

Exponential Random Graph Models for Network Data

David Hunter

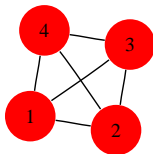
Department of Statistics
Penn State University

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Outline

- 1 **Statistical Models for Networks**
 - What's a network?
 - What's an ERGM?
- 2 **Difficulties of fitting the ERGM**
 - Why MLE is difficult
 - Change Statistics and Maximum Pseudolikelihood
- 3 **Favored Approach: Approximate MLE via MCMC**
 - Law of Large Numbers to the Rescue
 - Obtaining samples via MCMC
 - A Numerical Example

What is a network?

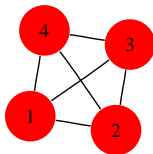


Definition

A representation of "relational data" in the form of a mathematical graph: A set of nodes along with a set of edges connecting some pairs of nodes.

- Edges can have directions and/or values. . .
. . . but for now, we'll assume undirected, binary (either on or off) edges.
- Notation: A symmetric matrix x of 0's and 1's.

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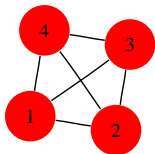
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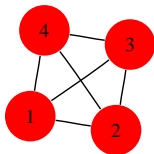


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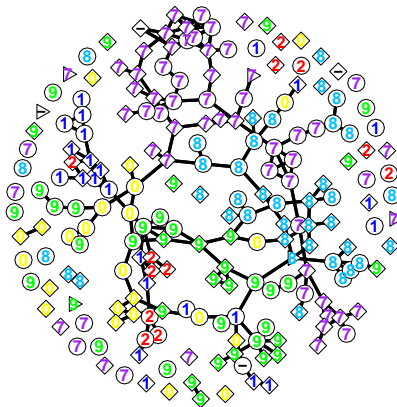
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Example Network: High School Friendship Data

School 10: 205 Students



- An edge indicates a mutual friendship.
- Colored labels give grade level, 7 through 12.
- Circles = female, squares = male, triangles = unknown.

Why study networks?

Many applications, including

- Epidemiology: Dynamics of disease spread
- Business: Viral marketing, word of mouth
- Telecommunications: WWW connectivity, phone calls
- Counterterrorism: Robustifying/attacking networks
- Political Science: Coalition formation dynamics
- ...

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What is an ERGM?

Exponential Random Graph Model (ERGM)

$$P_{\theta}(X = x) \propto \exp\{\theta^t s(x)\}$$

or

$$P_{\theta}(X = x) = \frac{\exp\{\theta^t s(x)\}}{c(\theta)},$$

where

- X is a random network on n nodes (a matrix of 0's and 1's)
- θ is a vector of parameters
- $s(x)$ is a known vector of graph statistics on x

Whence the name ERGM?

Exponential Family

Whenever the density of a random variable may be written

$$f(x) \propto \exp\{\theta^t s(x)\},$$

the family of all such random variables (for all possible θ) is called an **exponential family**.

- Since the random graphs in our model form an exponential family, we call the model an **exponential random graph model**.
- “ERGM” is easier to pronounce than “EFRGM”!

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Maximum Likelihood Estimation

The model:

$$P_{\theta}(X = x) = \frac{\exp\{\theta^t s(x)\}}{c(\theta)}, \text{ where } s(x^{\text{obs}}) = 0$$

- It follows that $c(\theta)$ is a normalizing “constant”:

$$c(\theta) = \sum_{\substack{\text{all possible} \\ \text{graphs } y}} \exp\{\theta^t s(y)\}.$$

- Replacing $s(x)$ by $s(x) - s(x^{\text{obs}})$ leaves $P_{\theta}(X = x)$ unchanged; thus, we “recenter” $s(x)$ so that $s(x^{\text{obs}}) = 0$.

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- The loglikelihood function is

$$\ell(\theta) = -\log c(\theta) = \log \sum_{\text{all possible graphs } y} \exp\{\theta^t s(y)\}.$$

- Merely evaluating (let alone maximizing) $\ell(\theta)$ is somewhat computationally burdensome. . .

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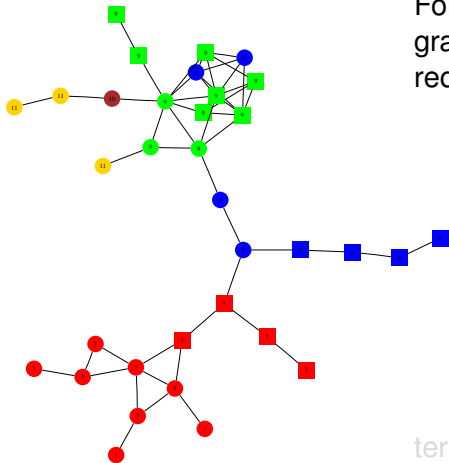
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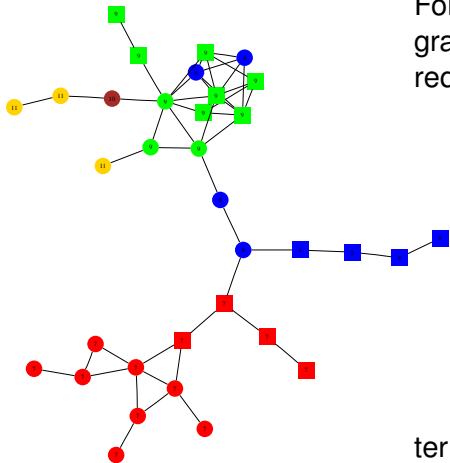


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Conditional log-odds of an edge

Notation: For a network x and a pair (i, j) of nodes,

- $x_{ij} = 0$ or 1 , depending on whether there is an edge
- x_{ij}^c denotes the status of all pairs in x other than (i, j)
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Let's calculate the ratio of the two respective probabilities:

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$$\frac{P(X_{ij} = 1 | X_{ij}^c = x_{ij}^c)}{P(X_{ij} = 0 | X_{ij}^c = x_{ij}^c)} = \frac{\exp\{\theta^t s(x_{ij}^+)\}}{\exp\{\theta^t s(x_{ij}^-)\}}$$

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Notation: For a network x and a pair (i, j) of nodes,

- $\Delta(s(x))_{ij}$ denotes the vector of change statistics,

$$\Delta(s(x))_{ij} = s(x_{ij}^+) - s(x_{ij}^-).$$

So $\Delta(s(x))_{ij}$ is the conditional log-odds of edge (i, j) .

$$\log \frac{P(X_{ij} = 1 | X_{ij}^c = x_{ij}^c)}{P(X_{ij} = 0 | X_{ij}^c = x_{ij}^c)} = \theta^t \Delta(s(x))_{ij}$$

Maximum Pseudolikelihood: Alternative to MLE?

- What if we approximate the marginal $P(X_{ij} = 1)$ by the conditional $P(X_{ij} = 1 | X_{ij}^c = x_{ij}^c)$?
- Then the X_{ij} are independent with

$$\log \frac{P(X_{ij} = 1)}{P(X_{ij} = 0)} = \theta^t \Delta(s(x^{\text{obs}}))_{ij},$$

so we obtain $\hat{\theta}$ using simple logistic regression.

- Result: The **maximum pseudolikelihood estimate**.
- Unfortunately, little is known about the quality of MPL estimates.

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MLE Revisited

- Remember, $c(\theta)$ is *really* hard to compute.
- However, suppose we fix θ_0 . A bit of algebra shows that

$$E_{\theta_0} [\exp \{(\theta - \theta_0)^t s(X)\}] = \frac{c(\theta)}{c(\theta_0)}.$$

- Thus, $c(\theta)/c(\theta_0)$ is the expectation of a function of a random network, where the random behavior is governed by the known constant θ_0 .

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Law of Large Numbers to the Rescue!

The LOLN suggests that we approximate an unknown population mean by a sample mean.

Thus,

$$\begin{aligned} c(\theta)/c(\theta_0) &= E_{\theta_0} \left(\exp \{ (\theta - \theta_0)^t s(X) \} \right) \\ &\approx \frac{1}{M} \sum_{i=1}^M \exp \{ (\theta - \theta_0)^t s(X^{(i)}) \}, \end{aligned}$$

where $X^{(1)}, X^{(2)}, \dots, X^{(M)}$ is a random sample of networks from the distribution defined by the ERGM with parameter θ_0 .

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$$\begin{aligned}
 \ell(\theta) - \ell(\theta_0) &= -\log \frac{c(\theta)}{c(\theta_0)} \\
 &= -\log E_{\theta_0} \left(\exp \left\{ (\theta - \theta_0)^t s(X) \right\} \right) \\
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Obtaining samples via MCMC

MCMC Idea:

Simulate a discrete-time Markov chain whose stationary distribution is the distribution we want to sample from.

We'll discuss two common ways to run such a Markov chain:

- Gibbs sampling
- A Metropolis algorithm



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- First, select a pair of nodes at random, say (i, j) .
- Decide whether to set $X_{ij} = 0$ or $X_{ij} = 1$ at the next time step according to the conditional distribution of X_{ij} given the rest of the network (X_{ij}^c).
- Based on an earlier calculation, we obtain

$$P_{\theta_0}(X_{ij} = 1 | X_{ij}^c = x_{ij}^c) = \frac{\exp\{\theta_0^t \Delta(s(x))_{ij}\}}{(1 + \exp\{\theta_0^t \Delta(s(x))_{ij}\})}$$

Note: To run the MCMC, the values of $s(x_{ij}^+)$ and $s(x_{ij}^-)$ are not needed; only the difference $\Delta(s(x))_{ij}$ matters.

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Metropolis algorithm

- First, select a pair of nodes at random, say (i, j) .
- Calculate the ratio

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- Accept the change of X_{ij} with probability $\min\{1, \pi\}$.
- This scheme generally has better properties than Gibbs sampling.

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- Theoretically, the estimated value of $\ell(\theta) - \ell(\theta_0)$ converges to the true value as the size of the MCMC sample increases, regardless of the value of θ_0 .
- However, this convergence can be agonizingly slow, especially if θ_0 is not chosen close to the maximizer of the likelihood.
- A choice that sometimes works is the MPLE (maximum pseudolikelihood estimate)

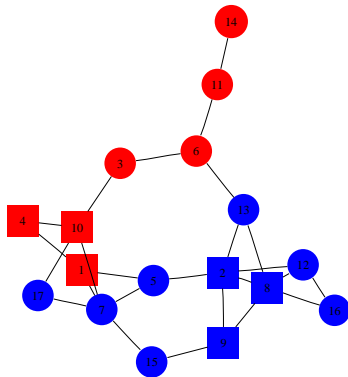
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How should θ_0 be chosen?

- Theoretically, the estimated value of $\ell(\theta) - \ell(\theta_0)$ converges to the true value as the size of the MCMC sample increases, regardless of the value of θ_0 .
- However, this convergence can be agonizingly slow, especially if θ_0 is not chosen close to the maximizer of the likelihood.
- A choice that sometimes works is the MPLE (maximum pseudolikelihood estimate)

A numerical example



```
=====
Summary of output
=====
```

```
Newton-Raphson iterations: 32
MCMC sample of size 10000
```

```
Monte Carlo MLE Results:
```

	theta0	estimate	s.e.	p-value
match.grade	1.0706	1.4118	0.4988	0.0054
dmatch.sex.0	1.0383	1.4660	0.7482	0.0522
dmatch.sex.1	-0.9387	-0.7195	0.6767	0.2897
triangle	1.1864	1.0389	0.5750	0.0732
kstar1	9.3754	8.2408	5.3026	0.1226
kstar2	-8.1424	-7.5155	4.4219	0.0916
kstar3	5.2464	5.0092	3.3080	0.1324
kstar4	-2.4226	-2.4512	1.8068	0.1773

```
Log likelihood of g: -78.52976
```

Some Useful References

- Frank, O. and D. Strauss (1986), Markov graphs, *JASA*
- Geyer, C. J. and E. Thompson (1992), Constrained Monte Carlo maximum likelihood for dependent data, *J. Roy. Stat. Soc. B*
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- Wasserman, S. and P. Pattison (1996), Logit models and logistic regression for social networks: I. An introduction to Markov graphs and p^* , *Psychometrika*