COLUMBIA UNIVERSITY
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Estimation of Exponential Ranomd Graph Models for Large Social Networks via Graph Limits

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Acknowledgement

- This research is supported by NSF.
- Joint work with Ran He

Outline

Introduction

Method

Results

Discussion

$$
\begin{aligned}
p_{\boldsymbol{\beta}}(G) &= \exp\left\{\sum_{i=1}^{k} \beta_i T_i(G) - \psi(\boldsymbol{\beta})\right\} \\
&= \exp\left\{\boldsymbol{\beta}' \boldsymbol{T}(G) - \psi(\boldsymbol{\beta})\right\},
\end{aligned}
$$

where $\boldsymbol{T}(G) = (T_1(G), \cdots, T_k(G))$ and

$$
\psi(\boldsymbol{\beta}) = \log \sum_{G \in \mathcal{G}_n} \exp\left(\boldsymbol{\beta}' \boldsymbol{T}(G)\right).
$$

Existing methods for estimation

- Pseudolikelihood approach
- Markov chain Monte Carlo based approach

Our approach

- is based on graph limits and a theoretical framework proposed by Chatterjee and Diaconis.
- uses techniques such as two dimensional simple function approximation to generalize the method.
- is an iterative algorithm to approximate the MLE.

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Graph limits based approach

- Lovasz, Szegedy, Borgs and their coauthors develop a unifying theory of graph limits.
- Convergent graph sequences have a limit object, which can be represented as symmetric *measurable* functions, i.e, $w : [0,1]^2 \to [0,1]$ that satisfy $w(x,y) = w(y,x)$ for all $x, y \in [0,1]$.
- w-random graph of size n can be generated by
  - first assigning x_i, $i = 1, \ldots, n \sim \text{unif}[0,1]$ to the n nodes,
  - and $e_{ij} \sim \text{Bernoulli}(w(x_i, x_j))$.
- Every finite simple graph G can also be represented as a graph limit w^G in a natural way. Split the interval $[0,1]$ into n equal intervals $J_1, \cdots, J_n$, where $n = |V(G)|$. For $x \in J_i$, $y \in J_j$, define

$$w^G(x,y) = \begin{cases} 1 & \text{if } ij \in E(G), \\ 0 & \text{otherwise.} \end{cases}$$

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- Chatterjee and Diaconis propose a quotient space of w, in which every simple graph G has an equivalence class $\widetilde{G}$, and define a distance $\delta_{\square}$ such that $(\widetilde{\mathcal{W}}, \delta_{\square})$ is a metric space.
- $\delta_{\square}(\widetilde{f}, \widetilde{g}) := \inf_{\sigma} d_{\square}(f, g_{\sigma})$, $g_{\sigma}(x, y) := g(\sigma x, \sigma y)$ and σ is a measure perserving bijection.
- Here $d_{\square} = \sup_{S,T \subseteq [0,1]} \left| \int_{S \times T} [f(x, y) - g(x, y)] dxdy \right|$.
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Graph limits based approach (cont'd)

- ERGM graph can be written as:

$$p_n(G) := e^{n^2(T(\widetilde{G})-\psi_n)},$$

where $T : \widetilde{\mathcal{W}} \to \mathbb{R}$ be a bounded continuous function on the metric space $(\widetilde{\mathcal{W}}, \delta_\square)$.

- Example:

$$\begin{aligned} T(\widetilde{G}) &= \sum_{i=1}^{3} \beta_i t(H_i, \widetilde{G}) \\ &= \frac{2\beta_1(\text{\# edges in G})}{n^2} + \frac{6\beta_2(\text{\# two-stars in G})}{n^3} \\ &\quad + \frac{6(\beta_3 - 2\beta_2)(\text{\# triangles in G})}{n^3}. \end{aligned}$$

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Graph limits based approach (cont'd)

- Assume $\widetilde{w_0}$ is the graph limit of $\widetilde{G_n}$ as $n \to \infty$.
- For a graph G_n of size n, assuming w_0, we have

$$\begin{aligned} \log p_n(G_n) &= T(G_n) - \psi_n \\ &= \sum_{i=1}^{n} \sum_{j=i+1}^{n} \left[e_{ij} \log w_0(x_i, x_j) + (1 - e_{ij}) \log(1 - w_0(x_i, x_j)) \right], \end{aligned}$$

- Here x_i and x_j are random draws from the uniform distribution on $[0, 1]$.
- As $n \to \infty$, we then have

$$\lim_{n \to \infty} \psi_n = \sup_{\tilde{w} \in \widetilde{W}} \left(T(\tilde{w}) - I(\tilde{w}) \right),$$

where

$$\begin{aligned} I(\tilde{w}) &= \iint_{[0,1]^2} I(w(x, y)) dx dy \\ I(u) &= \frac{1}{2} u \log u + \frac{1}{2} (1 - u) \log(1 - u) \end{aligned}$$

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Graph limits based approach (cont'd)

- When n is large, almost all random graphs G_n drawn from ERGM induced by T are close to w random-graphs F when $T(\widetilde{F}) - I(\widetilde{F})$ is maximized.
- Based on these findings, Chatterjee and Diaconis remarked that one can approximate MLE, by evaluating $\psi(\beta)$ on a fine grid in β space and then carrying out the maximization by classical methods such as a grid search.

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Two-dimensional simple functions approximation

- For any m, split $[0,1]^2$ into m^2 lattices with equal area,

$$A_{ij} = \left\{(x,y) : x \in \left[\frac{i-1}{m}, \frac{i}{m}\right) \text{ and } y \in \left[\frac{j-1}{m}, \frac{j}{m}\right)\right\},$$

 where $i, j = 1, \cdots, m$. And let $\{c_{ij}\}$ be a sequence of real numbers between 0 and 1.

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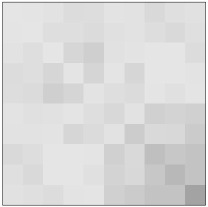
$$\hat{w}_m = \sum_{i,j=1}^{m} \hat{c}_{ij} \mathbf{1}_{A_{ij}}(x,y),$$

where $\{\hat{c}_{ij}; i,j = 1, \ldots m\} = \underset{\{c_{ij}; i,j=1,\ldots m\}}{\operatorname{argmax}} [T(w_m) - I(w_m)].$



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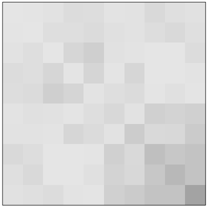

- For example, we can easily derive (for an ERGM model using *egdes*, *two-stars* and *triangles*.)

$$
\begin{aligned}
& T(w_m) - I(w_m) \\
= \quad & \frac{\beta_1}{m^2} \sum_{ij} c_{ij} + \frac{\beta_2}{m^3} \sum_{ijk} c_{ij} c_{jk} + \frac{\beta_3}{m^3} \sum_{ijk} c_{ij} c_{jk} c_{ik} \\
& - \frac{1}{2m^2} \sum_{ij} \left[c_{ij} \log c_{ij} + (1 - c_{ij}) \log(1 - c_{ij}) \right].
\end{aligned}
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Estimating parameters of ERGM via graph limits

- Give an initial value of β, $\beta^{(0)}$.
- For each t,
  - Given $\beta^{(t)}$, use simple function approximation to estimate $\tilde{w}^{(t)}$ by maximizing $T_{\beta^{(t)}}(\tilde{w}) - I(\tilde{w})$.
    The corresponding simple function is
    $$\hat{w}_m^{(t)} = \sum_{i,j=1}^{m} \hat{c}_{ij} \mathbf{1}_{A_{ij}}(x, y)$$
    and $\hat{\psi}^{(t)} = T_{\beta^{(t)}}\left(\widetilde{\hat{w}_m^{(t)}}\right) - I\left(\widetilde{\hat{w}_m^{(t)}}\right)$.
  - set $\beta^{(t+1)} = \underset{\beta}{\operatorname{argmax}} \log \hat{p}_n(\beta; G, \hat{w}_m^{(t)})$.
- Stop once $||\beta^{(t+1)} - \beta^{(t)}|| < \varepsilon$ for some fixed ε. And the corresponding $\beta^{(t+1)}$ is the GLMLE.

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Practical remarks

- Initial values: use w corresponding to the observed graph to find initial value of β.
- Updating w_m
- Updating β
  - For exponential family,
    $$E_\beta\left[\boldsymbol{T}(G)\right] = \nabla\psi(\beta)$$
    .
  - Thus the first derivative of the log-likelihood function for an ERGM graph G is
    $$\begin{aligned}\nabla \log p_n(\beta; G) &= n^2\left\{\boldsymbol{T}(G) - \nabla\psi(\beta)\right\}\\ &= n^2\left\{\boldsymbol{T}(G) - E_\beta\left[\boldsymbol{T}(G)\right]\right\}.\end{aligned}$$
- Computational complexity
  - Obtaining w_m^G in the initial step takes $O(n^2)$.
  - In each iteration, the computational complexity is $O(m^3)$.

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  - Obtaining w_m^G in the initial step takes $O(n^2)$.
  - In each iteration, the computational complexity is $O(m^3)$.

Practical remarks

- Initial values: use w corresponding to the observed graph to find initial value of β.
- Updating w_m
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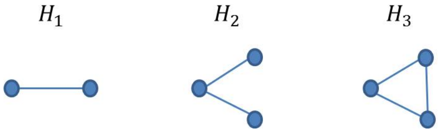
Outline

Results

- Can be used on large network.
- Outperform MCMC-based algorithm, especially when the network is large.
- Run faster then MCMC-based algorithm.

- Consider an ERGM using homomorphism densities $t(H_i, \cdot)$ as sufficient statistics, where H_1 is edge, H_2 is two-star and H_3 is triangle.



- The true value of the parameters β is $\beta = (-2, -1, 1)$.
- Using the R function `simulate.ergm` from the `ergm` package, we generate ERGM graphs of different sizes ($n = 100, 200, 500, 1000, 2000, 4000$) for this model.
- In each case, we simulate 100 graphs and apply our algorithm as well as MCMC algorithm (R function `ergm`) to model these data.
- We set $m = 10$

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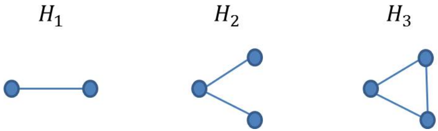

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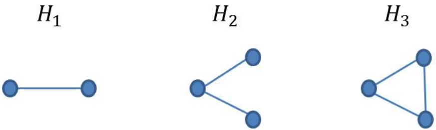

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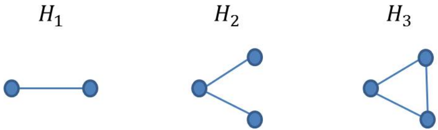

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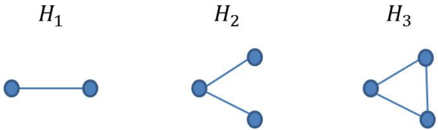

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Simulation study 1 (cont'd)

size n	GLMLE			MCMCMLE		
	Bias($\hat{\beta}_1$) se($\hat{\beta}_1$)	Bias($\hat{\beta}_2$) se($\hat{\beta}_2$)	Bias($\hat{\beta}_3$) se($\hat{\beta}_3$)	Bias($\hat{\beta}_1$) se($\hat{\beta}_1$)	Bias($\hat{\beta}_2$) se($\hat{\beta}_2$)	Bias($\hat{\beta}_3$) se($\hat{\beta}_3$)
100	−0.017 (0.206)	−0.429 (5.055)	0.929 (7.161)	0.042 (0.163)	−0.496 (1.738)	9.800 (7.638)
200	−0.022 (0.100)	0.137 (1.369)	0.075 (1.667)	0.033 (0.188)	−1.757 (3.968)	23.780 (18.074)
500	−0.490 (0.019)	0.285 (0.491)	0.079 (2.433)	−0.481 (0.069)	0.598 (1.725)	−9.748 (43.559)
1000	−0.922 (0.013)	0.045 (0.381)	0.154 (0.330)	−0.917 (0.048)	0.483 (2.660)	−27.233 (102.808)
2000	−1.347 (0.009)	−0.209 (0.347)	0.355 (0.255)	−1.346 (0.029)	0.458 (3.787)	−20.266 (188.530)
4000	−1.741 (0.007)	−0.417 (0.307)	0.547 (0.127)	−1.742 (0.023)	0.588 (6.431)	18.510 (379.371)

Simulation study 2

- W-random graph is a method to generate random graph using a given graph limit w.
  - Generate n independent numbers $X_1, \cdots, X_n$ from the uniform distribution $U(0, 1)$.
  - Connect nodes i and j by an edge with probability $w(X_i, X_j)$, independently for every pair.
- All other settings are the same as simulation study 1.

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100	0.110 (0.694)	−2.412 (16.639)	0.182 (10.243)	0.004 (0.150)	0.487 (1.546)	7.164 (8.593)
200	−0.018 (0.045)	0.357 (0.661)	−0.098 (2.275)	−0.015 (0.114)	0.803 (1.125)	−6.063 (17.025)
500	−0.009 (0.012)	0.223 (0.064)	−0.103 (0.127)	−0.031 (0.068)	0.979 (0.661)	−1.681 (8.269)
1000	−0.009 (0.006)	0.225 (0.021)	−0.125 (0.040)	−0.031 (0.051)	0.962 (0.520)	−0.557 (5.283)
2000	−0.007 (0.003)	0.219 (0.021)	−0.110 (0.045)	−0.031 (0.030)	0.982 (0.307)	−1.263 (4.180)
4000	−0.007 (0.002)	0.212 (0.017)	−0.094 (0.029)	−0.035 (0.024)	1.029 (0.240)	−1.452 (2.960)

Real data analysis

- We apply our method to two real large social networks from Slashdot, a technology-related news website that has a large specific user community.

	nodes	edges	two-stars	triangles	transtivity ratio
Slashdot0811	77,360	469,180	68,516,301	551,724	0.02416
Slashdot0902	82,168	504,230	74,983,589	602,592	0.02411

- Although MCMC-based approach works in theory for large networks, it fails in practice, primarily because these two networks are too large to be coerced to objects to which the `ergm` function can be applied. Our GLMLE algorithm still works.
  - *Slashdot0811*: $(-4.5109, -1.5863, 1.6871)$, running time for obtaining w^G is 392 seconds, while that of estimation is 153 seconds.
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- In order to compare our method with MCMC-based approach, we obtain a random subnetwork G_{sub} from the *Slashdot0902* network via link-tracing-based sampling method. It contains 376 nodes, $1,609$ edges, $48,915$ two-stars and $1,661$ triangles.
- Besides the above model, we consider another model:

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\begin{aligned}
T(\widetilde{G}) &= \beta_1(\text{edges density}) + \beta_2(\text{triangle percent}) \\
&= \frac{2\beta_1(\text{\# edges in G})}{n^2} \\
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Real data analysis (cont'd)

Method	$\hat{\beta}$	corresponding w	$\frac{1}{n^2}\log(p_n)$
Model 1			
MCMCMLE	$(-2.5161, 3.3917, 43.2382)$	w_1	-44.1442
GLMLE	$(-1.8415, -0.7689, 0.7705)$	w_2	-0.0558
Model 2			
MCMCMLE	$(-1.6072, 0.1206)$	w_3	-0.1408
GLMLE	$(-2.1921, 0.0714)$	w_4	-0.0518

Visualization of graph limit objects used

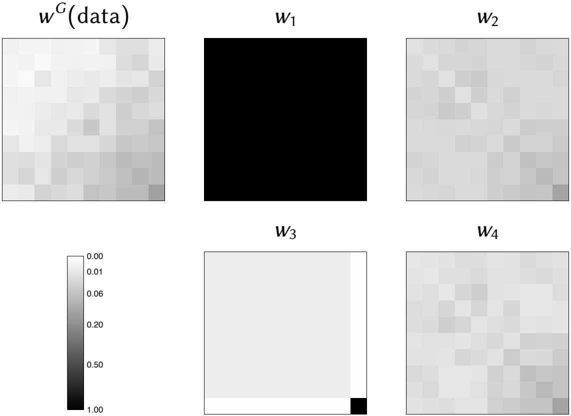

Figure : Heat map of graph limits w_1,w_2,w_3,w_4 and the graph limit representation of G_{sub}, w^G, as in above table. The different shades of gray represent the values of $w(x, y) \in [0, 1]$, with black being 1 and white 0.

Hypothesis testing

- We conduct a likelihood ratio test based on the approximate likelihood values for a number of models to test whether the values of each parameter in GLMLE is statistically significant.

Model	log-likelihood	Deviance	Deviance d.f.	p-value
Model 1				
NULL	-48997.19	—	—	—
T_1 only	-8085.31	40911.88	1	$< 1 \times 10^{-16}$
T_1 and T_2	-8019.34	65.97	1	4.44×10^{-16}
model 1	-7887.76	131.58	1	$< 1 \times 10^{-16}$
Model 2				
NULL	-48997.19	—	—	—
T_1 only	-8085.31	40911.88	1	$< 1 \times 10^{-16}$
model 2	-7321.27	764.04	1	$< 1 \times 10^{-16}$

Future work

- Choosing m.
- Examine the numerical stability.
- Apply our algorithm to more general exponential random graph models.

Thank you!