

# Are we there yet?

## When to stop a Markov chain while generating random graphs

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Office of Advanced Scientific Computing Research

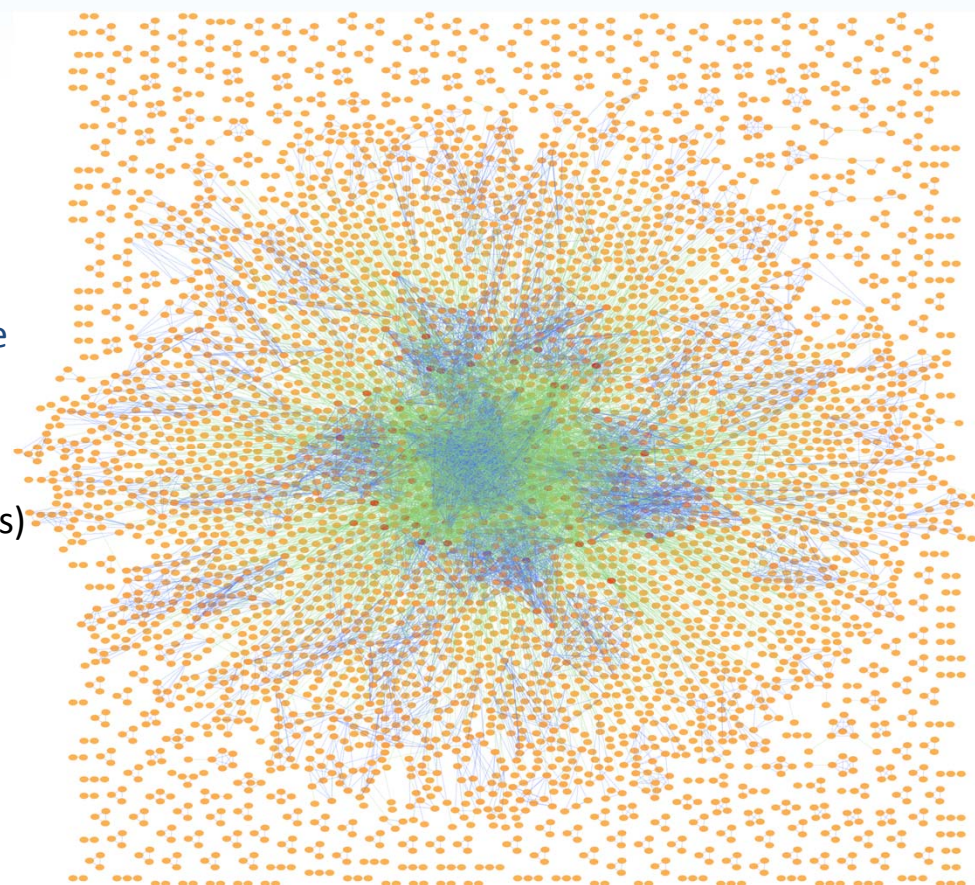


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# Why generate random graphs?

- Enable sharing of surrogate data
  - Computer network traffic
  - Social networks
  - Financial transactions
- Statistical analysis
  - Sample uniformly from a specified space
- Testing graph algorithms
  - Scalability
  - Versatility (e.g., vary degree distributions)
  - Characterizing algorithm performance
- Insight into...
  - Generative process
  - Community structure
  - Comparison
  - Evolution
  - Uncertainty



Block Two-Level Erdős-Rényi (BTER) graph;  
image courtesy of Nurcan Durak.

# Markov Chains: common method to generate random graphs

- For this talk, a Markov chain (MC) is a graph whose nodes are realizations of a graph with desired features
  - Normally, MC graph is never constructed
  - We generate its vertices, as we walk on the graph
- A random walk on an MC (with the right features) can yield a random graph.
- To generate a random graph using an MC
  - Find an arbitrary node of the MC
  - Take a loooong random walk
  - You will arrive at a uniform random vertex of the graph
    - given that you have a “good” MC
- Challenges
  - Generating a graph with given properties
  - Rewiring a graph to preserve desired features
  - Patience

# Math can prove convergence, but cannot grant you patience

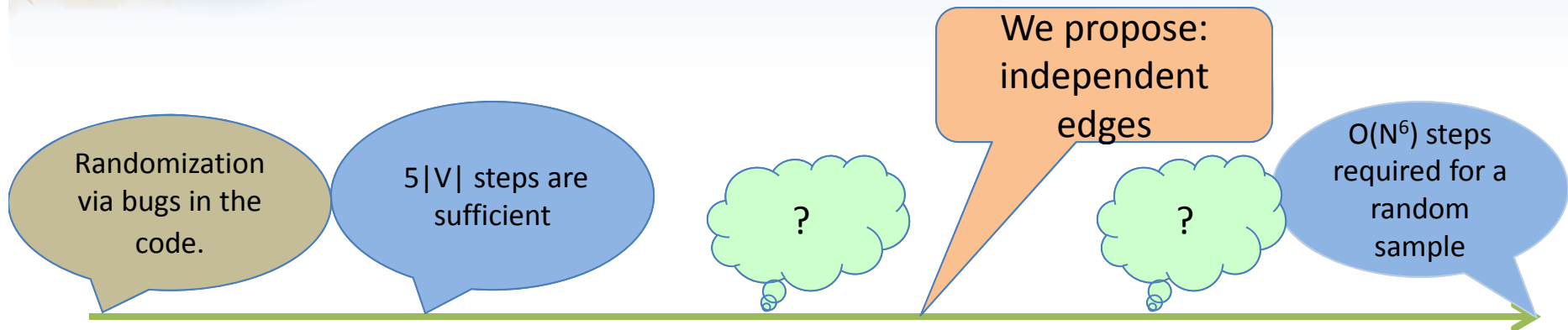


Source: <http://metsmerizedonline.com/wp-content/uploads/2013/02/Are-We-There-Yet.jpg>

Can we find principled and practical metrics to think about convergence?

- In theory, we need to prove the MC eventually produces a random graph.
- In practice, bounds for convergence may be impractical or nonexistent.
- Practitioners use unprincipled methods.
  - e.g., 10K steps on the MC
- Interpretations of statistical tools may be hard.
  - What does Gelman Rubin test mean from a graphs perspective?

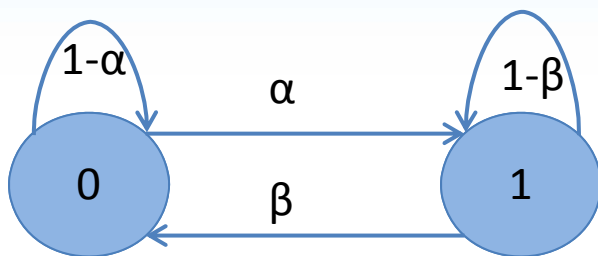
# Can we find principled and practical metrics for convergence?



- What is a mathematically sound definition of “random enough?”
- Goals: practical, sound, and interpretable.
- An imperfect analogy:
  - To solve  $Ax=b$ , we do not compute  $A^{-1}b$ , we compute an  $x$ , that yields a small residual for  $Ax-b$ .
  - We learn how to deal with this imperfection.



# Testing independence of edges



State 0: edge is absent

State 1: edge is present

$\alpha$ : probability that the edge will be inserted

$\beta$ : probability that the edge will be deleted

$$T = \begin{bmatrix} 1-\alpha & \alpha \\ \beta & 1-\beta \end{bmatrix}$$

T: transition matrix of the edge

- Assume the addition/deletion of an edge can be approximated as a Markov process.
- The full Markov chain (MC) can be approximated as a collection of smaller Markov chains.
- Convergence of the smaller MCs is a necessary condition for convergence of the full MC.

# Convergence of smaller Markov chains

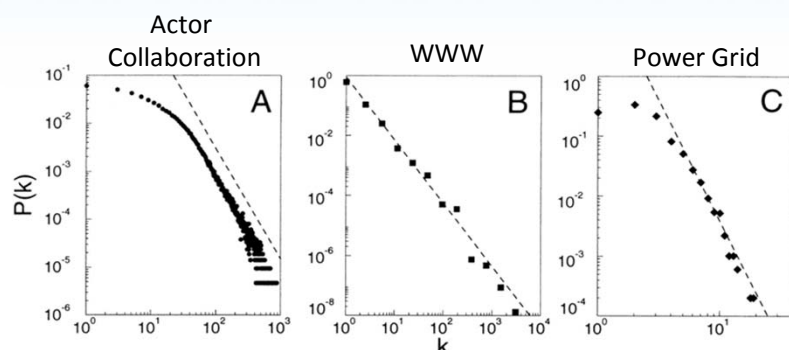
- Eigenvalues of  $T$  are  $1$  and  $1 - (\alpha + \beta)$
- Eigenvalues form a basis, so initial state  $v$  can be written as  $v = c_1 e_1 + c_2 e_2$ .
- After  $N$  iterations, we have

$$p = T^N v = c_1 e_1 + c_2 (1 - (\alpha + \beta))^N e_2$$

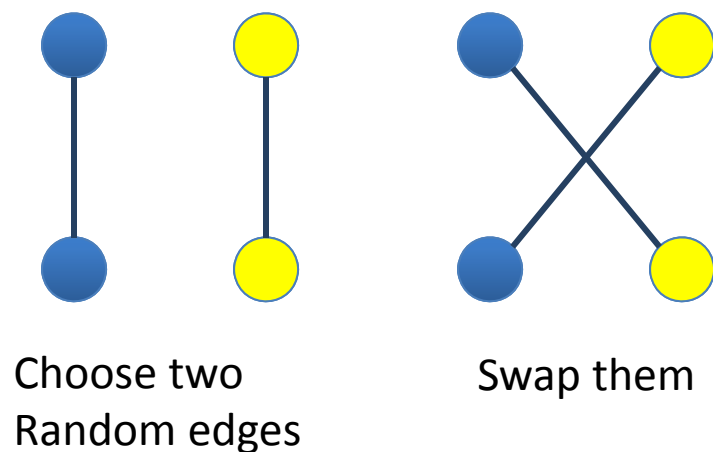
- The second term decays and  $p$  converges to  $c_1 e_1$ , which indicates the probability the edge is present/absent in a random graph.
- For tolerance  $\varepsilon$ , the number of iterations required,  $N$ , is

$$N = \ln(1 / \varepsilon) / (\alpha + \beta)$$

# Preserving the degree distributions



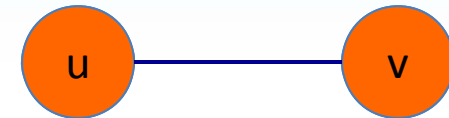
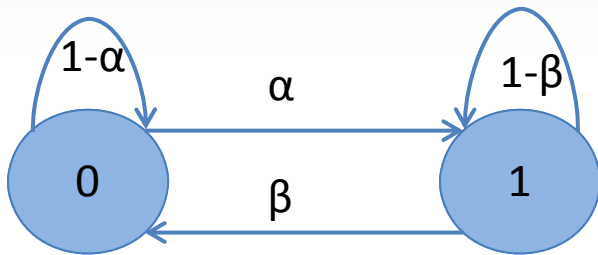
A.-L. Barabasi and R. Albert. Emergence of scaling in random networks. *Science*, 286(5349):509-512, 1999.



- Degree distribution is like a histogram of degrees.
- It is one of the critical features that distinguish real graphs from arbitrary sparse graphs.
- Rewiring scheme has long been used to perturb graphs while preserving the degree distribution.
  - Converges in  $O(|E|^6)$ -time.
- Havel and Hakimi described the first algorithm to construct a graph with a given degree distribution.



# Transition matrix for preserving degree distribution



$d_u$ : degree of vertex  $u$

$m$ : total number of edges

$\alpha$ : probability that the edge will be inserted

$\beta$ : probability that the edge will be deleted

$$N = \ln(1 / \epsilon) / (\alpha + \beta)$$

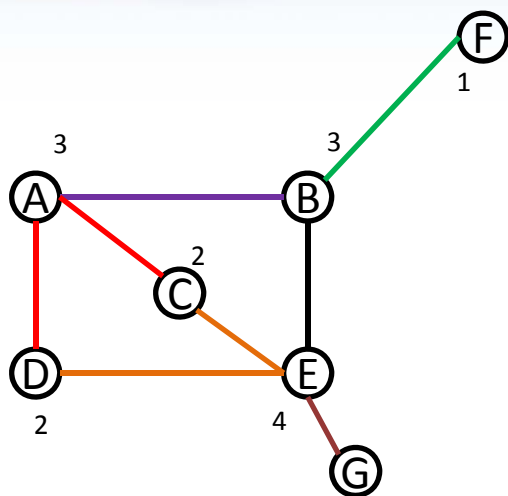
$$\alpha = \frac{d_u d_v}{2m^2} \quad \beta = 1 - \left(1 - \frac{1}{m}\right)^2$$

$$\alpha + \beta \geq \frac{2}{m}$$

To generate a graph with independent edges with a specified degree distribution we need

$$N = \frac{m}{2} \ln \epsilon^{-1}$$

# Joint Degree Distribution



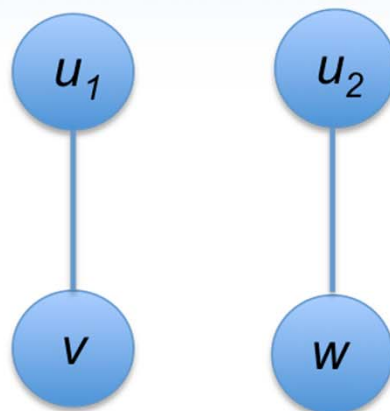
Degree	1	2	3	4
1	0	0	1	1
2	.	0	2	2
3	.	.	1	1
4	.	.	.	0

- Joint Degree Distribution (JDD) specifies the number of *edges* between vertices of specified degrees.
- *JDD provides more information about a graph.*
  - *The degree distribution is implicitly defined by JDD.*
- *Work on JDD is more recent and sparse.*

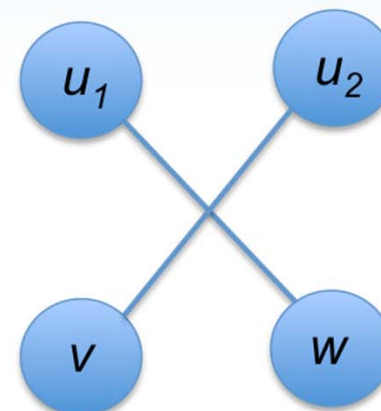
# Preserving JDD



**Step 1:** Pick an edge  $(u_1, v)$ , and pick one of its vertices, e.g.,  $u_1$



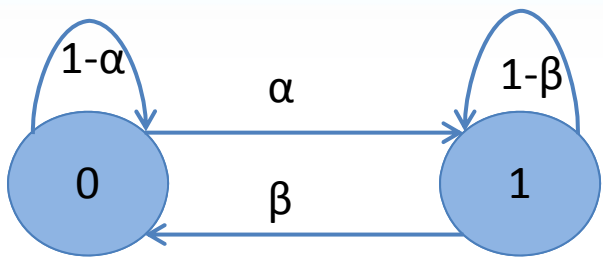
**Step 2:** Pick another edge  $(u, w)$ , such that  $d(u_1) = d(u_2)$  or  $d(u_1) = d(w)$



**Step 3:** Swap edges

- This Markov chain can be used to construct uniformly random instances of a graph with a specified degree distribution.
- No theoretical bounds on convergence.
- A graph with a specified (feasible) joint degree distribution can be constructed in linear time.
- Stanton & P., *ACM J. Experimental Algorithmics*, 2012

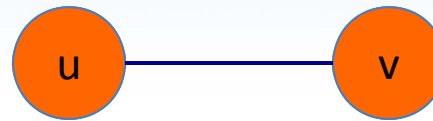
# Transition matrix for preserving degree distribution



$\alpha$ : probability that the edge will be inserted

$\beta$ : probability that the edge will be deleted

$$N = \ln(1 / \epsilon) / (\alpha + \beta)$$



$d_u$ : degree of vertex  $u$     $m$ : # edges

$f(d_u)$ : #vertices of degree  $d_u$

$J(d_u, d_v)$ : #edges between  $d_u$  and  $d_v$

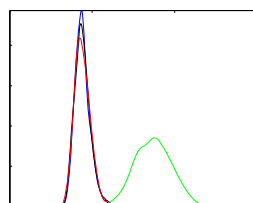
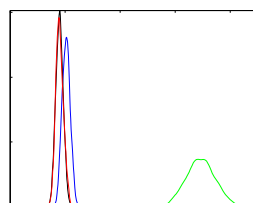
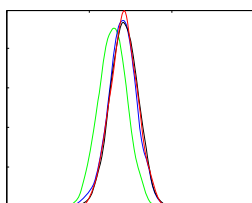
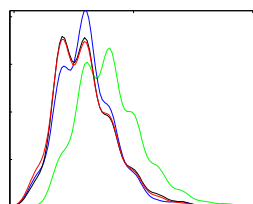
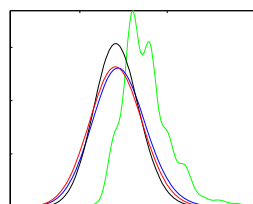
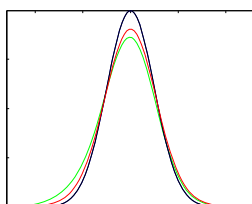
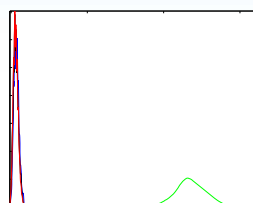
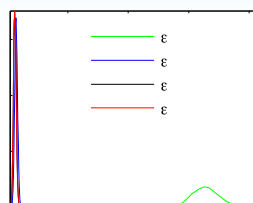
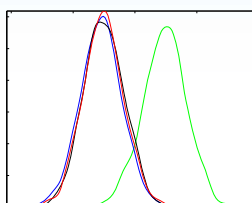
$$\beta = \frac{1}{m} + \frac{f(d_u) - 1}{2mf(d_u)} + \frac{f(d_v) - 1}{2mf(d_v)}$$

$$\alpha \cong \frac{2J(d_u, d_v)}{mf(d_u)f(d_v)} \quad \alpha + \beta \geq \frac{1}{m}$$

To generate a graph with independent edges with a specified degree distribution we need

$$N = m \ln \epsilon^{-1}$$

# How does edge practice work in practice?



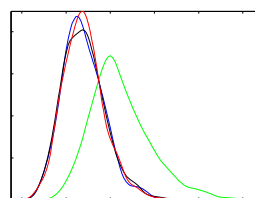
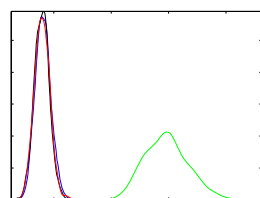
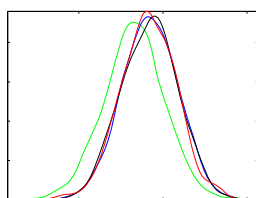
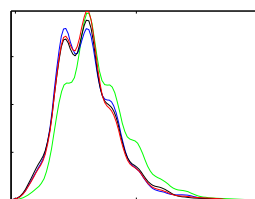
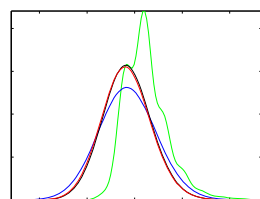
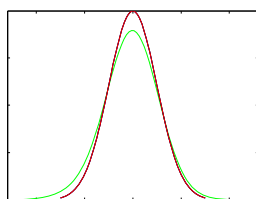
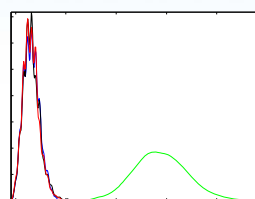
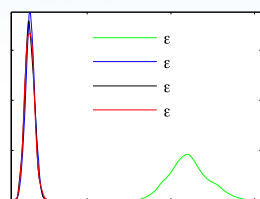
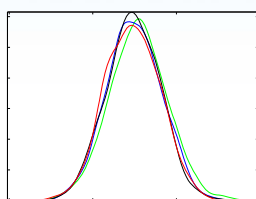
C. Elegans  
297 vertices,  
4296 edges

Netscience  
1461 vertices,  
5484 edges

Power  
4941 vertices,  
13188 edges

- Preserving degree distribution
- Errors correspond to  $0.5|E|$ ,  $2.5|E|$ ,  $5|E|$ , and  $7.5|E|$  iterations
- 1000 graphs generated starting from the original
- $5|E|$  iterations seem to be sufficient.

# Edge independence in practice



C. Elegans  
297 vertices,  
4296 edges

Netscience  
1461 vertices,  
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Power  
4941 vertices,  
13188 edges

- Preserving JDD
- Errors correspond to  $|E|$ ,  $5|E|$ ,  $10|E|$ , and  $15|E|$  iterations.
- 1000 graphs generated starting from the original
- $10|E|$  iterations seem as sufficient.

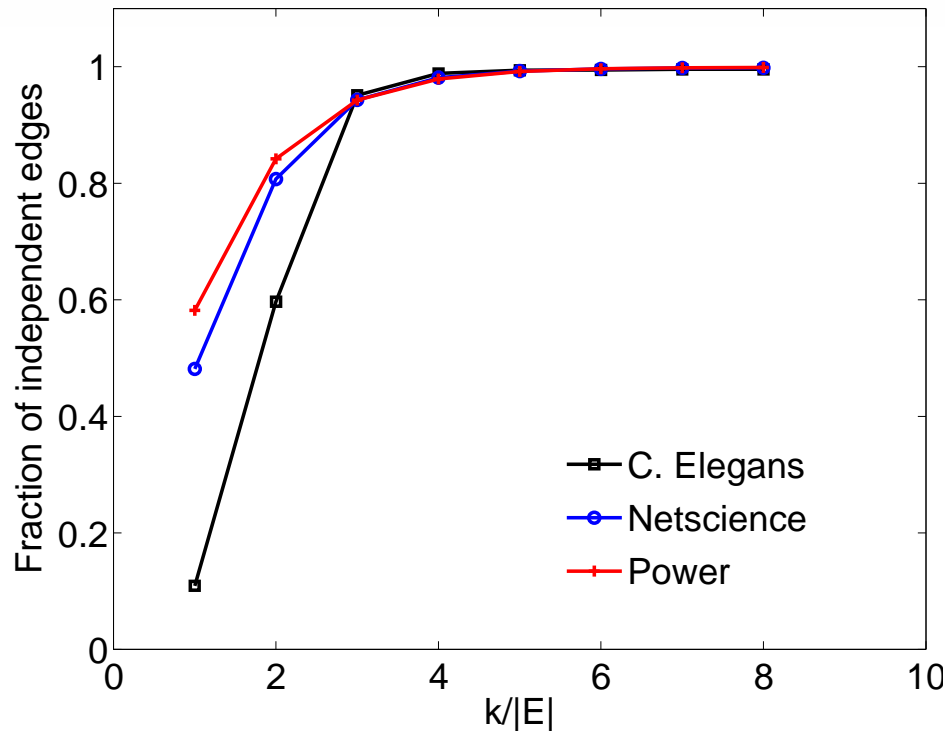


# Alternative way to measure independence

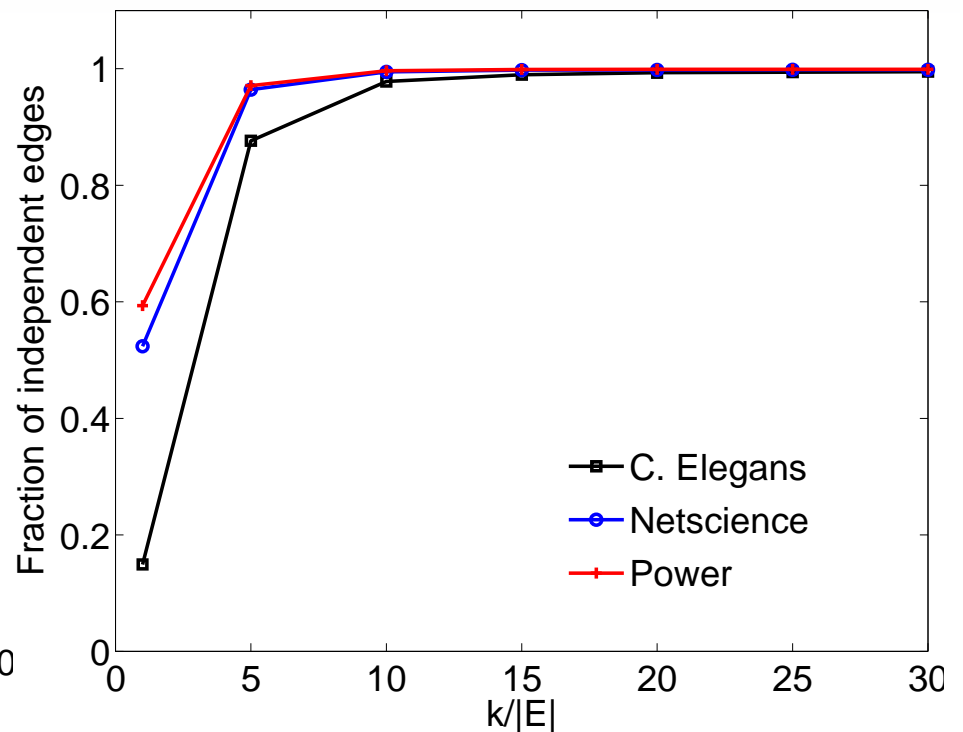
- Does knowing the current status (present/absent) of an edge help us predict its status in the next iteration better?
  - How about its status after 10 steps? 20 steps?
  - How many steps will be sufficient for the prediction to fail?
- The point we fail, the edge becomes independent
- A popular method in statistics
- Method:
  - Generate a long sequence
  - Fit a model to predict  $k$  steps ahead
  - Thin this sequence with smallest  $k$  for which the prediction fails

# Edges become independent rapidly

Preserving DD

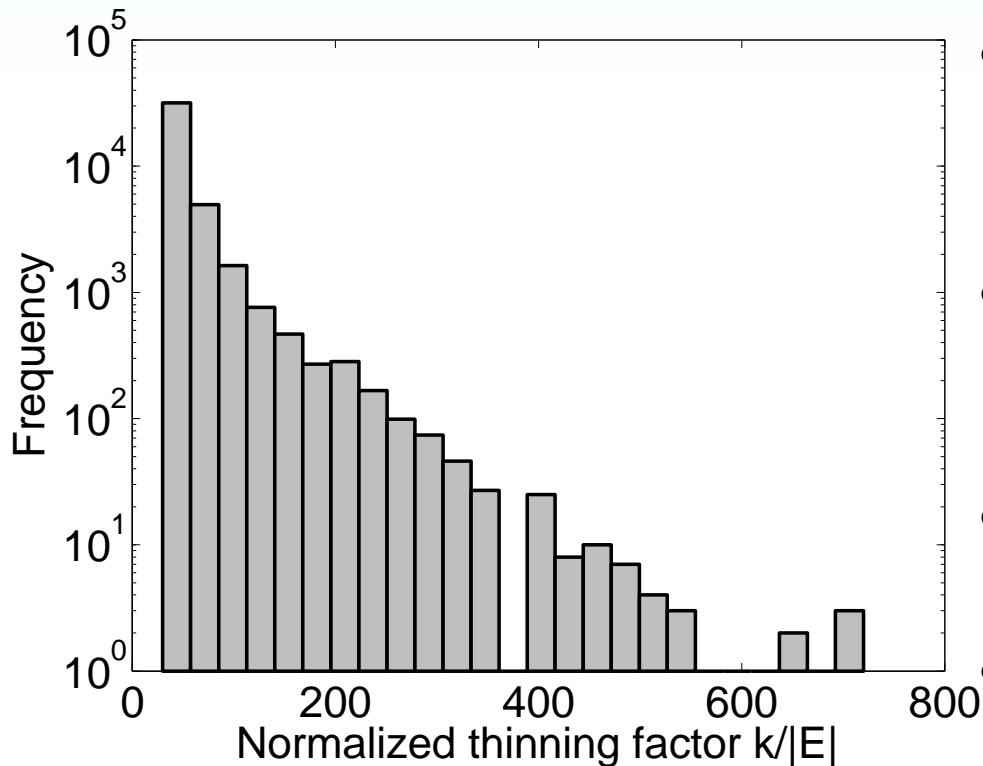


Preserving JDD



- All potential edges are included in the analysis.
- Only a few remain after  $7.5|E|$  and  $15|E|$  iterations for preserving DD and JDD, respectively.

# Some edges are tougher than others

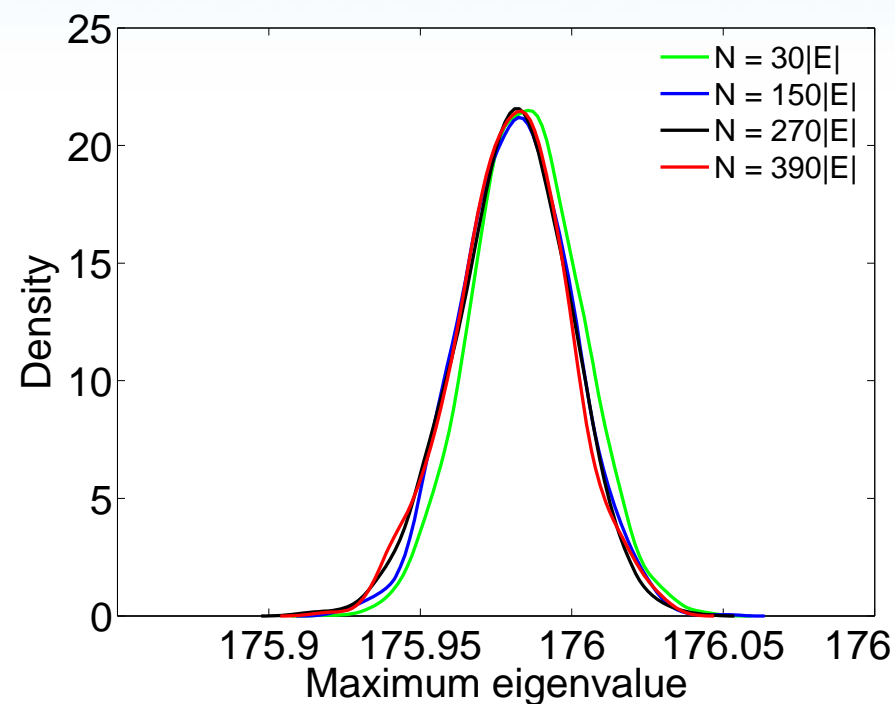
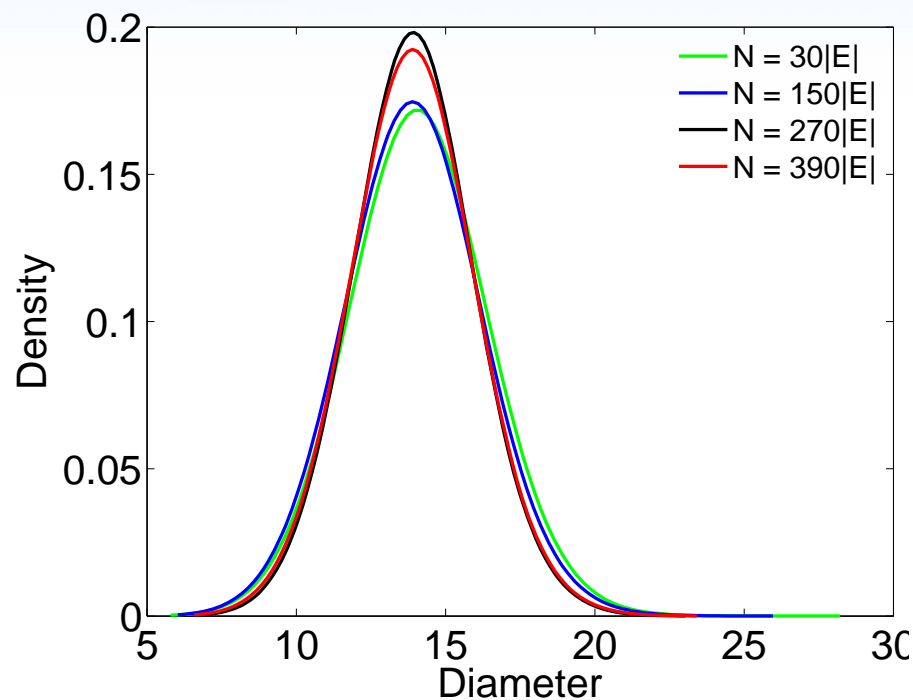


Soc-Epinions1

75879 vertices, 405740 edges

- Preserving JDD on Soc-Epinions
  - Edges are sampled down to 10%.
- After  $30|E|$  iterations 90% of the edges become independent.
- Most of the remaining ones are close to independence.
- There are a few outliers.

# Diminishing returns for extra steps



- Preserving JDD on soc-opinions1
- Distributions are very similar

# Conclusions

- Generating uniformly random instances of a graph with given properties is a fundamental problem in graph analysis.
- Markov chains are commonly used for this purpose, but guaranteeing/testing their convergence is a challenge.
- We proposed to use
  - edge independence as a practical metric.
  - smaller Markov chains for presence/absence of edges as a guide.
- We showed how the method applies to DD and JDD preserving MCs.
- Empirical studies on several graphs validated the approach.
- We are not guaranteeing convergence of the chain, but providing a metric that quantifies what is satisfied.
  - Results should be interpreted accordingly.
- The same approach can be used to guarantee independence of a bigger structures.

# A new workshop

- SIAM Workshop on Network Science
- Dates: July 7-8, 2013
- Place: San Diego, CA
- Co-located with SIAM Annual Meeting
- There will be a call for posters
- Contact:
  - Ali Pinar ([apinar@sandia.gov](mailto:apinar@sandia.gov)), Sandia National Labs
  - Madhav Marathe ([mmarathe@vbi.vt.edu](mailto:mmarathe@vbi.vt.edu)), Virginia Tech



# Relevant Publications

- J. Ray, A. Pinar, and C. Seshadhri, “A stopping criterion for Markov chains when generating independent random graphs,” arXiv:1210.8184.
- J. Ray, A. Pinar, and C. Sehadhri, “Are we there yet? When to stop a Markov chain while generating random graphs,” Proc. WAW 12. .
- I. Stanton and A. Pinar, “Constructing and uniform sampling graphs with prescribed joint degree distribution using Markov Chains,” ACM Journal on Experimental Algorithmics, Vol. 17, No. 1, 2012.
- I. Stanton and A. Pinar, “Sampling graphs with prescribed joint degree distribution using Markov Chains,” ALENEX’11.