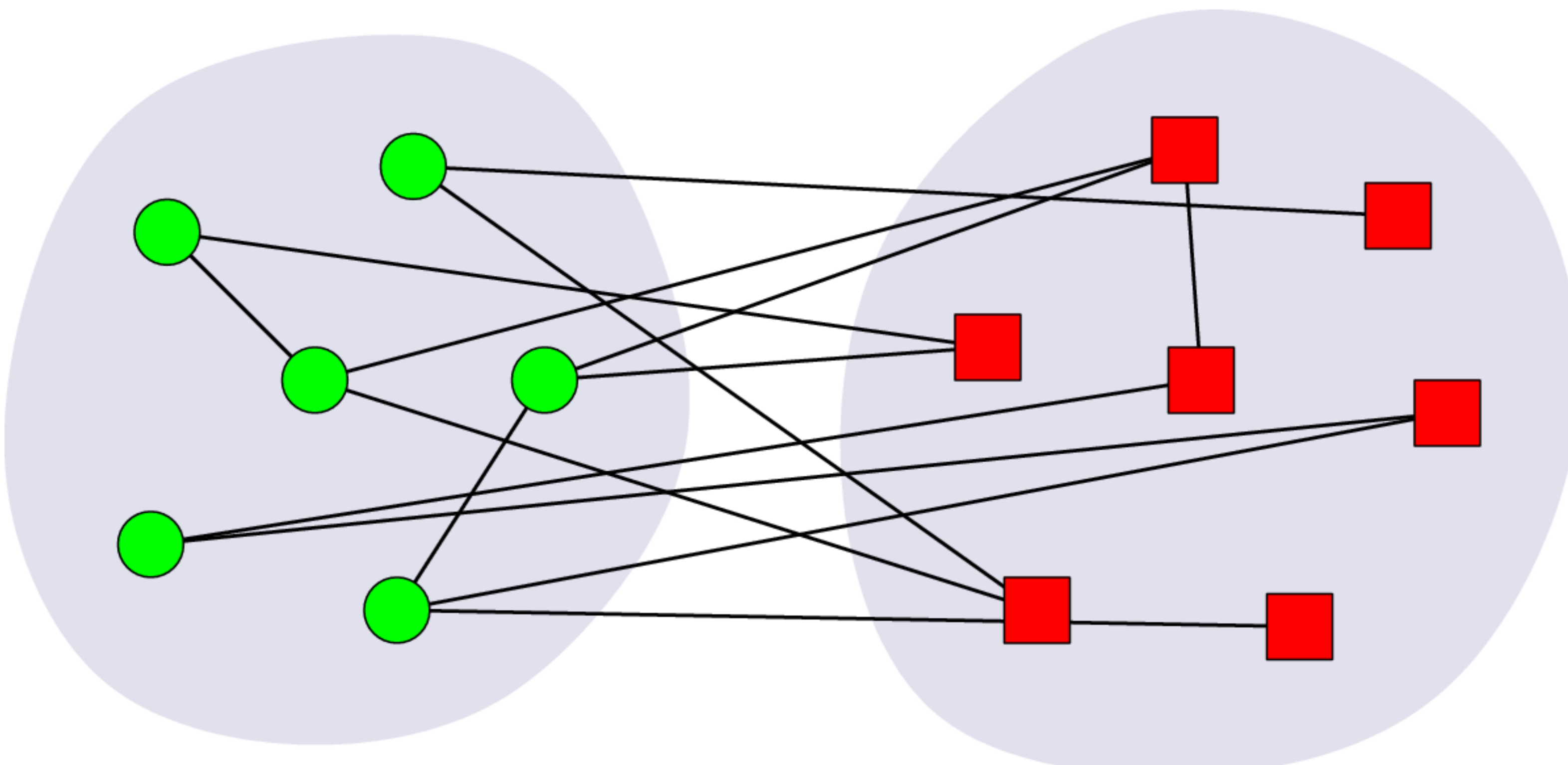
Dividing into more than two groups

- Simplest approach is repeated division into two groups
  - Divide in two, then divide those parts in two, etc.
- Stop when there is no division that will increase the modularity
  - But this is precisely when the subgraph is indivisible
  - Stop when there are no positive eigenvalues of the modularity matrix

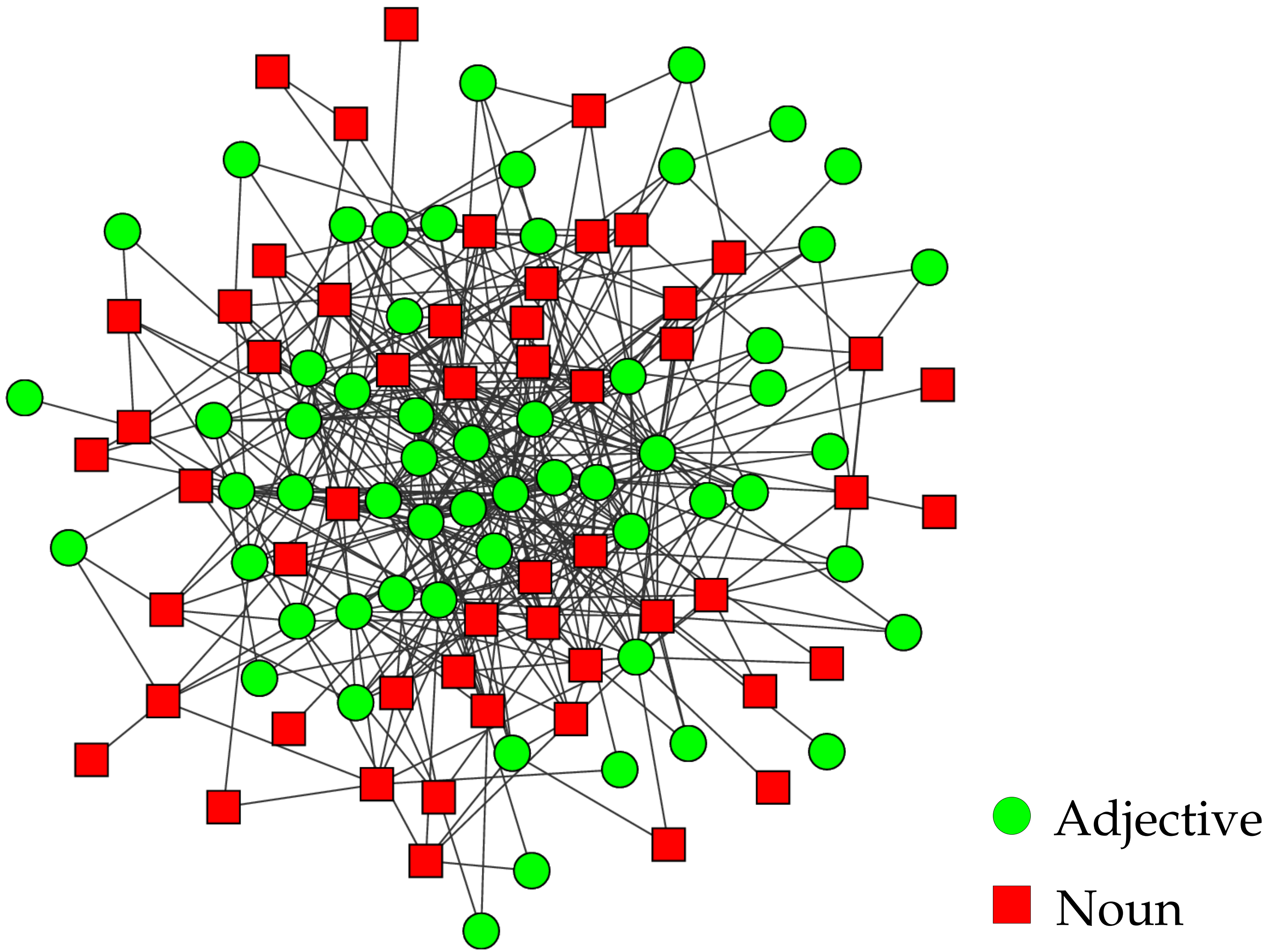
Negative eigenvalues

- Unlike the Laplacian, the modularity matrix has negative eigenvalues
- These tell us about *minimization* of the modularity
- A division with negative modularity has *fewer* edges than expected within communities (or more than expected between communities)

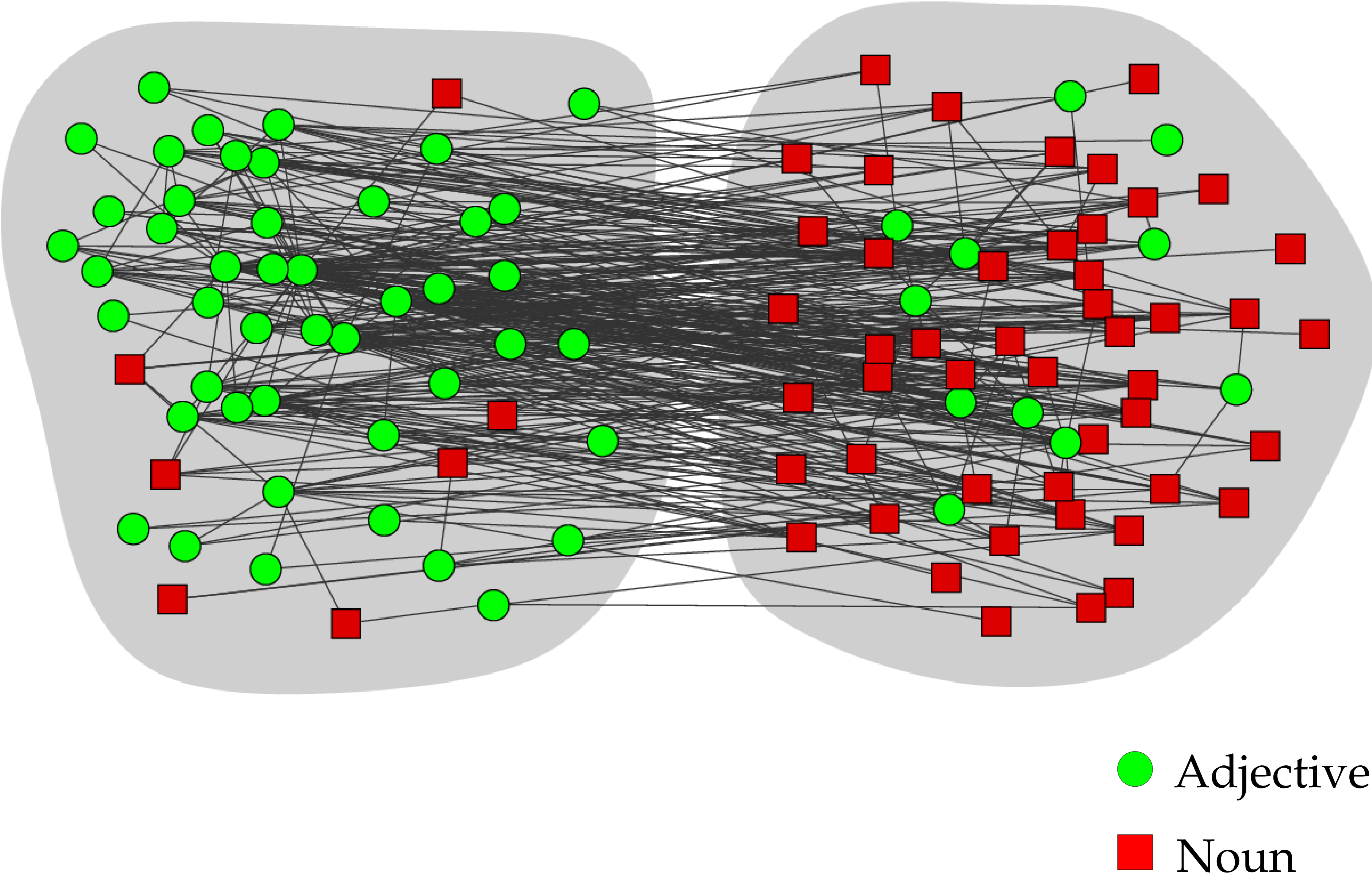
- This corresponds to a network with bipartite structure
- Or *k*-partite in the general case



Network of word adjacencies



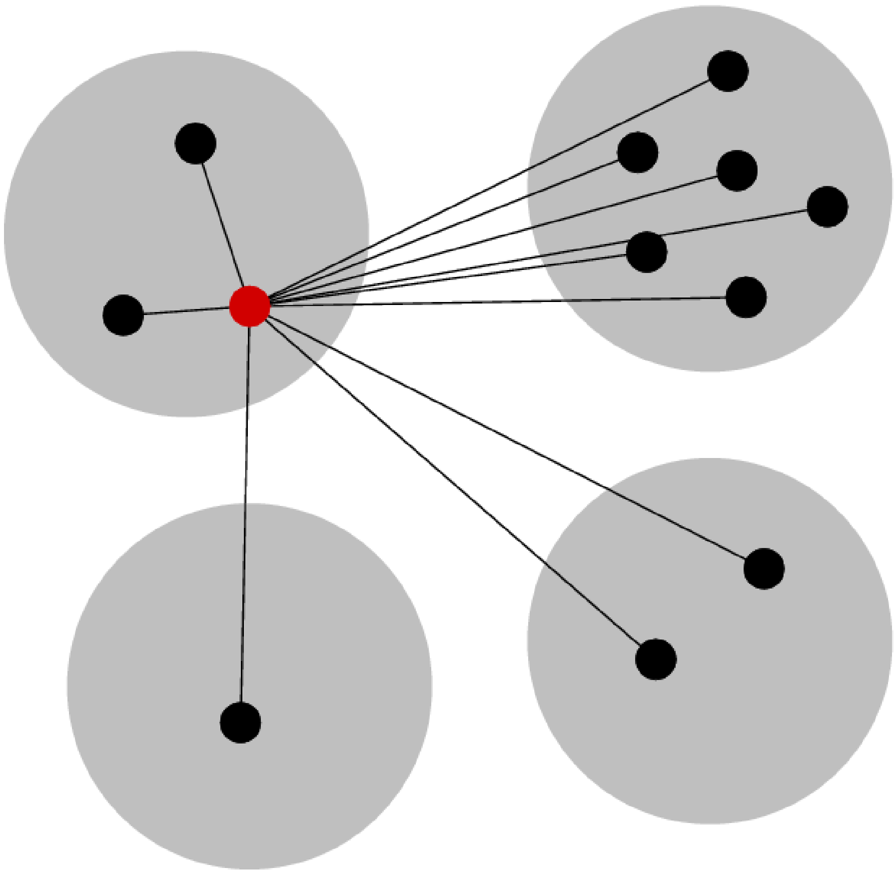
Network of word adjacencies



Vertex classification

(Newman and Leicht 2007)

- We specify a very broad set of possible structures that we are interested in:



Definition of the model

- There are three kinds of quantities in this approach:
  - Observed data: the pattern of edges observed between the vertices. These are given to us by the experimenter.
  - Missing data: We assume that the vertices divide into c groups. We denote the group to which vertex i belongs by g_i. These are missing data.
  - Model parameters: these describe the patterns of connection between vertices in different groups.

Definition of the model

Directed case:

$$\pi_r = \text{probability of being in group } r$$

and

$$\theta_{ri} = \text{probability of a link to vertex } i$$

These satisfy

$$\sum_{r=1}^{c} \pi_r = 1, \qquad \sum_{i=1}^{n} \theta_{ri} = 1.$$

Likelihood and log-likelihood

- The likelihood is

$$\Pr(A, g|\pi, \theta) = \Pr(A|g, \pi, \theta) \Pr(g|\pi, \theta)$$

- Here

$$\Pr(A|g, \pi, \theta) = \prod_{ij} \theta_{g_i,j}^{A_{ij}}, \quad \Pr(g|\pi, \theta) = \prod_i \pi_{g_i}$$

- So

$$\Pr(A, g|\pi, \theta) = \prod_i \left[\pi_{g_i} \prod_j \theta_{g_i,j}^{A_{ij}} \right]$$

$$\mathcal{L} = \ln \Pr(A, g|\pi, \theta) = \sum_i \left[\ln \pi_{g_i} + \sum_j A_{ij} \ln \theta_{g_i,j} \right]$$

- Unfortunately, we don't know the values of the missing data, so we can't evaluate this expression
- However, we can make a pretty good guess at the values of the missing data if we know A, π, and θ. More specifically, we can calculate the probability that g_i takes a particular value r thus:

$$q_{ir} = \Pr(g_i = r | A, \pi, \theta) = \frac{\Pr(A, g_i = r | \pi, \theta)}{\Pr(A | \pi, \theta)}.$$

- The numerator we can calculate by summing $\Pr(A,g | \pi,\theta)$ over all the gs except g_i
- The denominator is fixed by the normalization

- The result is:

$$q_{ir} = \frac{\pi_r \prod_j \theta_{rj}^{A_{ij}}}{\sum_s \pi_s \prod_j \theta_{sj}^{A_{ij}}}.$$

- This looks odd: we're saying you can calculate q_{ir} given the model and the data, and then we're going to calculate the model from q_{ir} and the data?

- Yes, but we have to do it self-consistently. . .

Expected likelihood

- We can now make a guess about the value of the log-likelihood. Our best guess is just the expectation value:

$$
\begin{aligned}
\overline{\mathcal{L}} &= \sum_{g_1=1}^{c} \ldots \sum_{g_n=1}^{c} \Pr(g|A,\pi,\theta) \sum_i \Big[\ln \pi_{g_i} + \sum_j A_{ij} \ln \theta_{g_i,j} \Big] \\
&= \sum_{ir} \Pr(g_i = r|A,\pi,\theta) \Big[\ln \pi_r + \sum_j A_{ij} \ln \theta_{rj} \Big] \\
&= \sum_{ir} q_{ir} \Big[\ln \pi_r + \sum_j A_{ij} \ln \theta_{rj} \Big].
\end{aligned}
$$

- Now it's a straightforward matter to maximize this with respect to π and θ to find the best values. The result is:

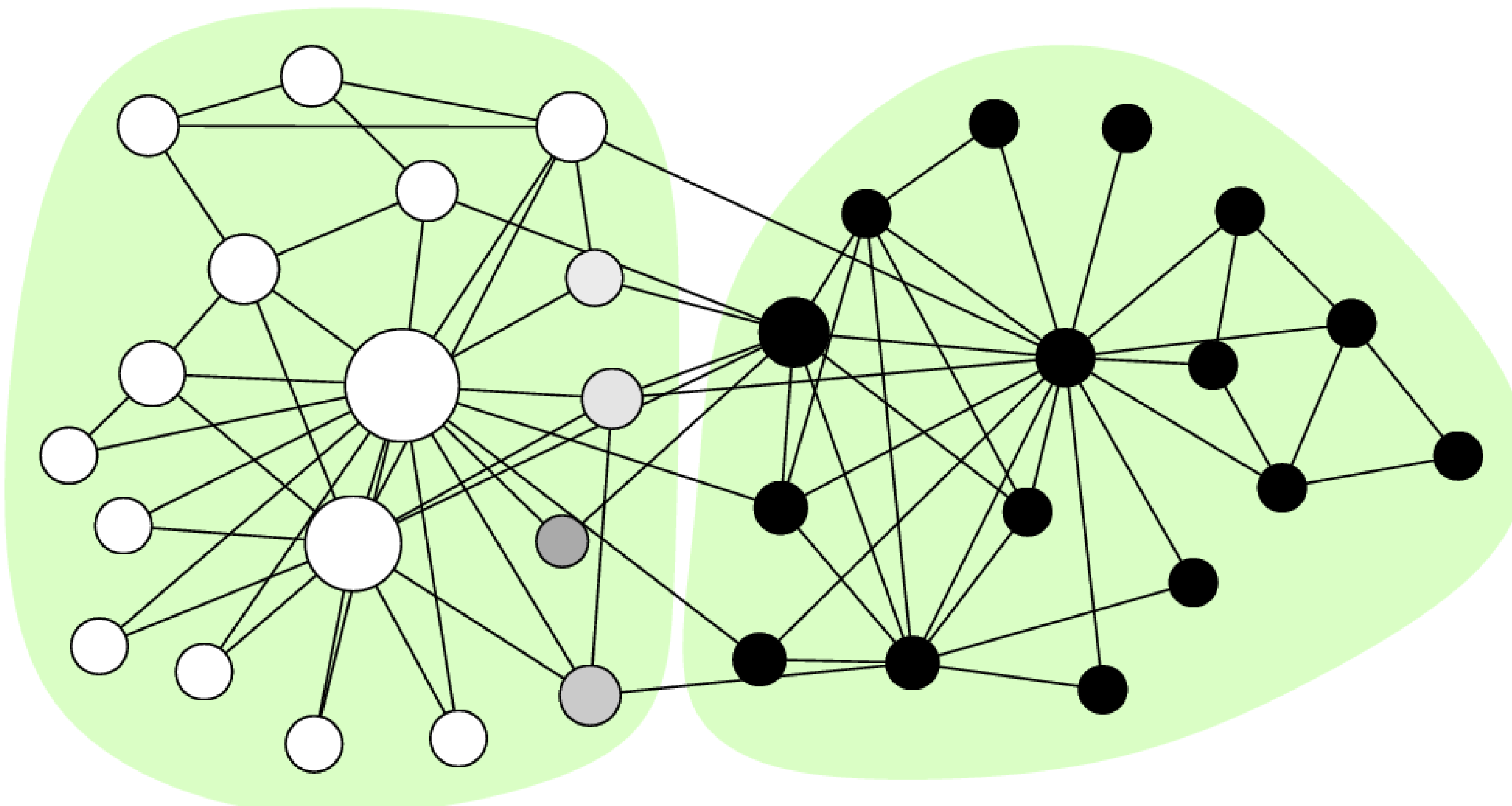
$$\pi_r = \frac{1}{n}\sum_i q_{ir}, \qquad \theta_{rj} = \frac{\sum_i A_{ij} q_{ir}}{\sum_i k_i q_{ir}},$$

- So we have π and θ in terms of q and we have q in terms of π and θ
- To find a self-consistent solution to both sets of equations, we iterate from a suitable set of starting values

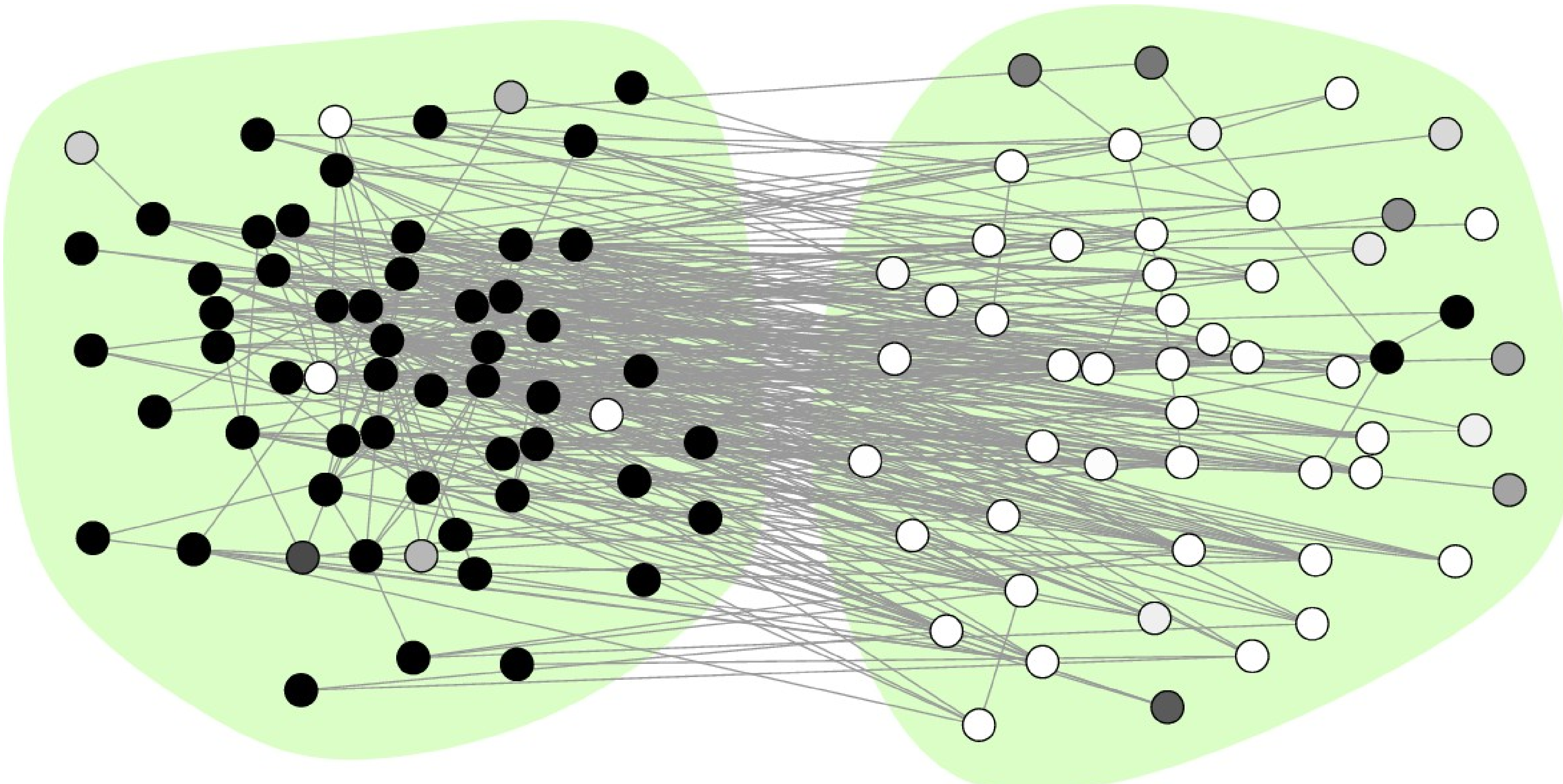
Expectation-Maximization Algorithm

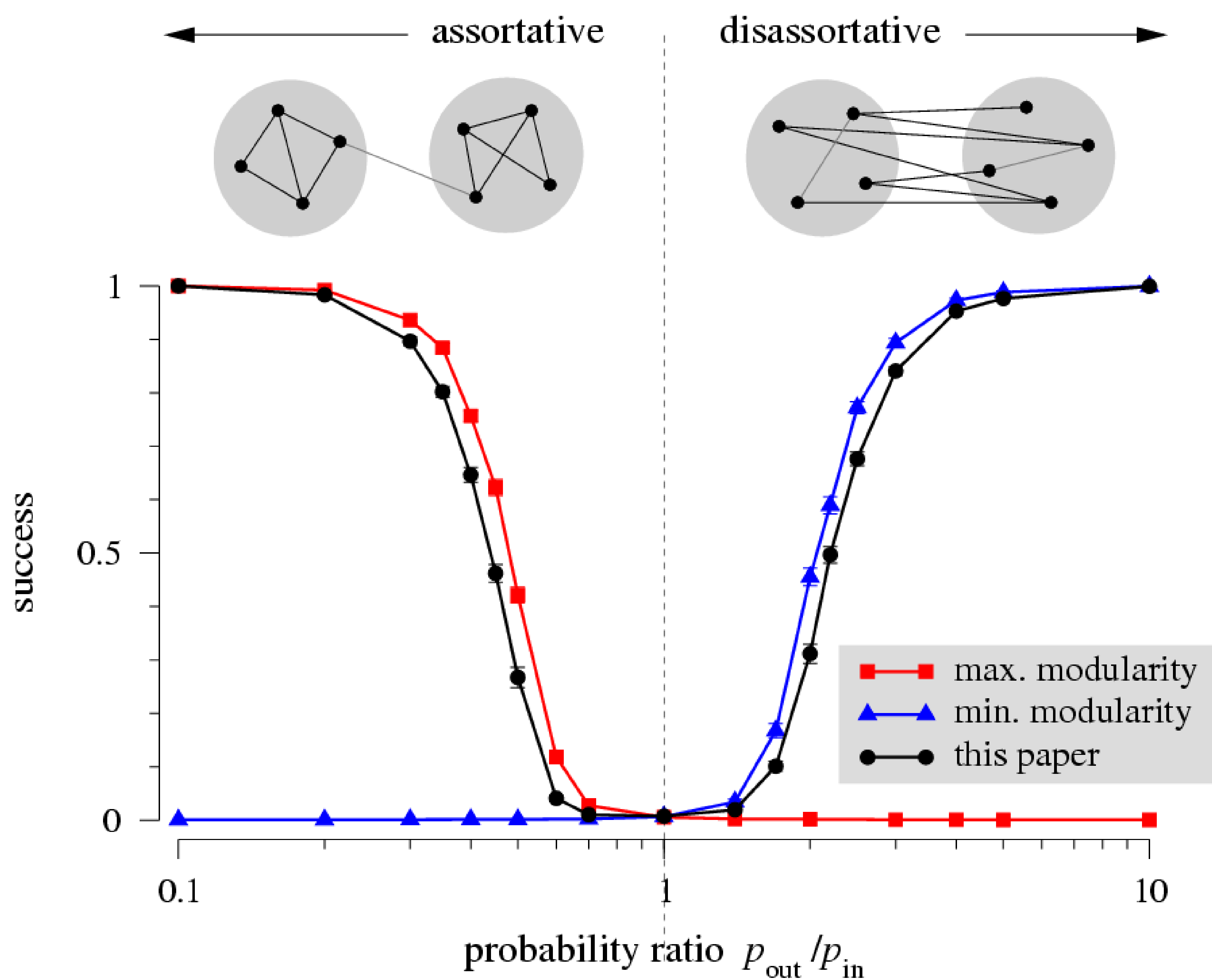
- Has a number of clear advantages:
  - Very simple: just a few lines of computer code to implement the method
  - Fast: typically only a few seconds to analyze even a large network
  - Simultaneously tells us how to group the vertices in the network and what the appropriate definition is for the groups
- Derivation is more complicated for undirected case, but the final equations are exactly the same

Example: Social network

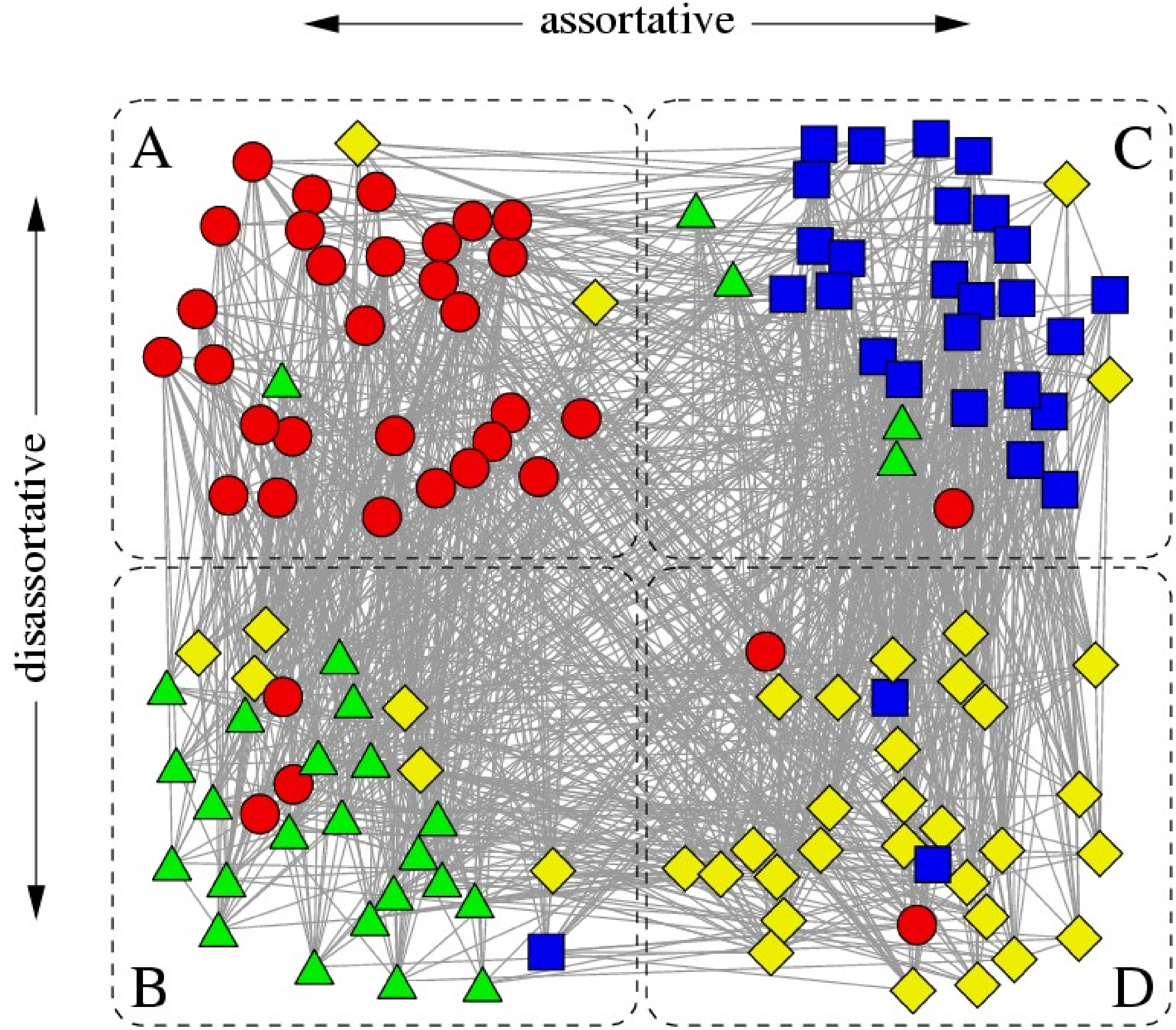


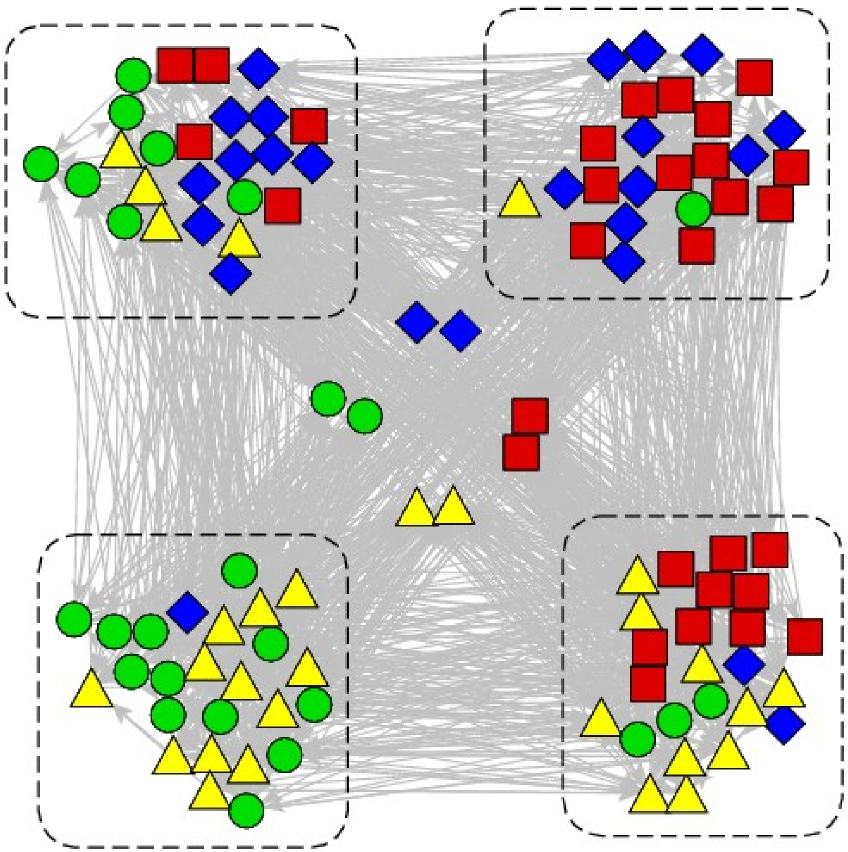
Example: Lexical network



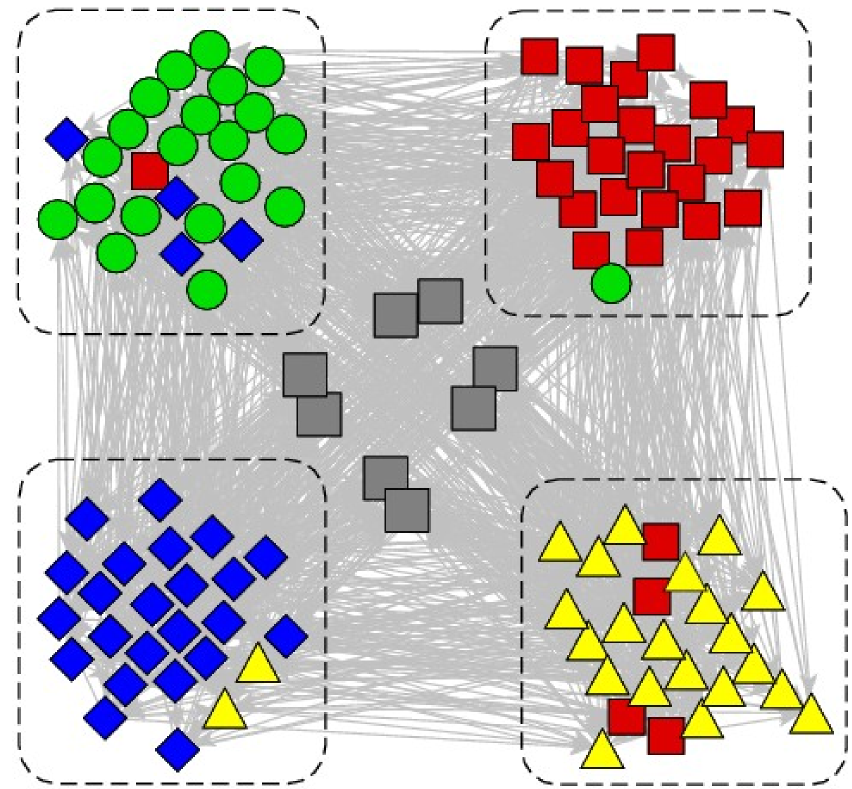


assortative
disassortative
1
0.5
0
success
0.1
1
10
probability ratio p_{out}/p_{in}
max. modularity
min. modularity
this paper


assortative
disassortative
A
B
C
D



Ordinary community detection



EM algorithm

- References:
  - See: http://www.umich.edu/~mejn/pubs.html

  - M. E. J. Newman and E. A. Leicht, *Proc. Natl. Acad. Sci.* (in press)
  - M. E. J. Newman, *Proc. Natl. Acad. Sci.* **103**, 8577-8582 (2006)
  - M. E. J. Newman, *Phys. Rev. E* **74**, 036104 (2006)
  - M. E. J. Newman and M. Girvan, *Phys. Rev E* **69**, 026113 (2004)
  - M. E. J. Newman, *Phys. Rev. E* **67**, 026126 (2003)
