Stanford CS224W: Generative Models for Graphs

CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
http://cs224w.stanford.edu

Motivation for Graph Generation

- So far, we have been **learning from graphs**
  - We assume the graphs are given

Image credit: Medium

Social Networks

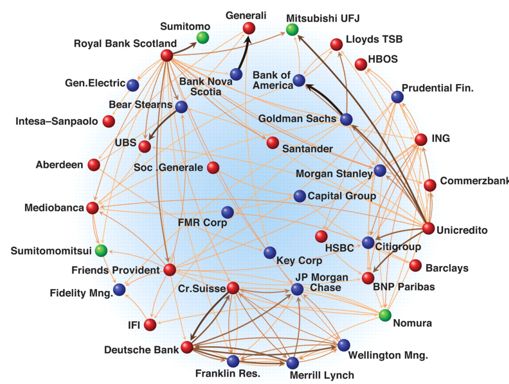


Image credit: Science

Economic Networks

Image credit: Lumen Learning

Communication Networks

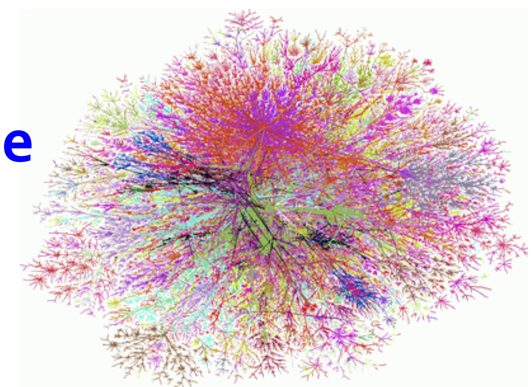
- **But how are these graphs generated?**

The Problem: Graph Generation

- We want to generate realistic graphs, using **graph generative models**

Graph Generative Model

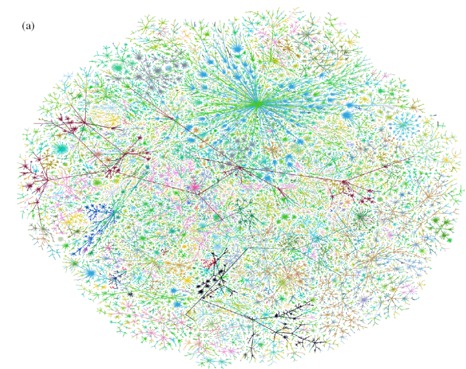
Generate $\Rightarrow$



Synthetic graph

which is similar to

$\sim$



Real graph

Why Do We Study Graph Generation

- **Insights** – We can understand the formulation of graphs
- **Predictions** – We can predict how will the graph further evolve
- **Simulations** – We can use the same process to general novel graph instances
- **Anomaly detection** - We can decide if a graph is normal / abnormal

Road Map of Graph Generation

- **Step 1: Properties of real-world graphs**
  - A successful graph generative model should fit these properties
- **Step 2: Traditional graph generative models**
  - Each come with different assumptions on the graph formulation process
- **Step 3: Deep graph generative models**
  - Learn the graph formulation process from the data
  - Cover in the next lecture

Stanford CS224W: Properties of Real-world Graphs

CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
http://cs224w.stanford.edu

Plan: Key Network Properties

We will characterize graphs by:

Degree distribution: $P(k)$

Clustering coefficient: C

Connected components: s

Path length: h

We have introduced these notions in Lecture 1&2. Here we give a quick recap.

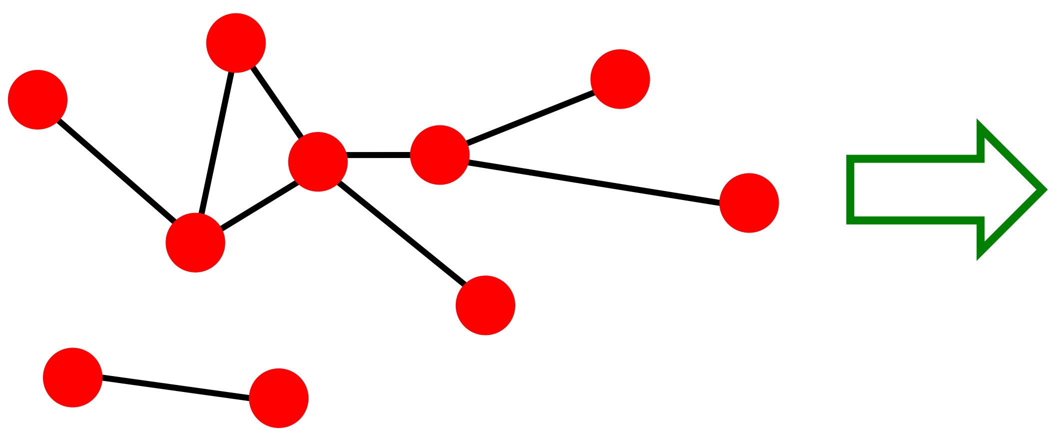
(1) Degree Distribution

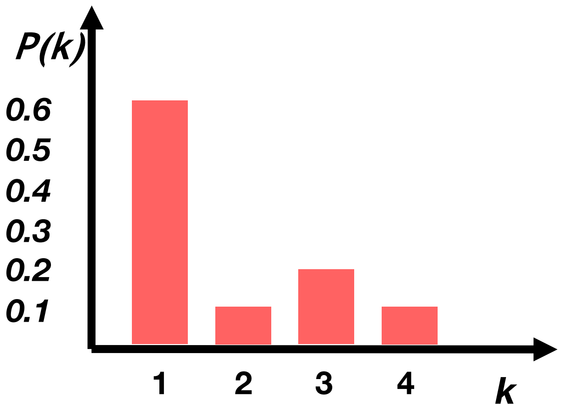
- **Degree distribution $P(k)$:** Probability that a randomly chosen node has degree k

  N_k = # nodes with degree k

- Normalized histogram:

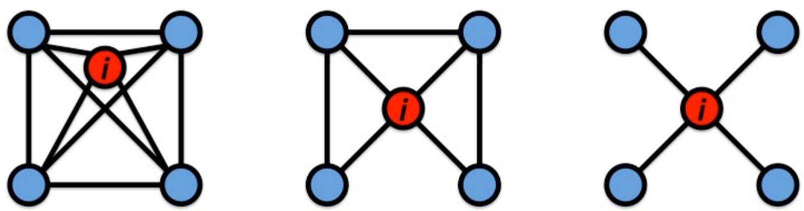
  $P(k) = N_k / N$ ➔ **plot**





(2) Clustering Coefficient

- **Clustering coefficient:**
  - How connected are $\boldsymbol{i}$'s neighbors to each other?
  - Node $\boldsymbol{i}$ with degree $\boldsymbol{k_i}$
  - $$C_i = \frac{2e_i}{k_i(k_i - 1)}$$ where e_i is the number of edges between the neighbors of node i



$C_i = 1$ $\qquad$ $C_i = 1/2$ $\qquad$ $C_i = 0$

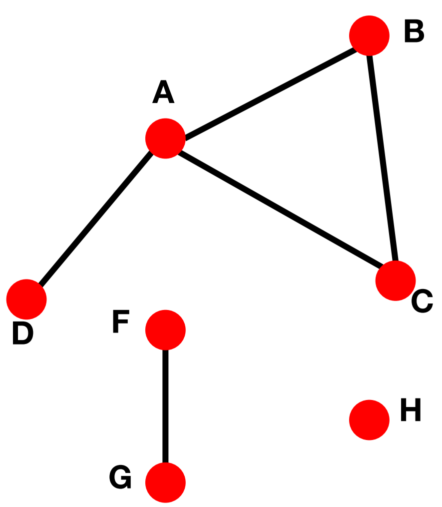
$C_i \in [0,1]$

- **Graph clustering coefficient:**
  - Take average over all the nodes

$$C = \frac{1}{N}\sum_{i}^{N} C_i$$

(3) Connectivity

- **Size of the largest connected component**
  - Largest set where any two vertices can be joined by a path
- **Largest component = Giant component**



How to find connected components:

- Start from random node and perform Breadth First Search (BFS)
- Label the nodes that BFS visits
- If all nodes are visited, the network is connected
- Otherwise find an unvisited node and repeat BFS

(4) Path Length

- **Diameter:** The maximum (shortest path) distance between any pair of nodes in a graph

- **Average path length** for a connected graph or a strongly connected directed graph

$$\bar{h} = \frac{1}{2E_{\max}} \sum_{i,j \neq i} h_{ij}$$

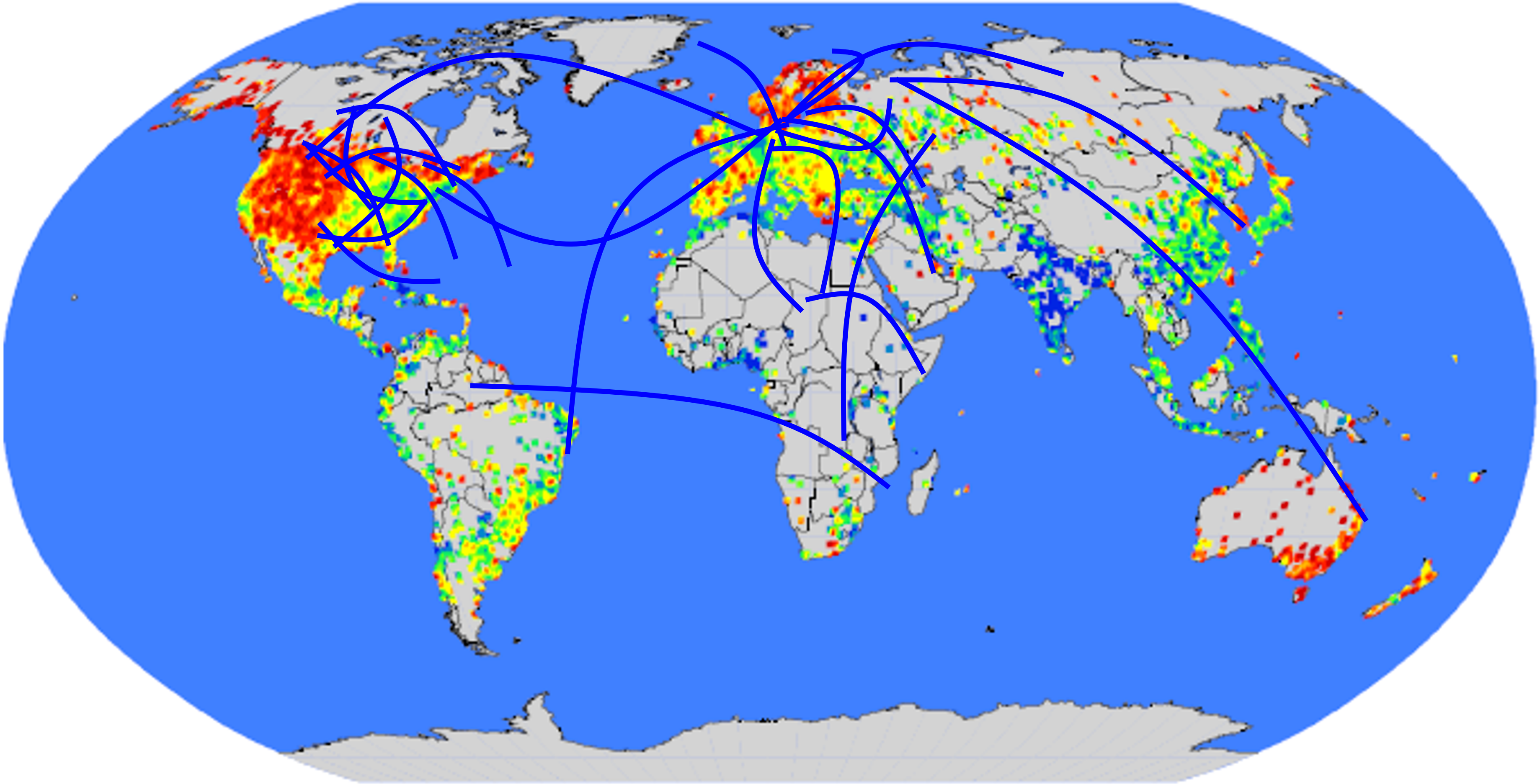
  - h_{ij} is the distance from node i to node j
  - E_{max} is the max number of edges (total number of node pairs) $= n(n-1)/2$

  - Many times we compute the average only over the connected pairs of nodes (that is, we ignore "infinite" length paths)

Case Study: MSN Graph

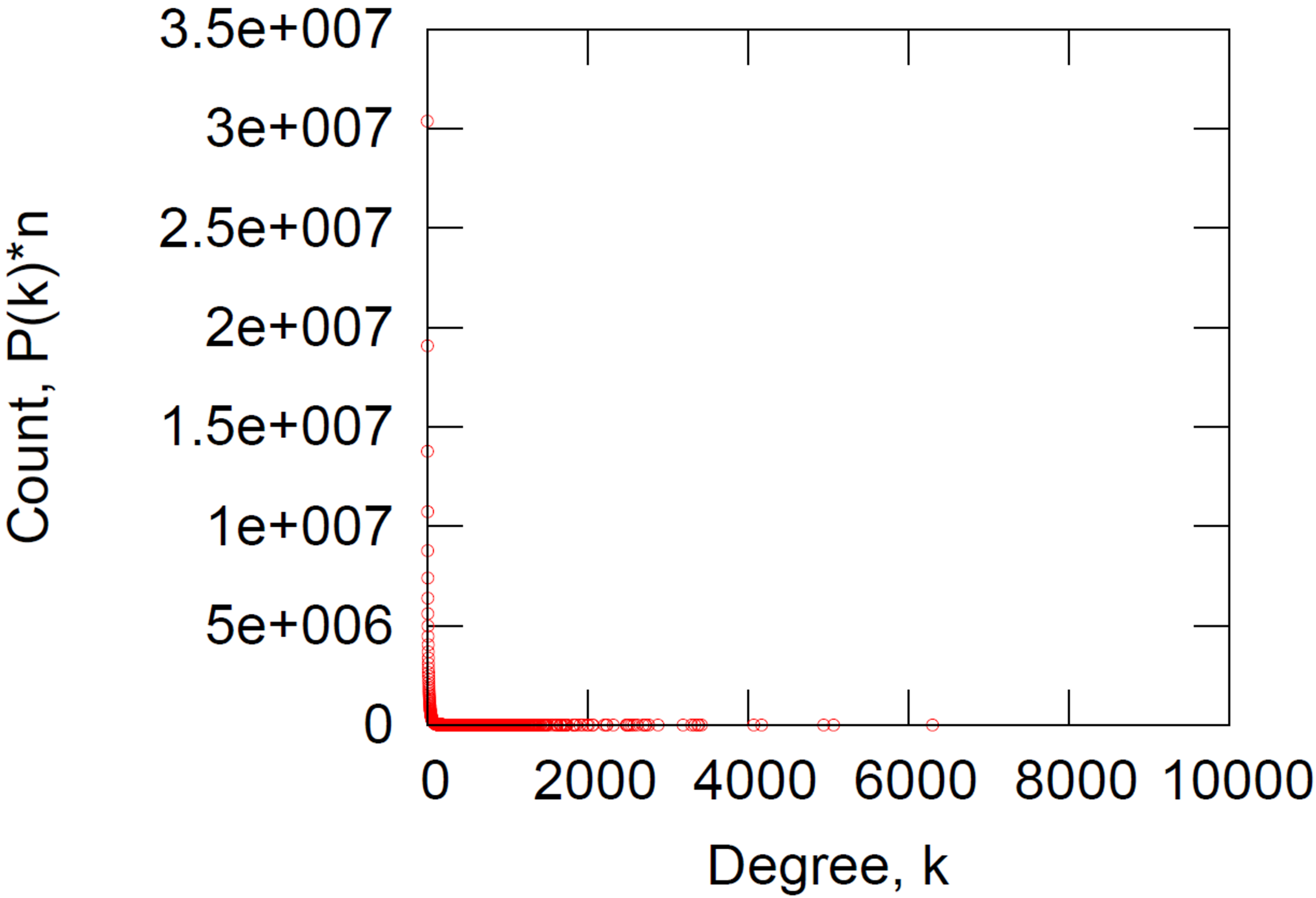
- **MSN Messenger:**
- **1 month of activity**
  - 245 million users logged in
  - 180 million users engaged in conversations
  - More than 30 billion conversations
  - More than 255 billion exchanged messages

Communication Network

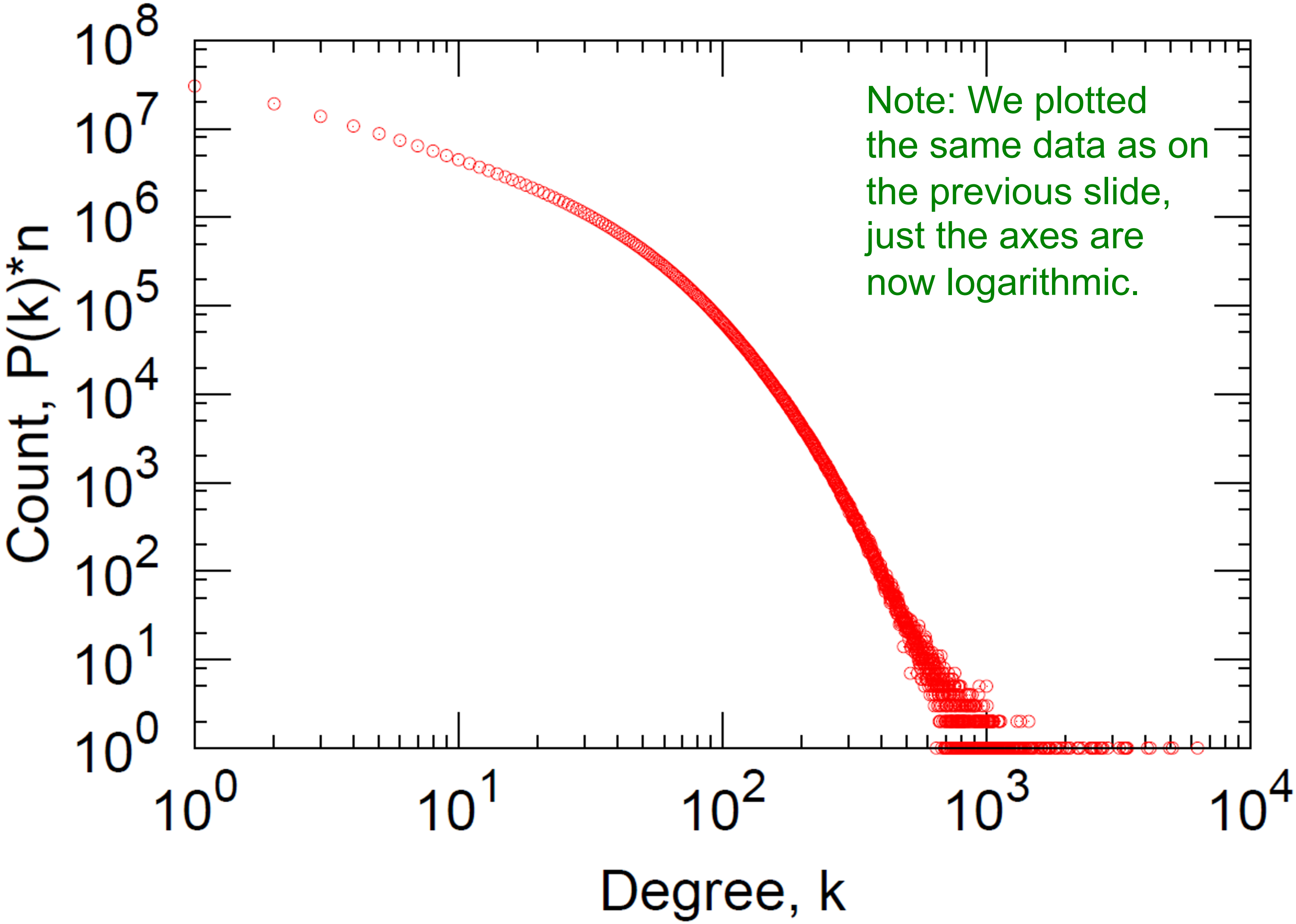


Network: 180M people, 1.3B edges

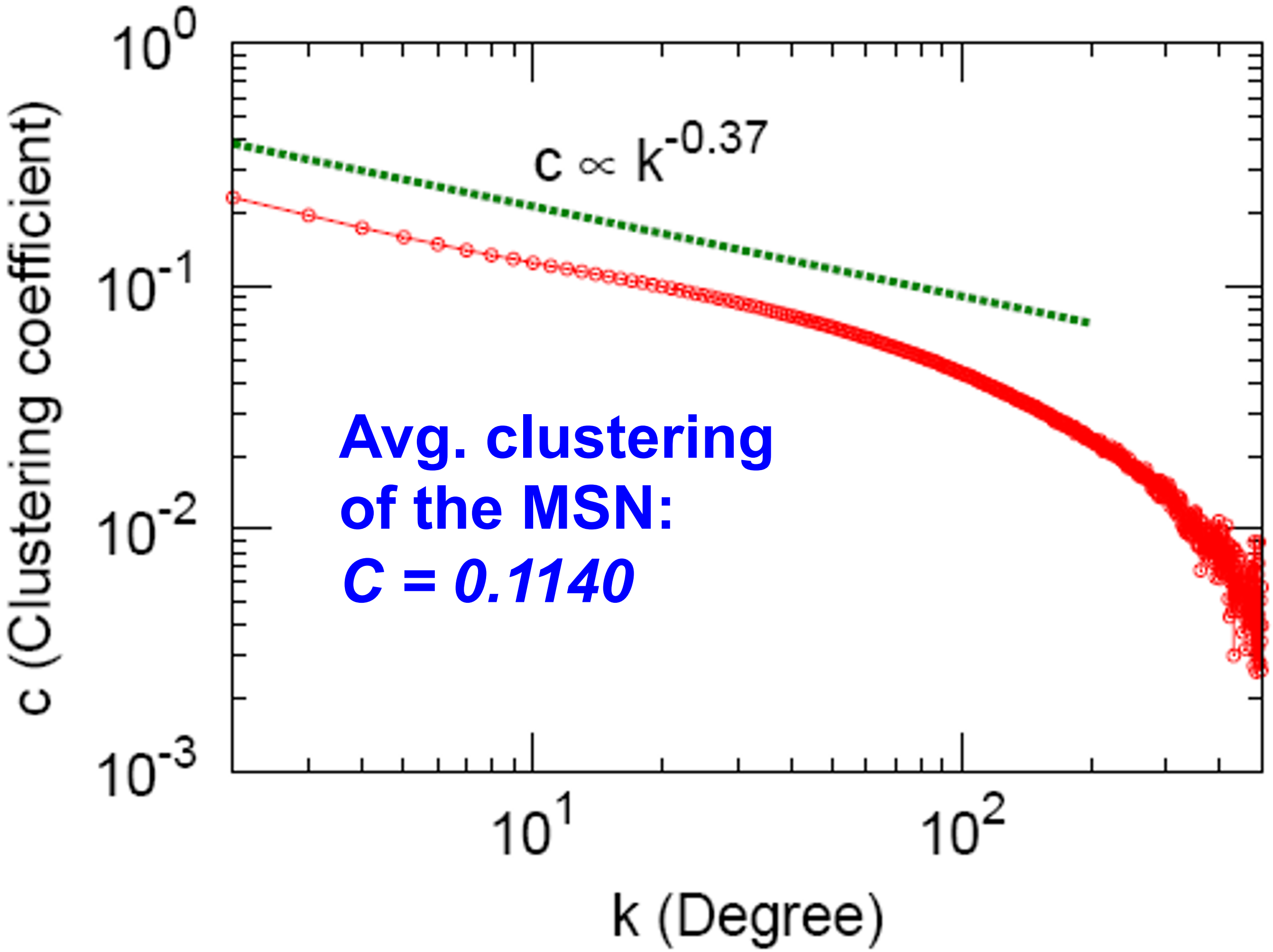
MSN: (1) Degree Distribution



MSN: Log-Log Degree Distribution

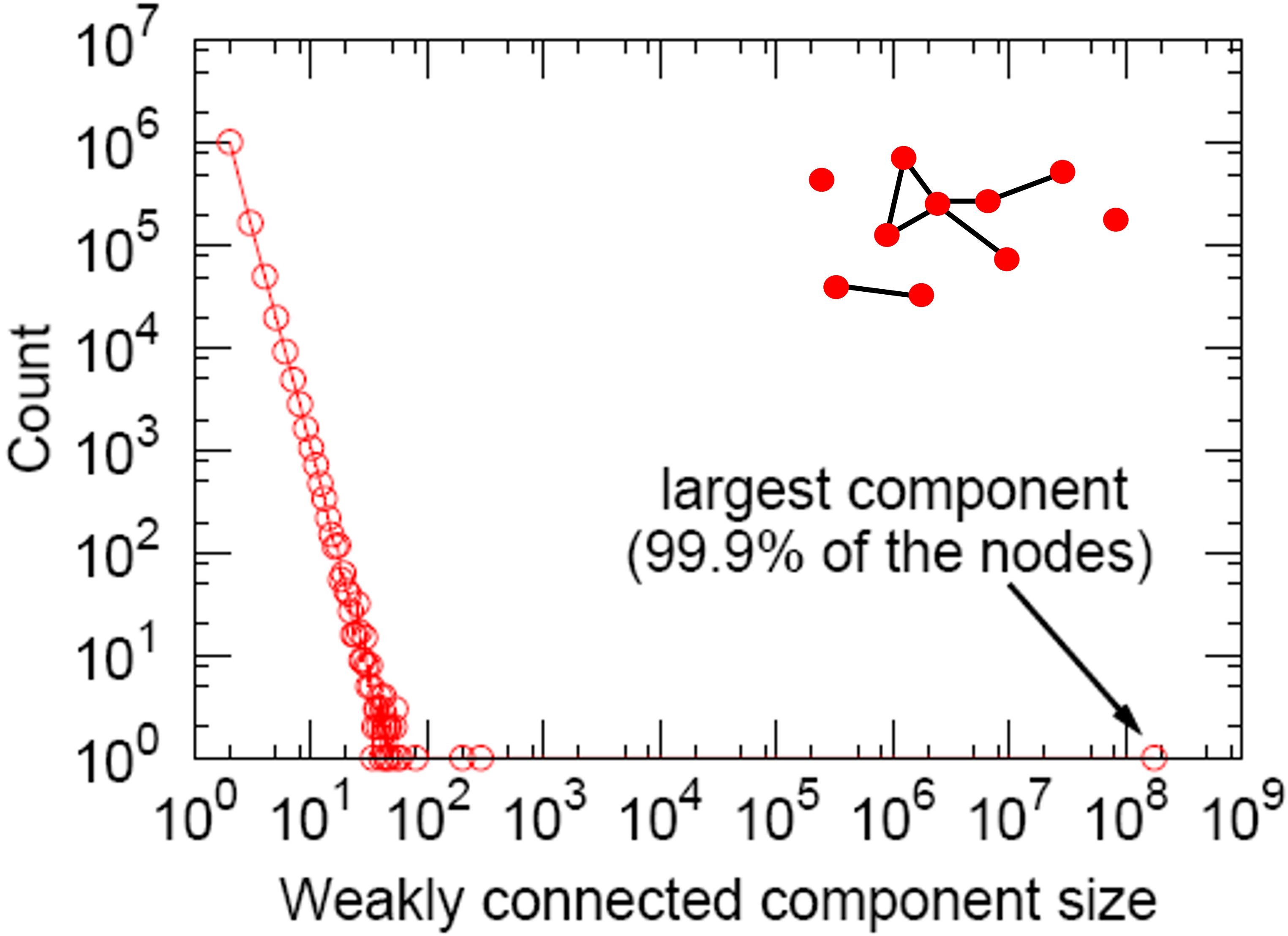


MSN: (2) Clustering

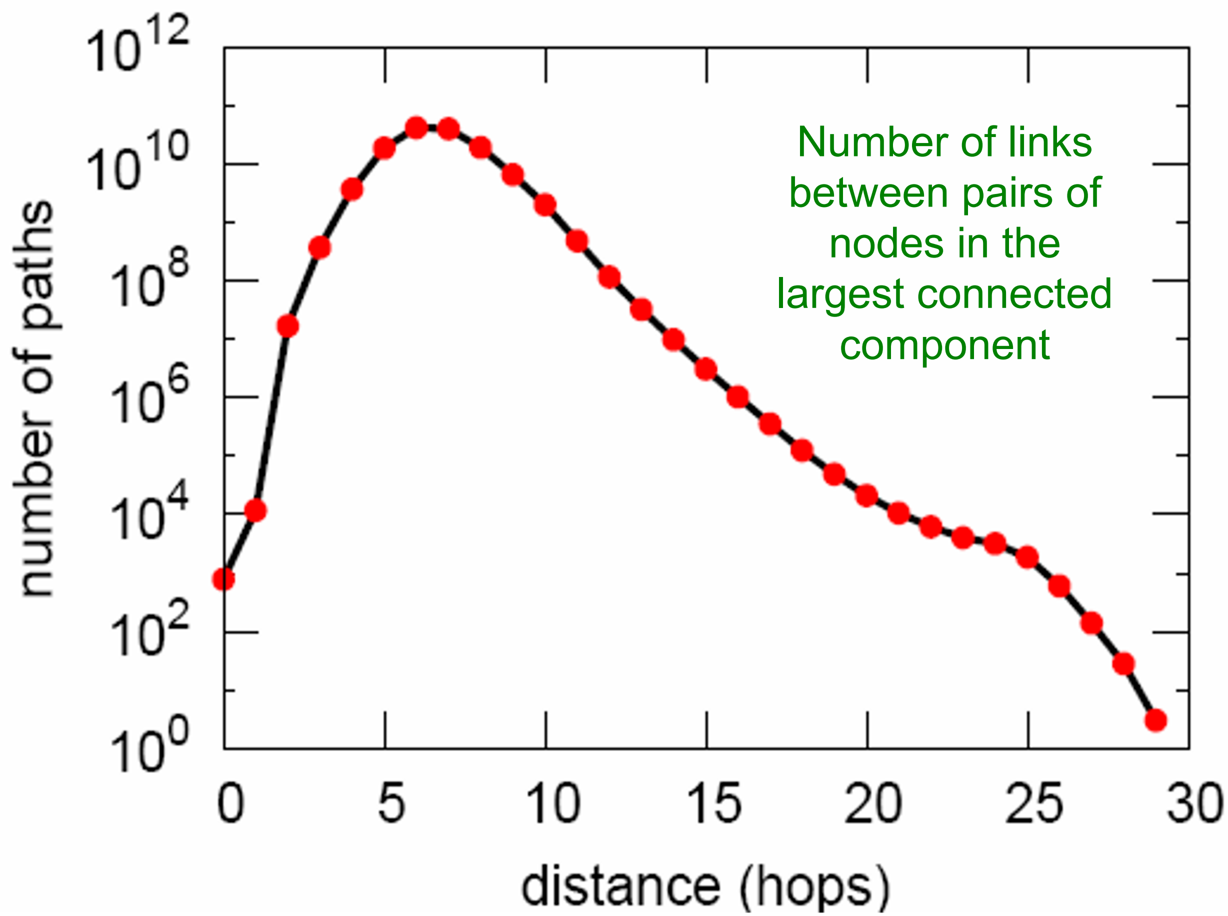


C_k: average C_i of nodes i of degree k: $C_k = \frac{1}{N_k} \sum_{i:k_i=k} C_i$

MSN: (3) Connected Components



MSN: (4) Path Length



Avg. path length **6.6**
90% of the nodes can be reached in < 8 hops

nodes as we do BFS out of a random node

Steps	#Nodes
0	1
1	10
2	78
3	3,96
4	8,648
5	3,299,252
6	28,395,849
7	79,059,497
8	52,995,778
9	10,321,008
10	1,955,007
11	518,410
12	149,945
13	44,616
14	13,740
15	4,476
16	1,542
17	536
18	167
19	71
20	29
21	16
22	10
23	3
24	2
25	3

MSN: Key Network Properties

Degree distribution: *Heavily skewed; avg. degree = 14.4*

Clustering coefficient: *0.11*

Connectivity: *giant component*

Path length: *6.6*

Are these values "expected"?
Are they "surprising"?

To answer this, we need a model!

Stanford CS224W: Erdös-Renyi Random Graphs

CS224W: Machine Learning with Graphs

Jure Leskovec, Stanford University

http://cs224w.stanford.edu

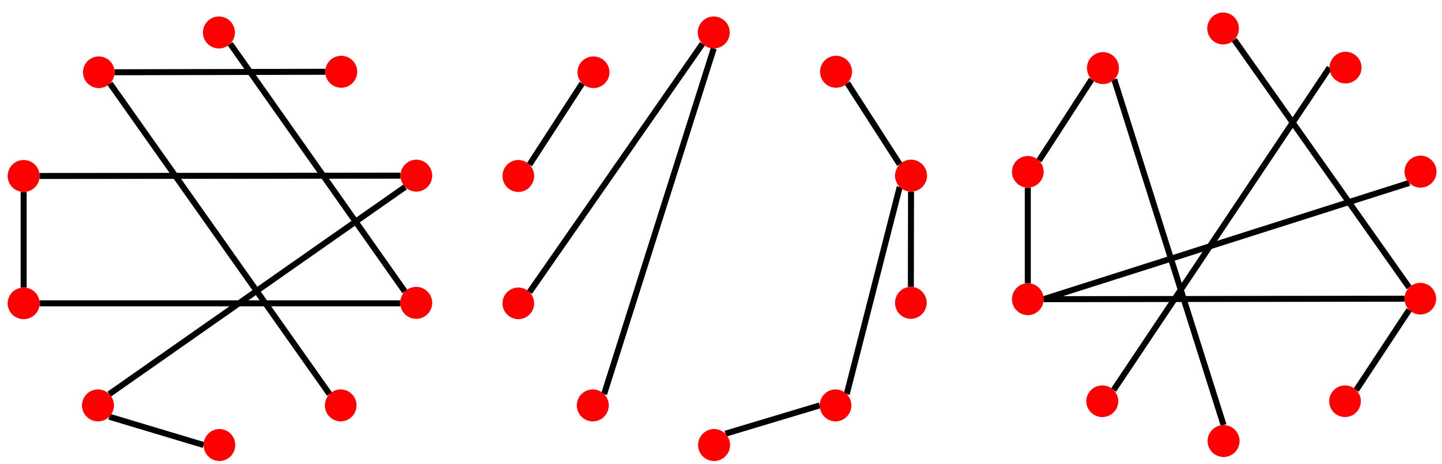
Simplest Model of Graphs

- **Erdös-Renyi Random Graphs** [Erdös-Renyi, '60]
  - **Two variants:**
    - G_{np}: undirected graph on n nodes where each edge (u,v) appears i.i.d. with probability p
    - G_{nm} : undirected graph with n nodes, and m edges picked uniformly at random

What kind of networks do such models produce?

Random Graph Model G_{np}

- ***n* and *p* do not uniquely determine the graph!**
  - The graph is a result of a random process
- We can have many different realizations given the same *n* and *p*



n = 10
p= 1/6

Properties of G_{np}

Degree distribution: $P(k)$

Clustering coefficient: C

Path length: h

What are the values of these properties for G_{np}?

(1) Degree Distribution of G_{np}

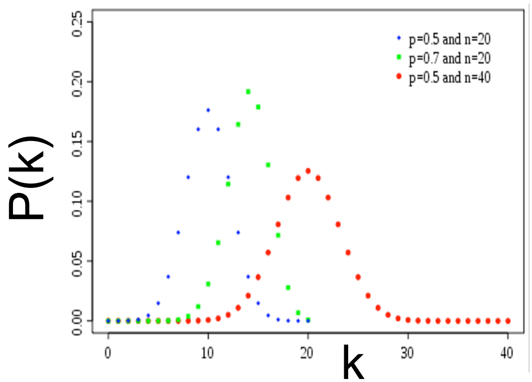
- **Fact:** Degree distribution of G_{np} is binomial.
- Let $P(k)$ denote the fraction of nodes with degree k:

$$P(k) = \binom{n-1}{k} p^k (1-p)^{n-1-k}$$

Select k nodes out of n-1

Probability of having k edges

Probability of missing the rest of the n-1-k edges



Mean, variance of a binomial distribution

$$\bar{k} = p(n-1)$$

$$\sigma^2 = p(1-p)(n-1)$$

(2) Clustering Coefficient of G_{np}

Remember: $$C_i = \frac{2e_i}{k_i(k_i-1)}$$

Where e_i is the number of edges between i's neighbors

Edges in G_{np} appear i.i.d. with prob. p

So, expected $E[e_i]$ is: $$= p\frac{k_i(k_i-1)}{2}$$

Each pair is connected with prob. p

Number of distinct pairs of neighbors of node i of degree k_i

Then $E[C_i]$: $$= \frac{p \cdot k_i(k_i-1)}{k_i(k_i-1)} = p = \frac{\bar{k}}{n-1} \approx \frac{\bar{k}}{n}$$

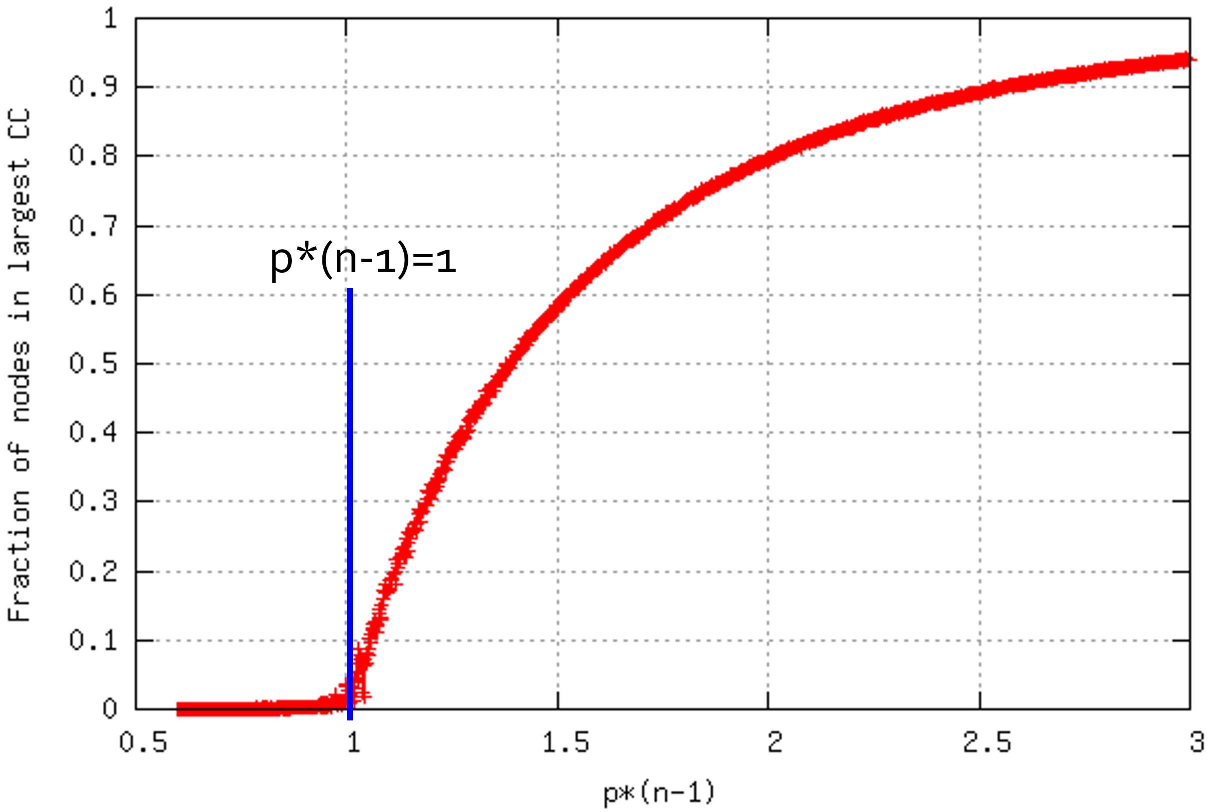
Clustering coefficient of a random graph is small.
If we generate bigger and bigger graphs with fixed avg. degree k (that is we set $p = k \cdot 1/n$), then C decreases with the graph size n.

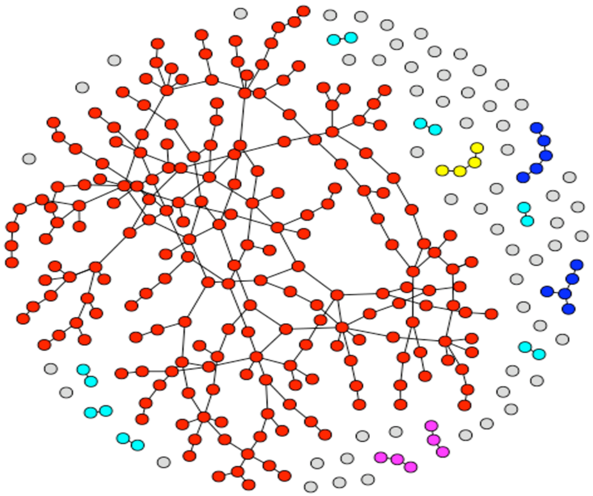
(3) Connected Components of G_{np}

- **Graph structure of G_{np} as p changes:**

- **Emergence of a giant component:**
- avg. degree $k=2E/n$ or $p=k/(n-1)$
  - **Degree $k=1-\varepsilon$:** all components are of size $\Omega(\log n)$
  - **Degree $k=1+\varepsilon$:** 1 component of size $\Omega(n)$, others have size $\Omega(\log n)$
    - Each node has at least one edge in expectation

G_{np} Simulation Experiment





Fraction of nodes in the largest component

G_{np}, n=100,000, k=$p(n-1)$ = 0.5 … 3

Network Properties of G_{np}

Degree distribution: $$P(k) = \binom{n-1}{k} p^k (1-p)^{n-1-k}$$

Clustering coefficient: $$C = p = \bar{k}/n$$

Connectivity: GCC exists when k>1.

Path length: ***next!***

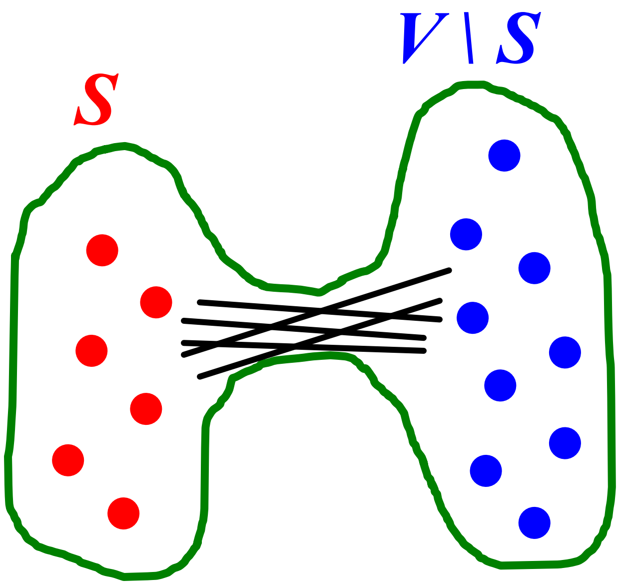
Def: Expansion

- Graph $G(V, E)$ has **expansion α**: if $\forall S \subseteq V$:

  $\#$ of edges leaving $S \geq \alpha \cdot \min(|S|, |V \setminus S|)$
- **Or equivalently:**

$$\alpha = \min_{S \subseteq V} \frac{\# edges\ leaving\ S}{\min(|S|, |V \setminus S|)}$$

这是为了考虑到
S大于V/2的情况

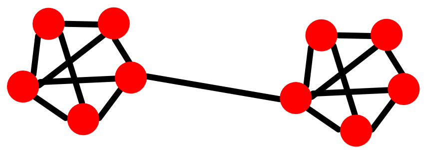


Expansion 表示S连出的点的比率

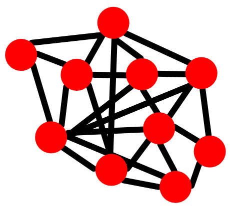
Expansion: Measures Robustness

$$\alpha = \min_{S \subseteq V} \frac{\#\,edges\ leaving\ S}{\min(|S|, |V \setminus S|)}$$

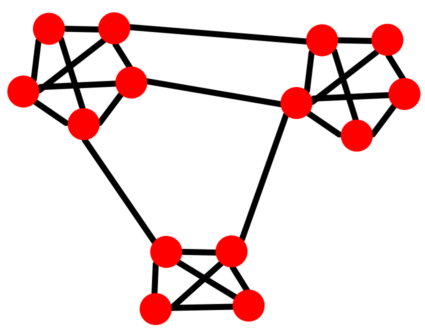
- Expansion is **measure of robustness:**
  - To disconnect l nodes, we need to cut $\geq \alpha \cdot l$ edges
- Low expansion:



- High expansion:

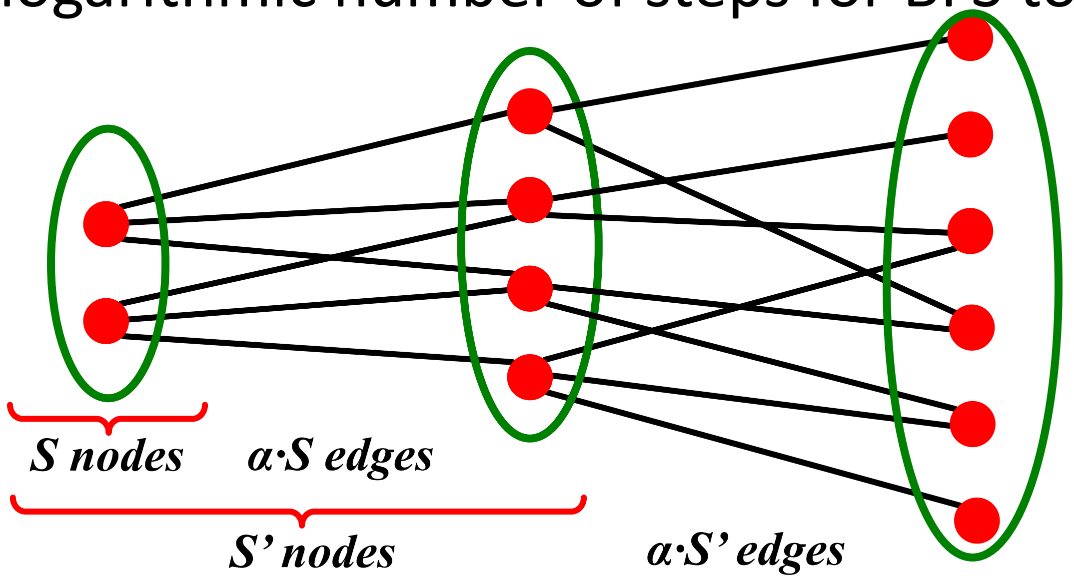


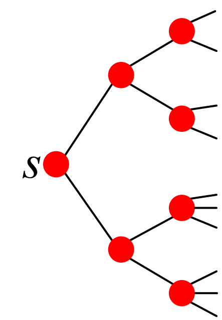
- Social networks:
  - "Communities"



Expansion: Random Graphs

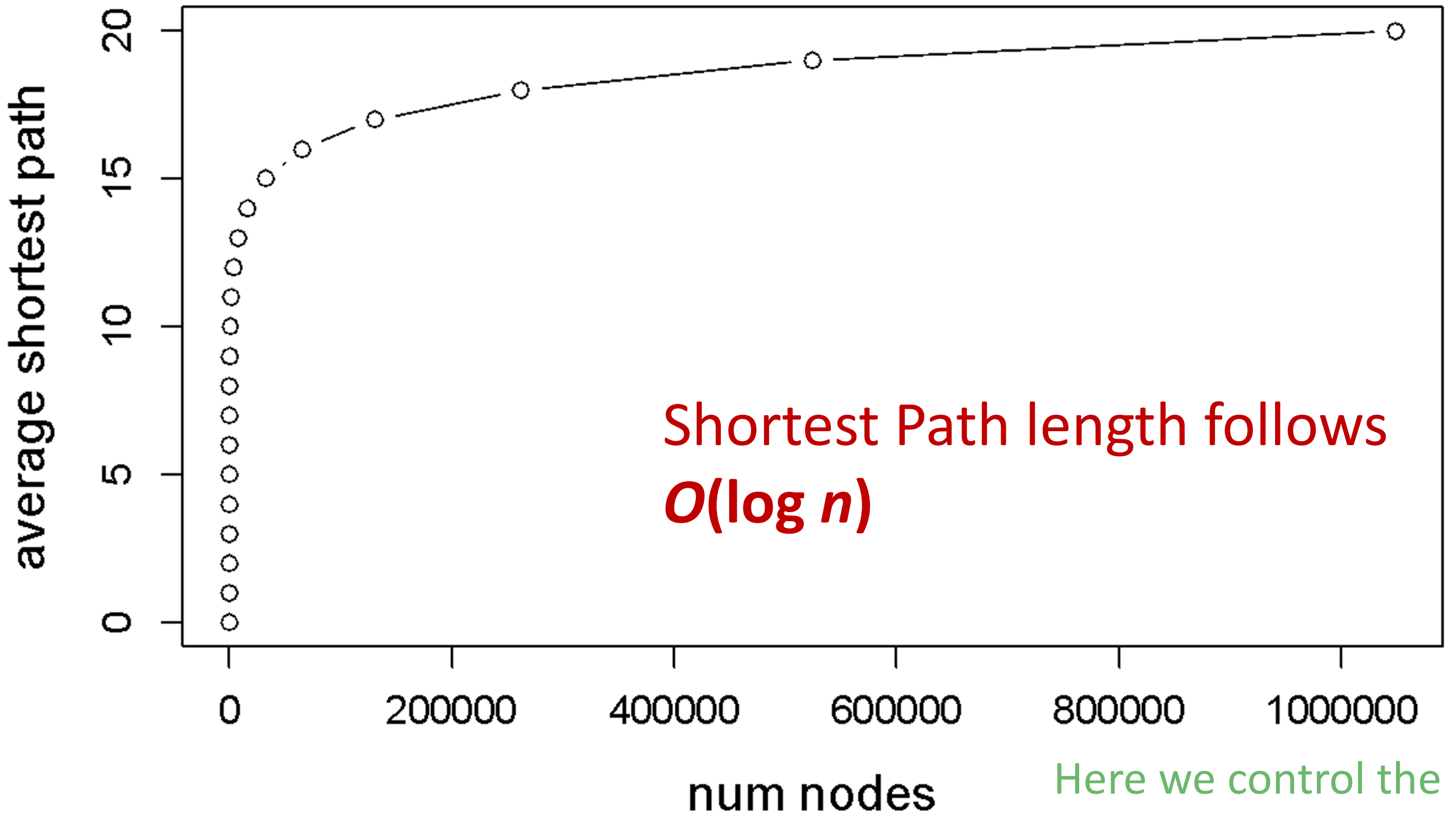
- **Fact:** In a graph on n nodes with expansion α for all pairs of nodes there is a path of lehth $O((\log n)/\alpha)$.
- **Random graph G_{np}:**
  For $\log n > np > c$, diam(G_{np}) $= O(\log n / \log (np))$
  - Random graphs have good expansion so it takes a logarithmic number of steps for BFS to visit all nodes





(4) Shortest Path of G_{np}

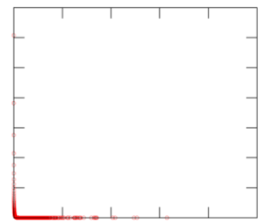
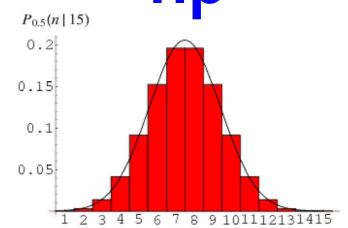
Erdös-Renyi Random Graph can grow very large but nodes will be just a few hops apart



Shortest Path length follows **$O(\log n)$**

Here we control the average degree to be constant

Back to MSN vs. G_{np}

	MSN	G_{np}	n=180M
Degree distribution:			
Avg. path length:	**6.6**	$O(\log n)$ $h \approx 8.2$	
Avg. clustering coef.:	0.11	$\bar{k} / n$ $C \approx 8 \cdot 10^{-8}$	
Largest Conn. Comp.:	99%	GCC exists when $\bar{k}>1$. $\bar{k} \approx 14$.	

Real Networks vs. G_{np}

- **Are real networks like random graphs?**
  - Giant connected component: ☺️
  - Average path length: ☺️
  - Clustering Coefficient: ☹️
  - Degree Distribution: ☹️
- **Problems with the random networks model:**
  - Degree distribution differs from that of real networks
  - Giant component in most real networks does NOT emerge through a phase transition
  - No local structure – clustering coefficient is too low
- **Most important: Are real networks random?**
  - The answer is simply: **NO!**

Stanford CS224W: The Small-World Model

CS224W: Machine Learning with Graphs

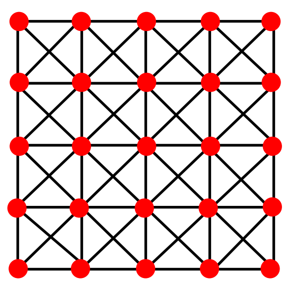
Jure Leskovec, Stanford University

http://cs224w.stanford.edu

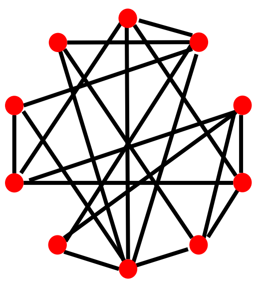
Motivation for Small-World

	MSN	G_{np}	n=180M	
Avg. path length:	**6.6**	$O(\log n)$ $h \approx 8.2$		☑
Avg. clustering coef.:	0.11	$\bar{k}/n$ $C \approx 8\cdot 10^{-8}$		☒

Can we have **high clustering** while also having **short paths**?



Vs.



Regular lattice graph:
High clustering coefficient
High diameter

G_{np} random graph:
Low clustering coefficient
Low diameter

Clustering Implies Edge Locality

- **Real networks have high clustering:**
  - **MSN network has 7 orders of magnitude larger clustering than the corresponding G_{np}!**
- **Other examples:**

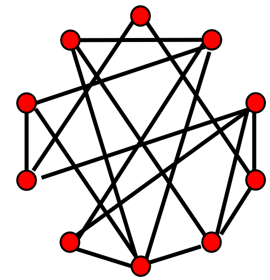
Avg. path length — Clustering coefficients

Network	Nodes	Degree	h_{actual}	h_{random}	C_{actual}	C_{random}
Film actor collaborations	225,226	61.00	3.65	2.99	0.79	0.00027
Power Grid	4,941	2.67	18.70	12.40	0.080	0.005
C. elegans	282	14.00	2.65	2.25	0.28	0.05

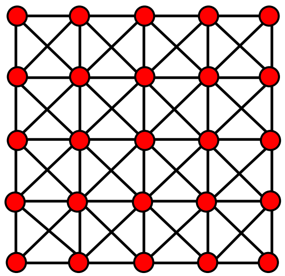
"actual" … real network
"random" … random graph with same avg. degree

The "Controversy"

- **Consequence of expansion:**
  - **Short paths:** $O(\log n)$
    - This is the smallest diameter we can get if we keep the degree constant.
  - But clustering is low!
- **But networks have "local" structure:**
  - **Triadic closure:** Friend of a friend is my friend
  - High clustering but diameter is also high
- **How can we have both?**



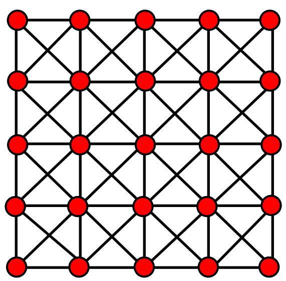
G_{np} random graph:
Low clustering coefficient
Low diameter



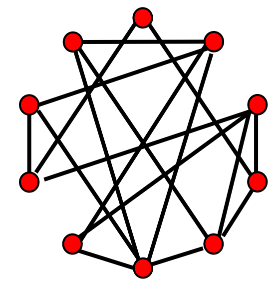
Regular lattice graph:
High clustering coefficient
High diameter

Small-world Graphs: Idea

- **Idea:** Interpolate between regular lattice graphs and G_{np} random graph



Interpolate



Regular lattice graph:
High clustering coefficient
High diameter

Small-world graph:
High clustering coefficient
Low diameter

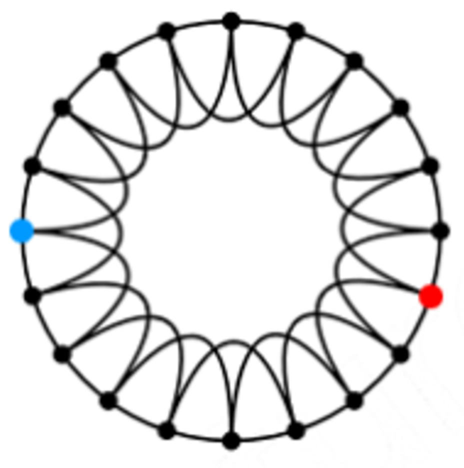
G_{np} random graph:
Low clustering coefficient
Low diameter

- **How do we interpolate between these two graphs?**

Our model must satisfies these two properties

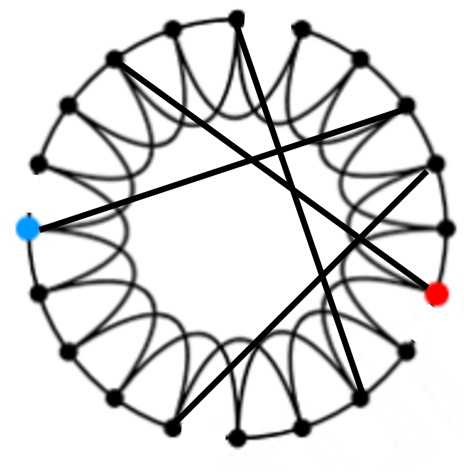
Solution: The Small-World Model

- **Small-World Model**
- Two components to the model:
- **(1) Start with a low-dimensional regular lattice**
  - (In our case we are using a ring as a lattice)
  - Has high clustering coefficient



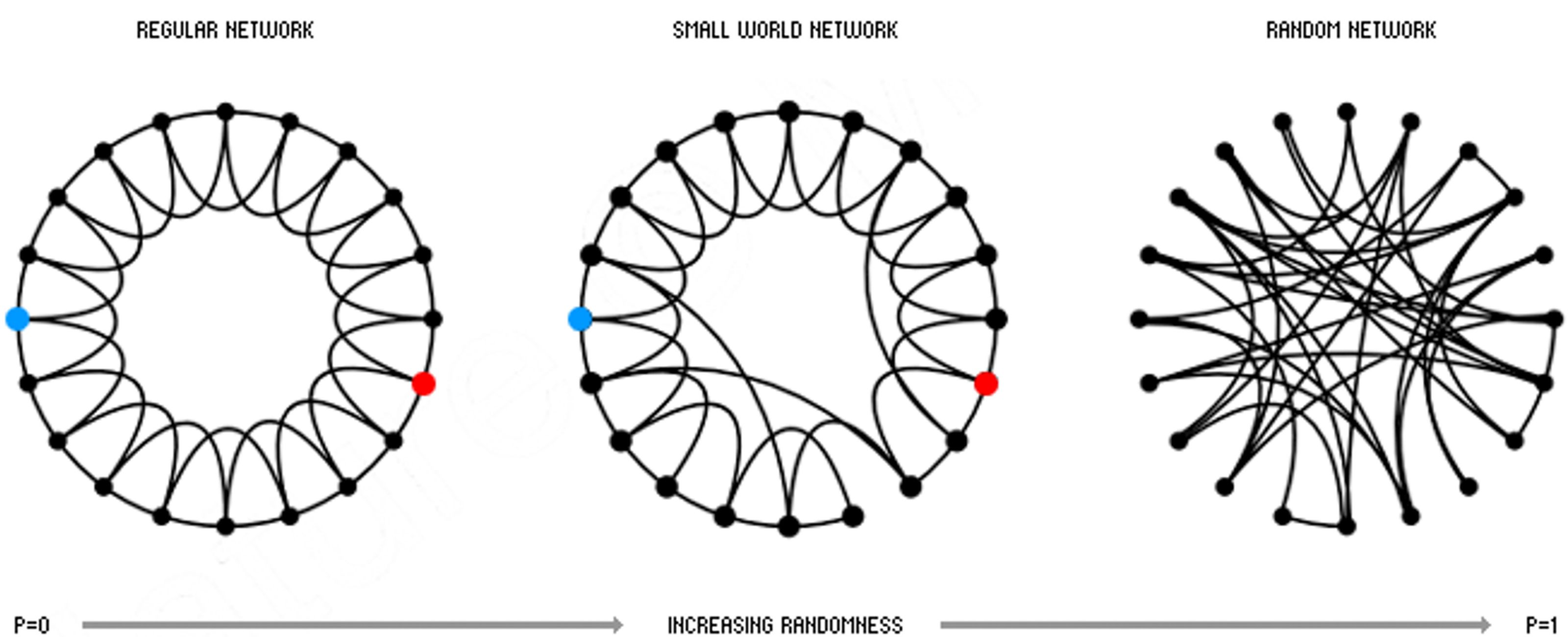
Solution: The Small-World Model

- **Small-World Model**
- Two components to the model:
- **(2) Rewire: Introduce randomness ("shortcuts")**
  - Add/remove edges to create shortcuts to join remote parts of the lattice
  - For each edge, with prob. p, move the other endpoint to a random node



[D. Wattts and S. Strogatz, Collective dynamics of 'small-world'networks, Nature]

The Small-World Model



High clustering
High diameter

High clustering
Low diameter

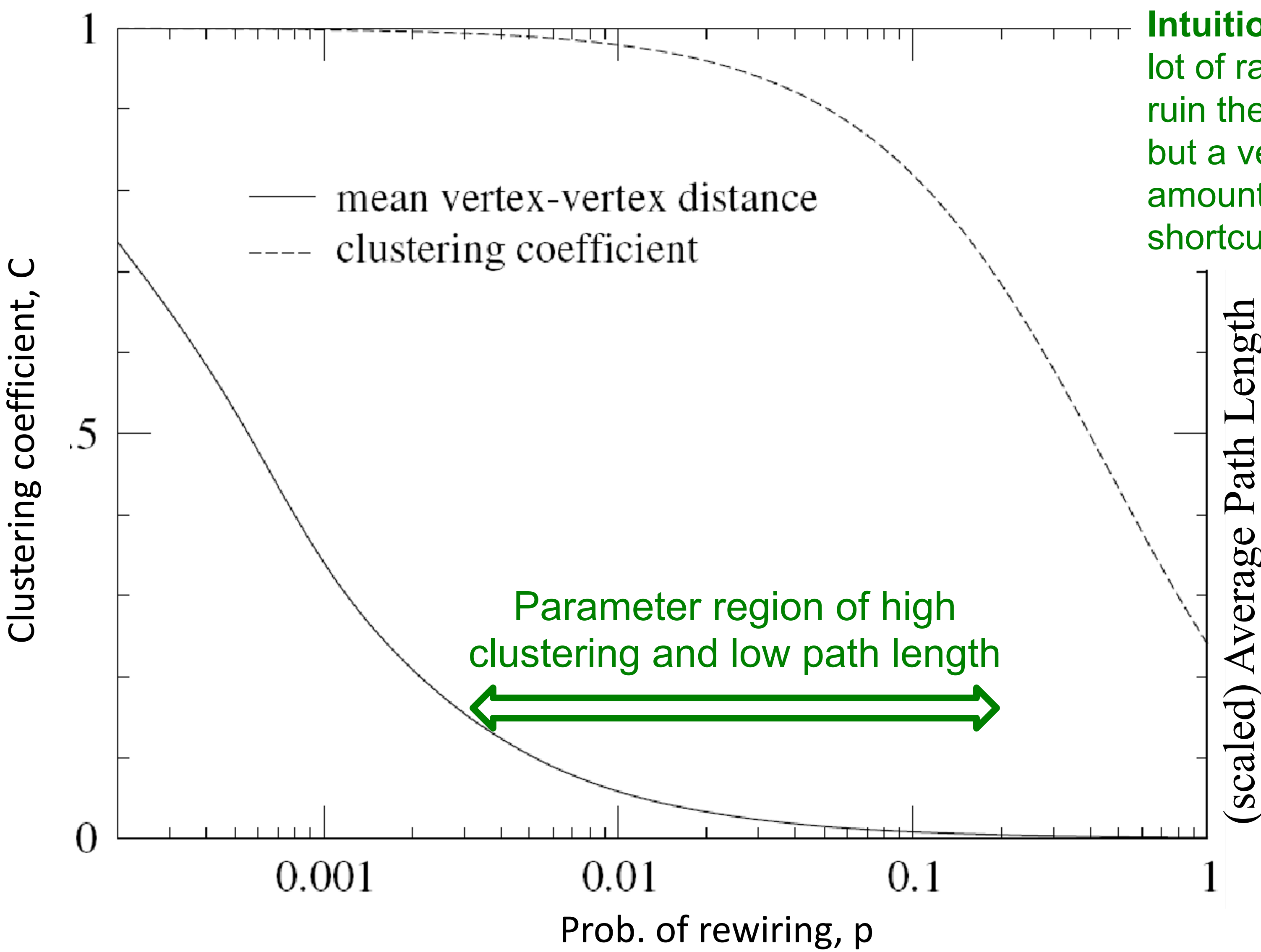
Low clustering
Low diameter

$h = \frac{N}{2\bar{k}}$ $\quad C = \frac{1}{2}$

$h = \frac{\log N}{\log \alpha}$ $\quad C = \frac{\bar{k}}{N}$

Rewiring allows us to "interpolate" between
a regular lattice and a random graph

The Small-World Model



Intuition: It takes a lot of randomness to ruin the clustering, but a very small amount to create shortcuts.

Small-World: Summary

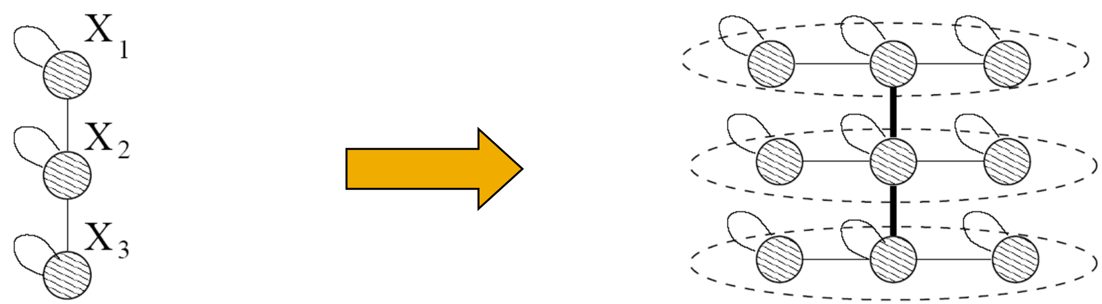
- **Could a network with high clustering be at the same time a small world?**
  - Yes! You don't need more than a few random links
- **The Small-World Model:**
  - Provides insight on the interplay between clustering and the small-world
  - Captures the structure of many realistic networks
  - Accounts for the high clustering of real networks
  - Does not lead to the correct degree distribution

Stanford CS224W: Kronecker Graph Model

CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
http://cs224w.stanford.edu

Idea: Recursive Graph Generation

- **How can we think of network structure recursively?** **Intuition:** Self-similarity
  - **Object is similar to a part of itself**: the whole has the same shape as one or more of the parts
- **Mimic recursive graph/community growth:**



Initial graph Recursive expansion

- **Kronecker product** is a way of generating self-similar matrices

Kronecker Graph

- **Kronecker graphs:**
  - **A recursive model of network structure**

1	1	0
1	1	1
0	1	1

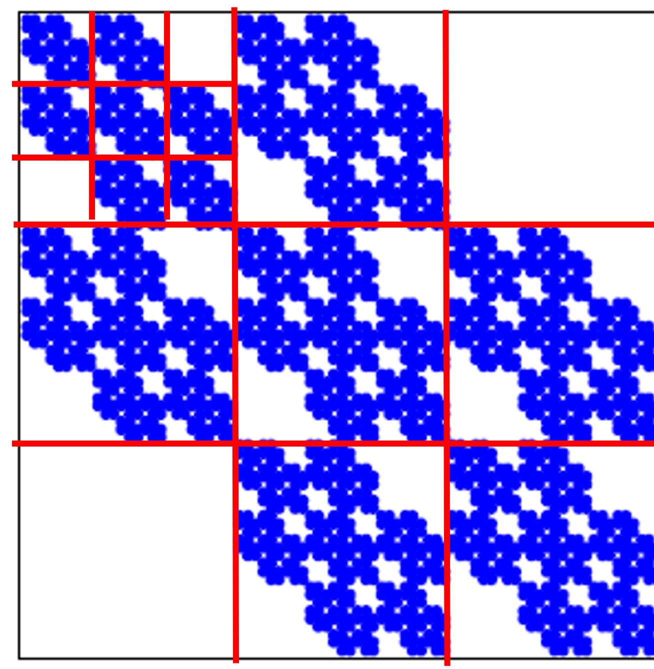
K_1

3 x 3

K_1	K_1	0
K_1	K_1	K_1
0	K_1	K_1

$$K_2 = K_1 \otimes K_1$$

9 x 9



81 x 81 adjacency matrix

Kronecker Product: Definition

- **Kronecker product** of matrices *A* and *B* is given by

$$\underset{N \times M}{\mathbf{C} = \mathbf{A}} \otimes \underset{K \times L}{\mathbf{B}} \doteq \underbrace{\begin{pmatrix} a_{1,1}\mathbf{B} & a_{1,2}\mathbf{B} & \dots & a_{1,m}\mathbf{B} \\ a_{2,1}\mathbf{B} & a_{2,2}\mathbf{B} & \dots & a_{2,m}\mathbf{B} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n,1}\mathbf{B} & a_{n,2}\mathbf{B} & \dots & a_{n,m}\mathbf{B} \end{pmatrix}}_{N*K \times M*L}$$

- Define a Kronecker product of two graphs as a Kronecker product of their **adjacency matrices**

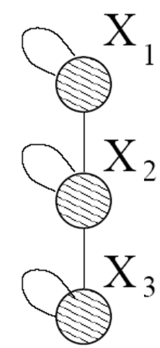
[PKDD '05]

Kronecker Graphs

- **Kronecker graph** is obtained by growing sequence of graphs by iterating the **Kronecker product over the initiator matrix K_1:**

$$K_1^{[m]} = K_m = \underbrace{K_1 \otimes K_1 \otimes \ldots K_1}_{\text{m } times} = K_{m-1} \otimes K_1$$

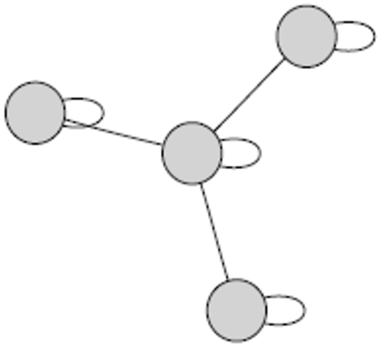
$$\begin{array}{|c|c|c|}\hline 1 & 1 & 0 \\ \hline 1 & 1 & 1 \\ \hline 0 & 1 & 1 \\ \hline \end{array}$$



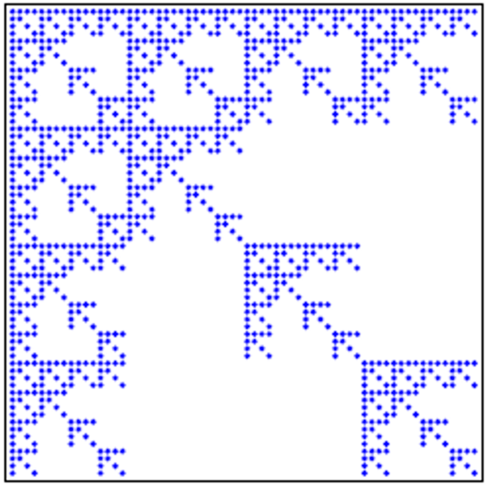
K_1

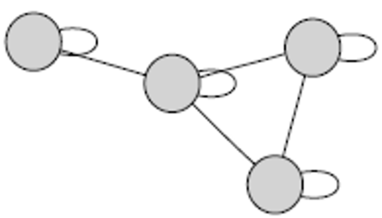
- **Note:** One can easily use multiple initiator matrices (K_1', K_1'', K_1''') (even of different sizes)

Kronecker Initiator Matrices

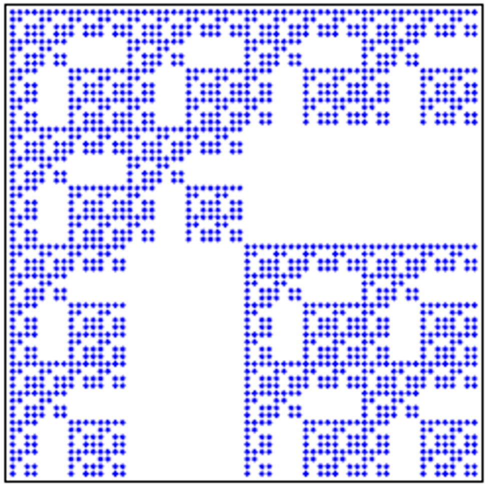


1	1	1	1
1	1	0	0
1	0	1	0
1	0	0	1





1	1	1	1
1	1	0	0
1	0	1	1
1	0	1	1



Initiator K_1 K_1 adjacency matrix K_3 adjacency matrix

Stochastic Kronecker Graphs

[PKDD '05]

- **Step 1:** Create N_1 x N_1 **probability matrix** Θ_1
- **Step 2:** Compute the k^{th} **Kronecker power** Θ_k
- **Step 3:** For each entry p_{uv} of Θ_k include an edge *(u, v)* in K_k with probability p_{uv}

0.5	0.2
0.1	0.3

Θ_1

Kronecker multiplication

0.25	0.10	0.10	0.04
0.05	0.15	0.02	0.06
0.05	0.02	0.15	0.06
0.01	0.03	0.03	0.09

$\Theta_2 = \Theta_1 \otimes \Theta_1$

Probability of edge p_{uv}

Instance matrix K_2

Flip biased coins

Generation of Kronecker Graphs

- **How do we generate an instance of a (Directed) stochastic Kronecker graph?**

Probability of edge p_{uv}

0.25	0.10	0.10	0.04
0.05	0.15	0.02	0.06
0.05	0.02	0.15	0.06
0.01	0.03	0.03	0.09

Flip biased coins

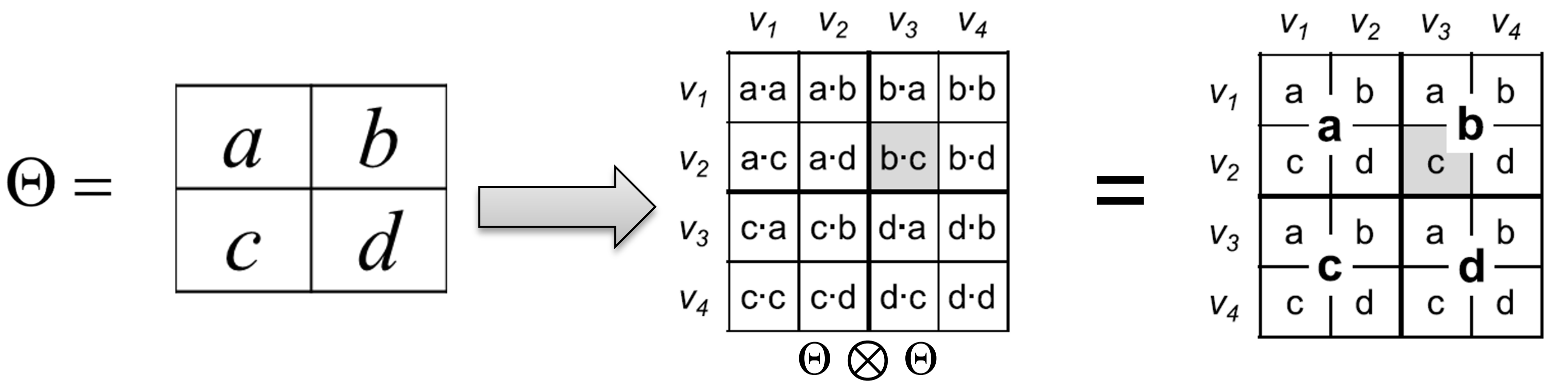
1	1	0	0
0	1	0	1
1	0	1	1
0	1	0	1

Need to flip n^2 coins!! Way too slow!!

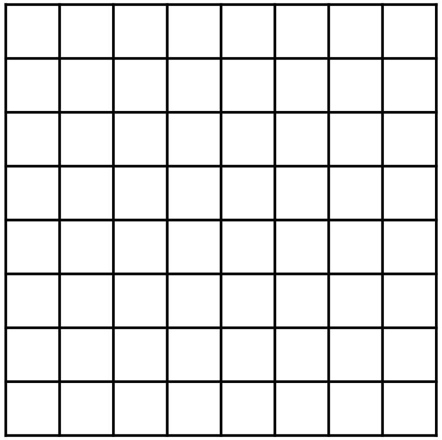
- **Is there a faster way? YES!**
- **Idea:** Exploit the recursive structure of Kronecker graphs
  - "Drop" edges onto the graph one by one

Generation of Kronecker Graphs

- **A faster way to generate Kronecker graph**



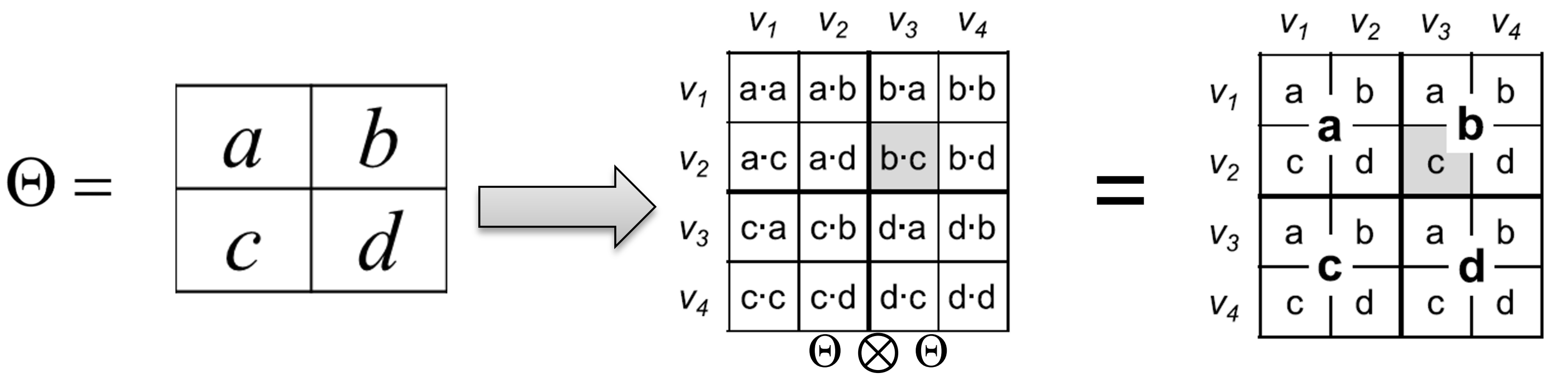
- **How to "drop" an edge into a graph G on n=2^m nodes**



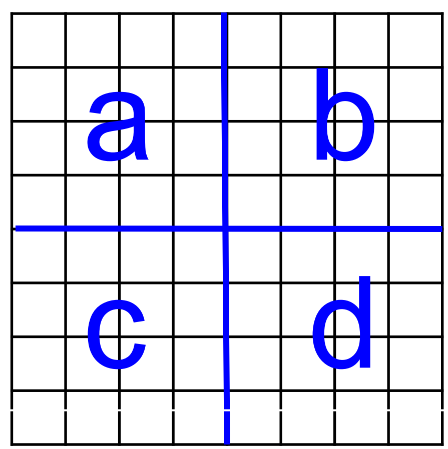
Adjacency matrix **G**

Generation of Kronecker Graphs

- **A faster way to generate Kronecker graph**



- **How to “drop” an edge into a graph G on $n=2^m$ nodes**



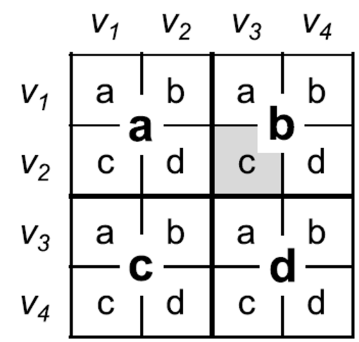
Adjacency matrix **G**

Generation of Kronecker Graphs

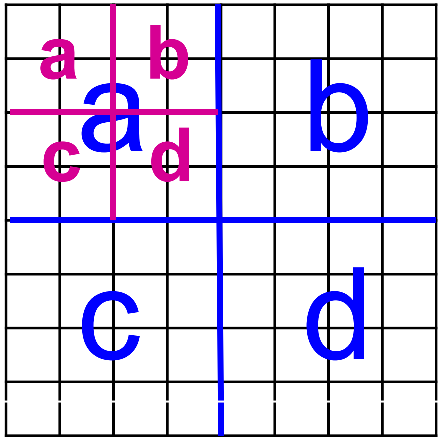
- **A faster way to generate Kronecker graph**

$$\Theta = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \Rightarrow \begin{array}{c|cccc} & v_1 & v_2 & v_3 & v_4 \\ \hline v_1 & a\cdot a & a\cdot b & b\cdot a & b\cdot b \\ v_2 & a\cdot c & a\cdot d & b\cdot c & b\cdot d \\ v_3 & c\cdot a & c\cdot b & d\cdot a & d\cdot b \\ v_4 & c\cdot c & c\cdot d & d\cdot c & d\cdot d \end{array} =$$

$\Theta \otimes \Theta$



- **How to "drop" an edge into a graph G on $n=2^m$ nodes**



Adjacency matrix **G**

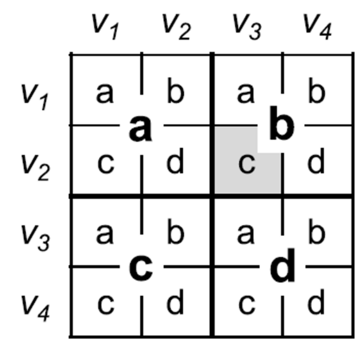
Generation of Kronecker Graphs

- **A faster way to generate Kronecker graph**

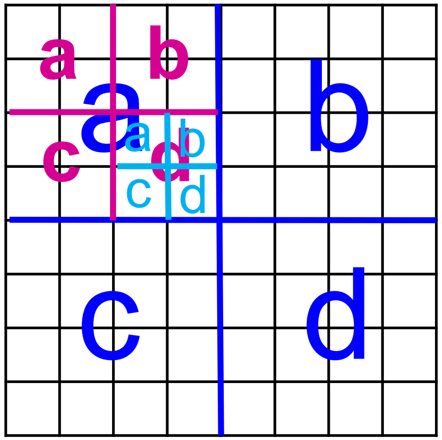
$$\Theta = \begin{array}{|c|c|} \hline a & b \\ \hline c & d \\ \hline \end{array} \Rightarrow \begin{array}{c|cc|cc|} & v_1 & v_2 & v_3 & v_4 \\ \hline v_1 & a\cdot a & a\cdot b & b\cdot a & b\cdot b \\ v_2 & a\cdot c & a\cdot d & b\cdot c & b\cdot d \\ \hline v_3 & c\cdot a & c\cdot b & d\cdot a & d\cdot b \\ v_4 & c\cdot c & c\cdot d & d\cdot c & d\cdot d \\ \hline \end{array}$$

$$\Theta \otimes \Theta$$

=



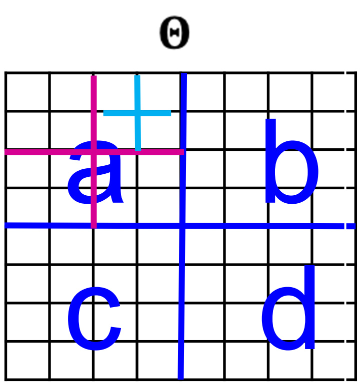
- **How to "drop" an edge into a graph G on $n=2^m$ nodes:**
- We may get a few edges colliding. We simply reinsert them.



Adjacency matrix **G**

Generation of Kronecker Graphs

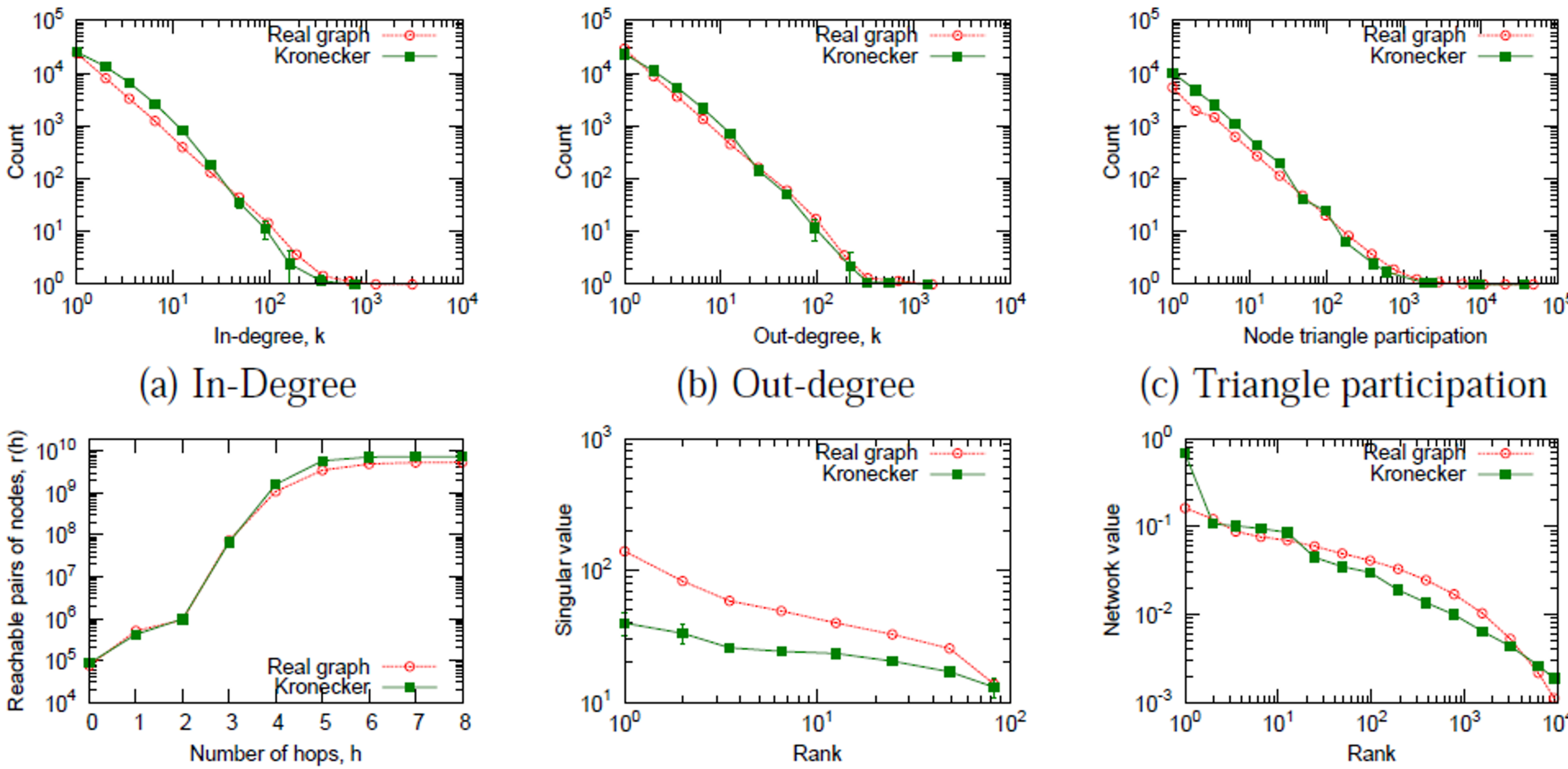
- **Fast Kronecker generator algorithm:**
  - For generating **directed graphs**
- **Insert 1 edge on graph G on $n = 2^m$ nodes:**
  - Create normalized matrix $L_{uv} = \Theta_{uv} / (\sum_{op} \Theta_{op})$
  - **For $i = 1 \ \ldots m$**
    - Start with $x = 0, y = 0$
    - Pick a row/column (u, v) with prob. L_{uv}
    - Descend into quadrant (u, v) at level i of G
      - **This means:** $x \mathrel{+}= u \cdot 2^{m-i}, y \mathrel{+}= v \cdot 2^{m-i}$
  - Add an edge (x, y) **to** G



Estimation: Epinions (n=76k, m=510k)

- Real and Kronecker are very close:

$$\Theta_1 = \begin{array}{|c|c|}\hline 0.99 & 0.54 \\ \hline 0.49 & 0.13 \\ \hline\end{array}$$



(a) In-Degree (b) Out-degree (c) Triangle participation

(d) Hop plot (e) Scree plot (f) “Network” value

Summary of the Lecture

- **Today: Traditional graph generative models**
  - Erdös-Renyi graphs
  - Small-world graphs
  - Kronecker graphs
  - All these models have **prior assumption of the graph generation processes**
- **Next: Deep graph generative models**
  - **Learn** the graph generation process **from raw data**