

# Inference and Simulation within the general ERGM framework

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Statistical Analysis of Networks  
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# Obtaining samples via MCMC

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

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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

# Gibbs sampling

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- Based on an earlier calculation, we obtain

$$P_{\eta_0}(Y_{ij} = 1 | Y_{ij}^c = y_{ij}^c) = \frac{\exp\{\eta_0 \cdot \Delta(g(y))_{ij}\}}{(1 + \exp\{\eta_0 \cdot \Delta(g(y))_{ij}\})}.$$

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

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

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# Maximum Likelihood Estimation

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$$\kappa(\eta) = \sum_{\substack{\text{all possible} \\ \text{graphs } z}} \exp\{\eta \cdot g(z)\}.$$

- Replacing  $g(y)$  by  $g(y) - g(y^{\text{obs}})$  leaves  $P_{\eta}(Y = y)$  unchanged; thus, we “recenter”  $g(y)$  so that  $g(y^{\text{obs}}) = 0$ .

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



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7,547,924,849,643,082,704,483,  
109,161,976,537,781,833,842,  
440,832,880,856,752,412,600,  
491,248,324,784,297,704,172,  
253,450,355,317,535,082,936,  
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terms.

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$$\mathbf{E}_{\eta_0} [\exp \{(\eta_0 - \eta) \cdot g(Y)\}] = \frac{\kappa(\eta_0)}{\kappa(\eta)}.$$

- Thus,  $\kappa(\eta_0)/\kappa(\eta)$  is the expectation of a function of a random network, where the random behavior is governed by the known constant  $\eta_0$ .

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Thus,

$$\begin{aligned}\kappa(\eta_0)/\kappa(\eta) &= \mathbf{E}_{\eta_0}(\exp\{(\eta_0 - \eta) \cdot g(Y)\}) \\ &\approx \frac{1}{m} \sum_{i=1}^m \exp\{(\eta_0 - \eta) \cdot s(Y_i)\},\end{aligned}$$

where  $Y_1, Y_2, \dots, Y_m$  is a random sample of networks from the distribution defined by the ERGM with parameter  $\eta_0$ .

# An approximate loglikelihood

- Using the LOLN approximation, we find that the difference in loglikelihoods is

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- Given a random sample of networks from  $P_{\eta_0}$ , we can thus approximate (and subsequently maximize) the loglikelihood shifted by a constant.

# How should $\eta_0$ be chosen?

- Theoretically, the estimated value of  $\ell(\eta) - \ell(\eta_0)$  converges to the true value as the size of the MCMC sample increases, regardless of the value of  $\eta_0$ .

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- However, this convergence can be agonizingly slow, especially if  $\eta_0$  is not chosen close to the maximizer of the likelihood.
- A choice that sometimes works is the MPLE (maximum pseudolikelihood estimate)

# Conditional log-odds of an edge

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

- $y_{ij} = 0$  or  $1$ , depending on whether there is an edge
- $y_{ij}^c$  denotes the status of all pairs in  $x$  other than  $(i, j)$
- $y_{ij}^+$  denotes the same network as  $x$  but with  $y_{ij} = 1$
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Conditional on  $Y_{ij}^c = y_{ij}^c$ ,  $Y$  has only two possible states, depending on whether  $Y_{ij} = 0$  or  $Y_{ij} = 1$ .



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Let's calculate the ratio of the two respective probabilities:

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$$\frac{P(Y_{ij} = 1 | Y_{ij}^c = y_{ij}^c)}{P(Y_{ij} = 0 | Y_{ij}^c = y_{ij}^c)} = \frac{\exp\{\eta \cdot g(y_{ij}^+)\}}{\exp\{\eta \cdot g(y_{ij}^-)\}}$$

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$$\log \frac{P(Y_{ij} = 1 | Y_{ij}^c = y_{ij}^c)}{P(Y_{ij} = 0 | Y_{ij}^c = y_{ij}^c)} = \eta \cdot [g(y_{ij}^+) - g(y_{ij}^-)]$$

# Conditional log-odds of an edge

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

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

$$\Delta(g(y))_{ij} = g(y_{ij}^+) - g(y_{ij}^-).$$

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

$$\log \frac{P(Y_{ij} = 1 | Y_{ij}^c = y_{ij}^c)}{P(Y_{ij} = 0 | Y_{ij}^c = y_{ij}^c)} = \eta \cdot \Delta(g(y))_{ij}$$

# Maximum Pseudolikelihood: Alternative to MLE?

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

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- The log-pseudolikelihood function is then

$$\ell\text{PL}(\eta) = \sum \log[P(Y_{ij} = y_{ij} | Y_{ij}^c = y_{ij}^c)]$$



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- Result: The **maximum pseudolikelihood estimate** is then the value that maximizes  $\ell\text{PL}(\eta)$  as a function of  $\eta$ .

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- Result: The **maximum pseudolikelihood estimate** is then the value that maximizes  $\ell\text{PL}(\eta)$  as a function of  $\eta$ .
- Unfortunately, little is known about the quality of MPL estimates.

# Implementation

- This has been implemented in the `ergm` package, available on CRAN.
- See <http://www.statnet.org> for more general code.
- Many different versions and ideas.
- See Volume 24 of the *Journal of Statistical Software*

# MCMC diagnostics

- The `ergm` package uses a Metropolis-Hastings algorithm to sample from the space of graphs given parameter values.
- It then uses the Geyer-Thompson device to estimate the MLE based on the sample of graphs.
- How do we know the MCMC algorithm has approximately converged, so that the graph sample can be used to get an accurate approximation of the MLE?
- We can use standard numerical and graphical diagnostics on graph statistics of the sampled graphs (i.e., statistics of the sampled graphs).

# mcmc.diagnostics

- The `mcmc.diagnostics` command computes many diagnostics from an `ergm` fit object.
- By default it produces *trace plots* and *density plots* of the statistics.
- In fact, an `ergm` output object contains the matrix of statistics from the MCMC run as component `$sample`. This matrix is actually an object of class `mcmc` and can be used directly in the `coda` package to assess MCMC convergence.
- Hence all MCMC diagnostic methods available in `coda` are available directly by calling `coda`.

# Example mcmc.diagnostics

```
data(florentine)
# Fit a simple model
gest <- ergm(flomarriage ~ edges + kstar(2))
summary(gest)
```

```
Call: ergm(formula = flomarriage ~ edges + kstar(2))
```

Monte Carlo Maximum Likelihood Results:

	Estimate	Std. Error	MCMC %	z value	Pr(> z )
edges	-1.541591	0.822422	0	-1.874	0.0609 .
kstar2	-0.008306	0.167888	0	-0.049	0.9605

---

Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

Null Deviance: 166.4 on 120 degrees of freedom  
Residual Deviance: 108.1 on 118 degrees of freedom

AIC: 112.1 BIC: 117.7 (Smaller is better. MC Std. Err. = 0.006)

# Example `mcmc.diagnostics`

```
mcmc.diagnostics(gest)
```

Sample statistics summary:

```
Iterations = 14336:262144
```

```
Thinning interval = 1024
```

```
Number of chains = 1
```

```
Sample size per chain = 243
```

1. Empirical mean and standard deviation for each variable,  
plus standard error of the mean:

	Mean	SD	Naive SE	Time-series SE
edges	-0.4815	4.076	0.2615	0.2615
kstar2	-1.5350	19.967	1.2809	1.2809

# Example mcmc.diagnostics

Sample statistics cross-correlations:

	edges	kstar2
edges	1.0000000	0.9540829
kstar2	0.9540829	1.0000000

Sample statistics auto-correlation:

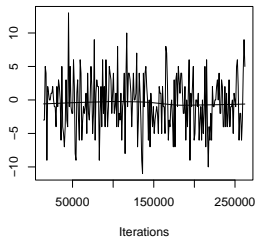
Chain 1

	edges	kstar2
Lag 0	1.00000000	1.000000000
Lag 1024	-0.01853626	0.008273854
Lag 2048	-0.07054771	-0.052840888
Lag 3072	0.03625916	-0.009676151
Lag 4096	0.02364600	-0.007372892
Lag 5120	0.02513591	0.026592066

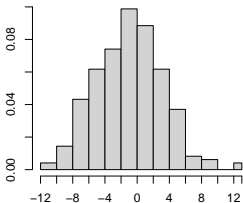


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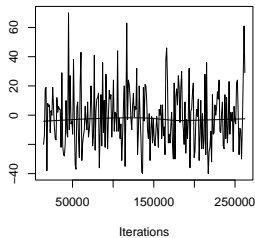
Trace of edges



Density of edges



Trace of kstar2



Density of kstar2

